

# MATERIALS SCIENCE MA(S)TERS

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Teacher Guides

Part 4



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**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**Physical and Colloid Chemistry for Material Scientists**

**Code: PCC**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

Physical Chemistry and Materials Science

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will discuss the methodological role of Physical Chemistry as the theoretical basis of the chemical field of knowledge, as well as its importance for Materials Science. The relationship between chemical transformations and physical phenomena will be considered. Students will also get acquainted with the classification and content of the main sections of modern Physical Chemistry. Particular attention will be paid to the sections that have now been formed as separate chemical disciplines, in particular Colloidal Chemistry, Quantum Chemistry, Electrochemistry, etc. The lecture will also cover the main groups of physical and chemical research methods, their purpose and application in Materials Science.

#### 3. Learning outcomes

- Understand the role of Physical Chemistry in the system of chemical knowledge and its importance for Materials Science.
- Understand the relationships between chemical transformations and physical phenomena.
- Familiarization with the sections of Physical Chemistry, the object and subject of their study.
- Understanding the purpose and capabilities of specific methods of physical and chemical research to study the properties of materials of various types.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – presenting examples of the use of physical and chemical research methods in the study of specific properties of materials of various types.

Discussion - encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. [https://en.wikipedia.org/wiki/Physical\\_chemistry](https://en.wikipedia.org/wiki/Physical_chemistry).
2. Keith J. Laidler, *The World of Physical Chemistry*, Oxford University Press, 1995.

#### 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

Basic concepts of Physical Chemistry

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture, students will become familiar with the basic concepts of Physical Chemistry, such as system, system state, system state function and its parameters (properties), process, process path, reversibility and irreversibility, etc. The issue of classification of systems, their parameters and processes in physical and chemical systems according to various criteria will also be discussed. Particular attention will be paid to real and ideal systems and their equations of state on the example of ideal and real gases. In addition, the correlation and interrelation of such concepts as energy, heat and process work, as well as types of work in physical and chemical systems will be considered.

### 3. Learning outcomes

- Familiarization yourself with the principles of modern classification of systems and processes.
- Understanding the differences between the description of ideal and real systems.
- Familiarization yourself with the equations of state of ideal and real gases.
- Understanding the physical meaning and relationship between energy, heat and work.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – comparative analysis of stable, unstable, and metastable states of the system.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "PROLOGUE. Energy, temperature, and chemistry" and "FOCUS 1. The properties of gases" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 1. Thermodynamics" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

**Chemical thermodynamics. Thermodynamic functions**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will focus on the thermodynamic approach to the analysis of physical and chemical systems. Particular attention will be paid to the four thermodynamic principles (laws) that underlie it, including their essence, formulations, and analytical expressions. The basics of thermochemistry, including Hess's and Kirchhoff's law and the concept of heat capacity, will be discussed. Students will also become familiar with thermodynamic functions that describe the state of a system and processes in it, namely entropy, enthalpy, internal energy, Gibbs energy, and Helmholtz energy. The concept of chemical potential, its relation to other thermodynamic functions will be discussed, and the application of the Lewis method to describe non-ideal systems, in particular the concepts of activity and fugacity, will be analyzed.

### 3. Learning outcomes

- Understand and be able to explain the essence of the four laws of thermodynamics and their place in the structure of chemical knowledge.
- Understandings of the physical meaning of the basic thermodynamic functions and know the relationships between them.
- Ability to calculate changes in the basic thermodynamic functions during chemical reactions and physicochemical processes under different conditions.
- Ability to use the relevant thermodynamic characteristics as criteria for equilibrium and spontaneity/directionality of processes under different conditions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – presenting of the examples of calculating changes in basic thermodynamic functions during chemical transformations and physicochemical processes.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "FOCUS 2. The First Law" and "FOCUS 3 The Second and Third Laws" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 2. The first law of thermodynamics", "Chapter 3. The second law of thermodynamics", "Chapter 4. Material equilibrium" and "Chapter 5. Standard thermodynamic functions" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

Phase equilibrium

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture, the conditions of phase equilibrium in heterogeneous systems will be discussed. Students will become familiar with first- and second-order phase transitions, as well as the representation of state diagrams of one-, two-, and three-component systems. The derivation and application of the Gibbs phase rule and the Clausius-Clapeyron equation will be discussed. Detailed attention will be paid to the principles and methods of thermal analysis, as well as the types of melting diagrams of binary systems of various types, both in the absence of chemical interaction and with the formation of new compounds, and their importance for materials science. The principles and technologies for the production of high-purity substances, in particular the zone melting method, will also be discussed.

### 3. Learning outcomes

- Understand the conditions of phase equilibrium.
- Ability to interpret phase diagrams of one-, two- and three-component systems.
- Ability to use the Gibbs phase rule for analysis of the phase diagrams of the systems of various types.
- Understanding of the principles of separation of liquid multicomponent systems of various types.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study - state diagrams of one-component (water, sulfur, CO<sub>2</sub>, carbon, helium) and two-component (Ag-Au, Pb-Cd, FeCl<sub>3</sub>-CuCl, etc.) systems.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "FOCUS 4. Physical transformations of pure substances" and "FOCUS 5. Simple mixtures. Topics 5C–5E" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 4. Material equilibrium", "Chapter 7. One-component phase equilibrium and surfaces" and "Chapter 12. Multicomponent phase equilibrium" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

Chemical thermodynamics of solutions

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will introduce students to theories of solutions, methods of expressing the composition of solutions, their classification, and the physical and chemical properties of ideal and non-ideal solutions. In particular, the issues of saturated vapor pressure over binary liquid solutions, Raoult's law and reasons for deviations from ideality (Henry's law), Gibbs-Konovalov laws, methods of separation of liquid mixtures, and solubility diagrams of three-component systems will be discussed. The solubility of gases, liquids, and solids, as well as the thermodynamics of mixing (dissolution) processes will also be considered. Particular attention will be paid to the nature and application of the colligative properties of solutions, namely the lowering of saturated vapor pressure over solutions of non-volatile substances, their lowering of freezing point and increasing of boiling point compared to a pure solvent, as well as osmotic pressure.

### 3. Learning outcomes

- Understand the reasons for and be able to explain the differences in the properties of ideal and non-ideal solutions.
- Familiarize yourself with the colligative properties of solutions and fields of their applications.
- Understand the need to use the Lewis method to describe non-ideal systems and its limitations.
- Ability to express the quantitative composition of solutions in various ways.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – values of the isotonic coefficient (van't Hoff factor) for various real systems.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapter "FOCUS 5. Simple mixtures. Topics 5A, 5B" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 9. Solutions" and "Chapter 12. Multicomponent phase equilibrium" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

Electrolyte solutions

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will focus on the description of equilibria in electrolyte solutions. In particular, students will become familiar with the types of electrolytes, as well as the Arrhenius theory, its application to describe the dissociation of weak electrolytes and hydrolysis processes, the role of solvent molecules in the processes of dissolution, solvation of ions, etc. The main provisions of the Debye-Hückel theory for strong electrolytes, the concept of ionic atmosphere, and the calculation of activity coefficients of ions will also be discussed. The most important part of the lecture will be the consideration of non-equilibrium phenomena in electrolyte solutions, namely diffusion and migration of ions. The dependence of the electrical conductivity of electrolyte solutions and ion mobility on concentration will be analyzed, as well as special cases of electrical conductivity in the liquid and solid phase, in particular, the relay mechanism of conductivity in the solutions of acids and bases and the nature of the conductivity of solid electrolytes.

### 3. Learning outcomes

- Understand and be able to explain the reasons for the differences in the properties of weak and strong electrolytes.
- Ability to calculate the ionic strength of a solution and ionic activity coefficients using the Debye-Hückel equation.
- Ability to explain the causes of changes in the electrical conductivity of electrolyte solutions with increasing concentration.
- Understand the mechanisms of abnormal electrical conductivity in electrolytes of different nature.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – mechanisms of abnormal electrical conductivity of solids and liquid solutions.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapter "FOCUS 5. Simple mixtures. Topic 5F" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 10. Nonideal solutions" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

Electrode potential and electrochemical cells

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture will cover the conditions of equilibrium at the interface between a metal electrode and an electrolyte solution, model concepts of the structure of a double electric layer and the mechanism of electrode potential occurrence. Students will become familiar with such basic electrochemical concepts as Galvani and Volta potentials, electrochemical potential, Nernst equation, galvanic/electrochemical cell, electrolyzer, electrode, electrolyte, electromotive force, etc. An important part of the lecture will be a discussion of the classification and structure of different types of electrodes, including the first and second types, redox, ion-selective, and enzymatic. The types of electrochemical cells and their thermodynamics will be discussed separately. The lecture will conclude with a discussion of the basics of electrochemical kinetics, namely the concepts of electrochemical process rate, overvoltage, and Faraday's laws of electrolysis.

### 3. Learning outcomes

- Understand physical sense and be able to explain the mechanism of electrode potential.
- Knowledge of the structure of the double electric layer and its role in the formation of the electrode potential.
- Ability to calculate the value of the electrode potential for different types of electrodes.
- Understand the differences between an electrochemical/galvanic cell and an electrolyzer.
- Understand the strength of an electric current as a measure of the rate of an electrochemical process and the causes of overvoltage.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – electrochemical systems used in commercial samples of chemical power sources.  
Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapter "FOCUS 6. Chemical equilibrium. Topics 6C, 6D" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 13. Electrochemical systems" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

**Surface layer and surface phenomena. Adsorption**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture, the equilibrium at the liquid-gas and solid-gas interfaces will be discussed, including the concept of interphase. Students will become familiar with the phenomena of wetting of the surface of solids and spreading of liquids, the edge (contact) angle and methods of its determination, the concepts of adhesion and cohesion, and their energy. Also discussed will be surface tension and surface activity, types of surfactants, surface excess and surface pressure, and the phenomenon of micelle formation. An important element of the lecture will be to familiarize students with the preparation and application of Langmuir-Blodgett layers. In addition, the differences between physical and chemical adsorption interactions on the surface of a solid will be analyzed. The adsorption of gases on a solid surface, the main provisions of the Henry and Langmuir monomolecular adsorption theories, the BET polymolecular adsorption theory will be discussed, and the corresponding adsorption isotherms will be analyzed.

### 3. Learning outcomes

- Understanding of the state of dynamic equilibrium at interfaces.
- Understand the differences between hydrophilic and hydrophobic surfaces, know the methods for finding the wetting edge angle.
- Know the types and structure of the molecules of surfactants and be able to explain the mechanism of their action.
- Understand main differences between physical and chemical adsorption.
- Knowledge of the main provisions of the theories of mono- and polymolecular adsorption.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – production and application of various types of Langmuir-Blodgett films for scientific and industrial needs.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "6. Surface Tension and Contact Angle: Application to Pure Substances" and "7. Adsorption from Solution and Monolayer Formation" in Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997, as well as chapters "3. Surface and Interfacial Tensions – Principles and Estimation Methods", "4. Fundamental Equations in Colloid and Surface Science", "6. Wetting and Adhesion" and "7. Adsorption in Colloid and Surface Science – A Universal Concept" in Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

### 6. Additional notes

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## Topics 9

### 1. The subject of the lecture

Chemical equilibrium

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will discuss the conditions of chemical equilibrium in homogeneous and heterogeneous systems, ways of expressing the equilibrium constant and their interrelation. The dependence of the equilibrium constant on temperature (van't Hoff's reaction isobar and isochore equations) will be analyzed separately. Particular emphasis will be placed on the essence of the van't Hoff's reaction isotherm equation and the differences between the use of Gibbs energy and Helmholtz energy as criteria for reversible and irreversible chemical processes. The application of the Le Chatelier-Braun principle to the assessment of equilibrium position shifts due to various factors will also be discussed in detail.

### 3. Learning outcomes

- Understand and be able to explain the dynamic nature of chemical equilibrium.
- Ability to write an expression for the constant of chemical equilibrium of any chemical process.
- Ability to interpret the results of the calculation of the Gibbs energy from the equation of the reaction isotherm.
- Understanding of Le Chatelier-Braun principle and the ability to use it to predict the direction of equilibrium position shift.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – expressions for equilibrium constants of homogeneous and heterogeneous industrial and native processes.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapter "FOCUS 6. Chemical equilibrium. Topics 6A, 6B" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 11. Reaction equilibrium in nonideal systems" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 10

### 1. The subject of the lecture

Chemical kinetics and catalysis

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will focus on the kinetic analysis of chemical systems. Students will become familiar with the basic concepts of chemical kinetics, such as velocity, rate constant, molecularity, order and activation energy of a chemical reaction, and the methodology for their calculation. The kinetic rate equations for simple and complex homogeneous reactions will be analyzed. Students will learn about the mechanism of influence of various factors on the rate of chemical transformations, primarily temperature increase and the introduction of catalysts. The kinetics of heterogeneous chemical transformations, namely the kinetic and diffusion domains of chemical transformations and the role of adsorption in heterogeneous reactions, will be discussed separately. Considerable attention will also be paid to the general principles of catalysis, its types, and the peculiarities of describing the kinetics of catalytic processes, including heterogeneous and enzymatic ones.

### 3. Learning outcomes

- Understand the physical sense of the main kinetic parameters.
- Ability to calculate the constant, order and activation energy of a chemical reaction from the obtained kinetic data.
- Knowledge of the basic principles and approaches used to describe the kinetics of chemical transformations.
- Understanding the mechanism of influence of various factors on the rate of chemical reactions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – the most important industrial catalytic reactions.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "FOCUS 17. Chemical kinetics. Topics 17A–17D" and "FOCUS 19. Processes at solid surfaces. Topic 19C" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 16. Reaction kinetics" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 11

### 1. The subject of the lecture

Basics of photochemistry

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will cover the basic principles of photochemistry. First of all, students will get acquainted with the laws of photochemistry, in particular the Grotthuss–Draper, the van't Hoff and Stark–Einstein laws, the Bouguer–Beer–Lambert equation, as well as the concept of quantum yield. The stages of primary and secondary photochemical transformations and the possibility of photochemical initiating chain processes will be analyzed. Their main stages will be discussed, as well as critical phenomena that may accompany chain reactions (thermal explosion and chain flash). The lecture will also familiarize students with the phenomenon of light radiation emission accompanying chemical transformations. The types of luminescence (by the method of its generation and the type of radiation transitions), the phenomenon of photosensitization, and their practical significance will be considered.

### 3. Learning outcomes

- Understand the essence of the processes of interaction of matter with light.
- Understand and be able to explain the basic laws of photochemistry.
- Understand the mechanism and consequences of critical phenomena during chain processes.
- To know the methods of generation of the particles in an excited energy state and ways of its radiative and non-radiative de-excitation.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – methods of luminescence generation and their practical significance.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "FOCUS 17. Chemical kinetics. Topic 17G" in Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019, as well as "Chapter 20. Spectroscopy and photochemistry" in Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

### 6. Additional notes

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## Topics 12

### 1. The subject of the lecture

Disperse systems and their properties

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture will cover the classification of dispersed systems by the degree of dispersion, the aggregate state of the dispersed phase and the dispersed medium (suspensions, ashes, gels, emulsions, foams, aerosols, porous bodies, capillary systems, xerogels), as well as the nature of intermolecular interactions at the interface. The most important part of the lecture will be devoted to the discussion of methods for obtaining free-dispersed systems (dispersion and condensation), their physicochemical features, thermodynamics and kinetics of formation. In addition, the aggregation stability, coagulation mechanism (including by electrolytes, the Schulze-Hardy rule), and methods of stabilizing dispersed systems will be analyzed. Students will also become familiar with electrokinetic phenomena, molecular-kinetic, optical, structural and mechanical properties of dispersed systems, and their practical significance.

### 3. Learning outcomes

- Ability to classify dispersed systems according to various criteria.
- Ability to explain the differences, advantages and disadvantages of different methods of obtaining dispersed systems.
- Understanding of the mechanisms of coagulation of dispersed systems.
- Understand the relationships between the structure, properties and practical application of dispersed systems of various types.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – practical importance of the main types of dispersed systems.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should read chapters "8. Colloidal Structures in Surfactant Solutions: Association Colloids" and "13. Electrostatic and Polymer-Induced Colloid Stability" in Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997, as well as chapters "10. Colloid Stability – Part I: The Major Players", "11. Colloid Stability – Part II: The DLVO Theory – Kinetics of Aggregation", "12. Emulsions" and "13. Foams" in Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

### 6. Additional notes

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## Course content – laboratory classes

### General provisions

1. **Contents of the laboratory workshop from the *Physical and Colloidal Chemistry for Materials Scientists* course:**

The student must complete 10 laboratory tasks as part of a team or individually. Students perform laboratory work according to an individual schedule, which is provided to them by the teacher at the first introductory laboratory session. A necessary condition for a student's admission to laboratory classes is his prior familiarization with the rules of safety technology and safe methods of work in a chemical laboratory.
2. **Team formation:**
  - a. The laboratory work is performed by a team of 2-3 students.
  - b. The division into teams is carried out on an ongoing basis (for the entire duration of the set of laboratory tasks in Physical and Colloid Chemistry for Material Scientists course).
  - c. The team will be responsible for determining the roles of its members in each individual study.
  - d. The instructor will approve the research plan to ensure that the team is working toward its goals.

## Topics 1 – Lab 1

### 1. The subject of the laboratory classes

**Determination of the thermal effect of a chemical reaction**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to familiarize students with the practical features of the calorimetric method of research on the example of studying the thermal effect of the combustion reaction. Samples of both pure organic substances with known thermodynamic characteristics and other combustible materials (polymers, wood products, etc.) can be used in the course of the work. Students will be determined the bomb calorimeter constant (based on the results of burning a standard sample) and the thermal effect (enthalpy) of combustion of the sample under study. Depending on the individual assignment, students will additionally calculate the enthalpy of the combustion reaction at a temperature specified by the instructor or the enthalpy of phase transitions of the respective substances. Students will evaluate the instrumental error of the studies and compare the results of the thermodynamic characteristics calculations using the NIST database. The laboratory work will end with the preparation of a report on the performance of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- familiarize themselves with the safety rules for working with oxygen equipment;
- acquire practical skills in preparing samples for combustion in a calorimetric bomb;
- gain experience in conducting calorimetric studies and processing the experimental data obtained (kinetics of temperature change during the experiment);
- learn to calculate the enthalpy of chemical reactions and phase transitions based on experimental data;
- learn how to estimate the error of measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory equipped with a press for making samples and equipped with a bomb calorimeter.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the theoretical foundations of thermochemistry to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare two experimental samples: standard and experimental.
  - b. The team will successively conduct two calorimetric experiments, during which pre-prepared samples will be burned.

4. Results analysis:
  - a. Based on the results of experiments, the team will plot the time dependences of the temperature change.
  - b. Students will determine individually the true temperature changes of the calorimeter during two consecutive calorimetric experiments, calculate the calorimeter constant and the thermal effect of the combustion reaction of the substance under study.
  - c. Students will conduct individually, according to the received assignments, a calculation of other thermochemical parameters.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 2C. Thermochemistry / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. Chapter 2. The first law of thermodynamics / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

## 8. Optional information

Exercise manuals will be available



## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

Phase equilibrium in three-component liquid systems with limited solubility of components

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to acquaint students with the methodology of studying mutual solubility and constructing a solubility diagram of three-component liquid mixtures. During the execution of the work, mixtures of organic and inorganic solvents of different nature will be used, which differ significantly in their physical and chemical properties (primarily, polarity). Students will prepare a series (~10) of binary solutions of different composition and determine the point of change in the phase composition of the system as a result of adding a third component (titrant). Depending on the individual task, students calculate the composition of equilibrium three-component mixtures and construct a diagram of the mutual solubility of three liquids. Students will evaluate the error of the conducted research and draw conclusions about the mutual solubility of the system components and ways to achieve homogeneity in them. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a predefined composition;
- acquire practical skills in titration when the equivalence point corresponds to a change in the phase composition of the system (transition from a homogeneous to a heterogeneous system, or vice versa);
- gain experience in determining/representing the composition of a three-component system using the Gibbs-Roseboom triangle;
- learn how to construct solubility diagrams of three liquids with one region of layering in different coordinates;
- improve their ability to perform calculations during transition between different ways of expressing the composition of solutions;
- learn to estimate the error of measurements.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for preparing solutions and carrying out titrations.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the theoretical foundations of construction of state diagrams of three-component systems and their isobaric-isothermal sections (solubility diagrams) to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.

- b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team prepares a series of initial binary liquid solutions.
  - b. The team successively titrates the initial solutions with the third component until the phase composition of the solution changes.
4. Results analysis:
  - a. Students will individually calculate the equilibrium compositions of three-component systems based on titration results and construct solubility diagrams of the studied system in Gibbs-Roseboom coordinates.
  - b. The team will present the results of their researches.
  - c. Team members will discuss and compare their results with reference (literature) data.
  - d. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 5E. Phase diagrams of ternary systems / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. 12.12. Three-Component Systems / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

## 8. Optional information

Exercise manuals will be available

## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

#### Thermal analysis of two-component systems

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to acquaint students with the method of thermal analysis. Binary low-melting systems will be used during the work. Students will prepare a series (~10) of binary mixtures of different compositions, which will be sequentially melted and cooled up to the crystallization process begins. Based on the obtained experimental data on temperature changes during cooling, the cooling curves (dependencies  $T=f(t)$ ) of the studied mixtures will be constructed. Their analysis will make it possible to find the temperatures of crystallization beginning of the corresponding mixtures and the eutectic temperature of the binary system, on the basis of which its melting diagram will be constructed. Students will estimate the error of the conducted research and draw conclusions about the nature of the interaction of components in the system. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing mixtures of a predefined composition;
- master the method of studying the processes of melting and crystallization of substances (thermal analysis);
- be able to determine the melting and crystallization temperatures using a thermocouple;
- gain experience in the use of calibration graphs;
- learn how to construct a melting diagram of a binary system in the composition-temperature coordinates.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes, reagents and equipment necessary for the preparation of reagent mixtures, a thermocouple and equipment for recording the change in temperature (thermoEMS) over time.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the theoretical foundations of construction of state diagrams of two-component systems and their isobaric sections (melting diagrams) to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare a series of a series of binary low-melting mixtures.

- b. The team will melt and cool the prepared mixtures in sequence, recording the change in temperature over time using a thermocouple.
4. Results analysis:
  - a. Based on the obtained results, the team will construct the cooling curves of the investigated binary mixtures of different compositions.
  - b. The team will determine the breakpoints or temperature stops on the cooling curves and, based on these results, will construct a melting diagram of the studied system.
  - c. The team will present the results of their researches.
  - d. Team members will discuss and compare their results with reference (literature) data.
  - e. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 5D. Phase diagrams of binary systems: solids / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. 12.8. Two-Component Solid–Liquid Equilibrium / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

## 8. Optional information

Exercise manuals will be available

## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

#### Cryoscopy

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to familiarize students with the cryoscopic method of researches and the practical application of its results. During the work, aqueous or non-aqueous solutions of non-electrolytes, electrolytes, high molecular weight compounds, polymers, enzymes, etc. will be used. Students will prepare a series of solutions of different compositions, which will be successively cooled (analogously as a pure solvent) up to the solvent crystallization process begins. The cooling curves (dependencies  $T=f(\tau)$ ) of the solvent and the prepared solutions will be used to find their crystallization temperatures. Depending on the individual assignment, the molecular weights of the solute, dissociation constants of a weak electrolyte, ionic activity coefficients, isotonic coefficient values, etc. will be calculated from the found values of the depression of the freezing point of the solutions compared to the pure solvent. The students will evaluate the error of the research and draw conclusions about the nature of the interaction between the solvent and the solute, as well as its state in the system under study. The laboratory work will end with the preparation of a report on the relevant task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- familiarize themselves with the peculiarities of cryoscopic research;
- learn how to work with a Beckman thermometer;
- be able to determine the crystallization temperature of solvent and solutions based on cooling curves;
- learn how to use the results of cryoscopic studies;
- be able to evaluate the error of measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of solutions and is equipped with a cryostat with a Beckman thermometer.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the theory of solutions and their colligative properties to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will cool the pure solvent until it begins to crystallize, recording the change in temperature over time using a Beckman thermometer.

- b. The team will repeat these measurements for 2-3 solutions of the test substance at different concentrations.
4. Results analysis:
  - a. The team will plot the cooling curves of the solvent and the tested solutions based on the results.
  - b. The team will determine the freezing point of the pure solvent and the freezing point depressions of the tested solutions.
  - c. Students will individually calculate the molecular weights of the solute, dissociation constants of the weak electrolyte, ionic activity coefficients, etc. according to the individual assignment.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 5B. The properties of solutions / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. Chapter 12. Multicomponent phase equilibrium. 12.1–12.4 / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

## 8. Optional information

Exercise manuals will be available



## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### Thermodynamics of a galvanic cell

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to acquaint students with the methodology and features of potentiometric research and to investigate the influence of temperature and concentration on the magnitude of the electromotive force of a galvanic element. Chemical galvanic elements of the simple and complicated type will be used during the work. The students will construct a galvanic cell, measure its electromotive force for different concentration values of the electrolyte (electrolytes), and also investigate the change in electromotive force with increasing temperature. The thermodynamic characteristics of the galvanic element and the equilibrium constant of the potential-determining reaction will be calculated based on the obtained dependence  $E=f(T)$ . Students will draw conclusions about its direction, about the energetics of processes in a galvanic cell, and also estimate the error of the conducted research. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- familiarize themselves with the hardware design of potentiometric measurements;
- master the method of measuring the electromotive force;
- be able to apply their theoretical skills to the practical calculation of the electromotive force of a galvanic cell;
- learn to calculate the thermodynamic characteristics of a galvanic cell;
- be able to evaluate the error of potentiometric measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of electrolyte solutions, and is equipped with a model of a galvanic cell, a potentiometer and a thermostat.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the mechanism of electrode potential occurrence, types of electrodes and electrochemical cells to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will construct a galvanic cell accordingly to the research tasks.



- b. The team will measure the electromotive force of the galvanic cell over the specified temperature range, taking measurements every 1-2 K.
4. Results analysis:
  - a. Based on the obtained results, the team will plot the dependence of the electromotive force of the galvanic cell on temperature and calculate its temperature coefficient.
  - b. Students will find individually the theoretical value of the electromotive force of a galvanic cell, based on the reference data and concentrations of the electrolytes which they used.
  - c. Students will calculate individually changes of enthalpy, entropy, and Gibbs energy of a galvanic cell in the studied temperature range, as well as equilibrium constant for the potential-determining reaction.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 6C. Electrochemical cells. TOPIC 6D. Electrode potentials / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. Chapter 13. Electrochemical systems. 13.2–13.9 / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available

## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

**Electrical conductivity of electrolyte solutions.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of laboratory work is to acquaint students with the methodology and features of conductometry studies and to investigate the dependence of the electrical conductivity of electrolyte solutions on concentration. Both strong and weak electrolytes will be used during the work. Students will prepare a series of solutions of different concentrations and measure their electrical resistance. Based on the obtained results, the specific and equivalent (molar) conductivity of the investigated solutions and, in accordance with the individual task and the nature of the sample, the dissociation constant of the weak electrolyte, the mobility and activity coefficients of the ions in the solution of the strong electrolyte, etc. will be calculated. Students will draw conclusions about the influence of the concentration and nature of electrolyte on the electrical conductivity of its solutions, as well as estimate the error of the conducted research. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- familiarize themselves with the hardware design of conductometric measurements;
- master the method of measuring the resistance / specific electrical conductivity of electrolyte solutions;
- be able to apply their theoretical skills for the practical calculation of the thermodynamic characteristics of ions and electrolytes;
- learn how to estimate the error of conductometric measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of electrolyte solutions, and is equipped with a conductometric cell and a conductometer (or another device for measuring the electrical conductivity of solutions).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the non-equilibrium phenomena in electrolyte solutions to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare a series of electrolyte solutions of different concentrations in accordance with the research task.

- b. The team will measure the electric resistance / specific conductivity of the prepared solutions.
4. Results analysis:
  - a. Based on the obtained results, the team will calculate specific and equivalent (molar) conductivity of the studied solutions.
  - b. Students will plot individually the graphical dependences of conductivity on electrolyte concentration.
  - c. Students will calculate individually the thermodynamic parameters of electrolytes or ions, depending on the task.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. TOPIC 16B. Motion in liquids / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. Chapter 15. Transport processes. 15.5–15.6 / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

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## Topics 7 – Lab 7

### 1. The subject of the laboratory classes

Study of the rate of sucrose inversion

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to familiarize students with the methodology and features of kinetic studies on the example of the reaction of sucrose inversion. During the work, catalysts of different nature (strong and weak acids of different concentrations) will be used. The students will prepare a series of sucrose solutions of different concentrations and study the kinetics of sucrose hydrolysis by the polarimetric method. Based on the results obtained, the main kinetic characteristics of the process will be calculated, namely the rate constant, activation energy, reaction order, etc. according to the individual assignment. Students will draw conclusions about the influence of relevant factors (catalyst concentration, temperature, etc.) on the rate of chemical reaction, as well as evaluate the error of the research. The laboratory work will end with the preparation of a report on the implementation of the relevant task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- become familiar with the polarimetric method of research;
- master the method of kinetic research;
- apply homogeneous catalysis to the reaction under study;
- be able to process kinetic data to calculate the main kinetic characteristics of chemical transformations;
- learn how to estimate the error of kinetic measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of sucrose and catalyst solutions, and is equipped with a polarimeter.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the physical sense and methods of finding the main kinetic parameters (rate constant of reaction, its order and activation energy) to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare solutions of sucrose and catalyst according to the research tasks.
  - b. The team will conduct kinetic studies, namely, investigate the evolution of the specific angle of rotation of plane-polarized light after it is passed through the reaction mixture.

4. Results analysis:
  - a. Based on the results obtained, the team will plot the graphical dependencies of the change in the function of the angle of rotation of plane-polarized light on time.
  - b. Students will individually find the rate constant of the studied reaction of sucrose hydrolysis based on the constructed dependencies.
  - c. Students will individually calculate other kinetic parameters of reaction as appropriate to the task.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. FOCUS 17. Chemical kinetics. TOPICS 17A–17D / Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry*, Oxford University Press 2019;
2. Chapter 16. Reaction kinetics. 16.1–16.4, 16.15, 16.16 / Ira N. Levine, *Physical Chemistry*, McGraw-Hill Higher Education 2009.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

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## Topics 8 – Lab 8

### 1. The subject of the laboratory classes

#### Sedimentation analysis of dispersed systems

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to acquaint students with the methodology and features of sedimentation analysis of dispersed systems. During the execution of the work, powder dispersions of different nature and granulometric composition and, accordingly, different disperse medium (solvents) will be used. The students will prepare the series of suspensions of the investigated substance and study the kinetics of their sedimentation. Based on the obtained results, integral and differential curves of the distribution of dispersion particles will be constructed according to the size. Students will draw conclusions about the nature of the obtained distribution (mono- or bimodal), estimate the average particle radius and polydispersity of the sample, as well as the errors of the conducted researches. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- get acquainted with the types of dispersed systems and with methods of their production;
- become familiar with the sedimentation method of research;
- gain practical skills in determining the particle size distribution of colloidal particles by the rate of their sedimentation in a liquid dispersion medium;
- learn to process the kinetic data of sedimentation analysis to build size distribution curves of dispersed systems;
- learn how to estimate the error of measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of colloidal solutions, and is equipped with torsion scales.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the methods of the production and classification of dispersed systems, methods of the determination of their dispersion degree to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare suspensions of the studied substance in accordance with the research tasks.
  - b. The team will study the sedimentation rate of colloidal particles in a liquid dispersion medium.
4. Results analysis:



- a. The team will plot a sedimentation curve for the dispersed system under study based on the results.
  - b. Students will process individually the sedimentation curve using the method of tangents and plot the integral and differential curves of the distribution of the dispersion particle on size.
  - c. Students will individually calculate the polydispersity and average particle size of the studied dispersion.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
- a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. Chapter 2. Sedimentation and Diffusion and Their Equilibrium / Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
2. Chapter 8.3. Sedimentation and creaming (Stokes and Einstein equations) / Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available



## Topics 9 – Lab 9

### 1. The subject of the laboratory classes

#### Adsorption of surfactants on solid adsorbents

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to acquaint students with the phenomenon of sorption on a solid surface. Fine-dispersed adsorbents of various nature and, accordingly, various adsorbates with surface-active properties will be used during the work. Students will prepare a series of solutions of surfactants of different concentrations and find the change in their concentration in the solutions as a result of adsorption on a solid adsorbent. Based on the obtained results, the adsorption characteristics of adsorbents will be calculated depending on the nature of the adsorbate and external conditions. Students will draw conclusions about the nature of the adsorbent - adsorbate interaction, as well as estimate the errors of the conducted researches. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- get acquainted with the types of adsorption isotherms and methods of calculating adsorption characteristics;
- gain practical skills in conducting adsorption studies of surfactants on solid surfaces of various nature;
- be able to process the data of adsorption studies and calculate the specific adsorption characteristics of the adsorbent and the parameters of the surfactant molecules in the adsorption layer;
- learn to estimate the error of measurements and related calculations.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of colloidal solutions, and is equipped with a titration device.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the theory of adsorption on a solid surface, types of adsorption isotherms and methods of determining integral and specific adsorption parameters to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare solutions of surfactants of different concentrations and samples of adsorbent of the same mass.

- b. The team conducts adsorption of the surfactant with a suitable adsorbent.
  - c. The team experimentally will determine the change in the surfactant concentration in the solution as a result of adsorption.
4. Results analysis:
- a. Based on the obtained results, the team will calculate the specific adsorption of the surfactant and plot a graphical dependence of the amount of adsorption on the concentration of the surfactant.
  - b. Students will individually process the constructed graphical dependence and find the value of the maximum adsorption of the studied surfactant.
  - c. Depending on the individual task, students will calculate the constants of the Langmuir equation, the value of the specific surface of the adsorbent, the area of the surfactant molecule in the adsorption layer, etc.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
- a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. Chapter 7. Adsorption from Solution and Monolayer Formation / Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
2. Chapter 7. Adsorption in Colloid and Surface Science – A Universal Concept / Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available

## Topics 10 – Lab 10

### 1. The subject of the laboratory classes

**Study of the wetting phenomenon. Edge angle of wetting**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to acquaint students with the phenomenon of the wetting of surface of solids and the marginal wetting angle as a criterion of surface wettability. During the work, solid substrates of different nature and surfactants of different types will be used. Students will prepare the surface of substrates, as well as a series of surfactant solutions of various concentrations. They will measure the value of the marginal wetting angle and construct wetting isotherms based on the obtained results. Students will draw conclusions about the nature of the interaction between the surface of a solid and a liquid applied to its surface, as well as about the effect of the nature and concentration of the surfactant on the wetting efficiency. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- become familiar with the phenomenon of wetting the surface of a solid;
- become familiar with the methods of inversion of hydrophobic/hydrophilic properties of surfaces;
- gain practical skills in measuring the wetting edge angle of surfaces of different nature;
- be able to evaluate the adhesion of the process of wetting a solid surface;
- learn to evaluate the error of measurements.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of surfactant solutions, and is equipped with a device for measuring the marginal wetting angle of the surface of solid substrates.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the phenomenon of wetting of the surface of a solid body with liquids, the work of cohesion and adhesion, the thermal effects that accompany them, as well as methods of measuring the marginal angle of wetting to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:

- a. The team will prepare the solid substrates and aqueous solutions of the surfactants of various compositions for conducting of studies.
  - b. The team will measure the marginal wetting angles of substrate surfaces with surfactant solutions of various concentrations.
4. Results analysis:
- a. Based on the obtained results, the team will plot surface wetting isotherms of the studied solid substrate.
  - b. Students will individually process the obtained results, find the point of inversion of the extreme wetting angle and evaluate the value of the work of adhesion of the wetting process for the studied substrate.
  - c. The team will present the results of their researches.
  - d. Team members will discuss and compare their results with reference (literature) data.
  - e. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
- a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. Chapter 6. Surface Tension and Contact Angle: Application to Pure Substances / Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
2. Chapter 6. Wetting and Adhesion / Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available

## Topics 11 – Lab 11

### 1. The subject of the laboratory classes

**Determination of surface tension of aqueous surfactant solutions**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to acquaint students with surface-active substances (surfactants), the concepts of surface activity and surface tension, as well as the methods of measurement of surface tension. Water-soluble surfactants of various types will be used during the work. Students will prepare a series of aqueous solutions of surfactants of different concentrations and find their surface tension experimentally. Based on the obtained results, surface tension isotherms and adsorption isotherms will be constructed for each investigated surfactant. Students will calculate the molecular characteristics of surfactants in the adsorption layer, draw conclusions about the surface activity of the studied substances, and also estimate the error of the conducted studies. The laboratory work will end with the preparation of a report on the completion of the corresponding task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- improve their skills in preparing solutions of a given composition;
- become familiar with the concept of surface activity and the influence of various factors on its value;
- gain practical skills in measuring surface tension;
- be able to calculate the molecular characteristics of surfactants in the adsorption layer;
- learn how to estimate the error of measurements.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains dishes and reagents necessary for the preparation of surfactant solutions, and is equipped with a device for measuring surface tension.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the physical sense of the concepts of interphase, surface tension, surface activity, types of surfactants, as well as methods of the measuring of surface tension to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare the solutions of surfactants of different nature and concentration depending on the received tasks of studies.

- b. The team will measure the surface tension of the prepared solutions using different methods.
4. Results analysis:
  - a. Based on the obtained results, the team will plot isotherms of surface tension and adsorption isotherms of surfactants.
  - b. Students will individually differentiate the resulting adsorption curve and find the limiting value of surfactant adsorption.
  - c. Students will individually calculate the molecular characteristics of adsorption of the studied surfactant.
  - d. The team will present the results of their researches.
  - e. Team members will discuss and compare their results with reference (literature) data.
  - f. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
  - a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. Chapter 6. Surface Tension and Contact Angle: Application to Pure Substances / Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
2. Chapter 3. Surface and Interfacial Tensions – Principles and Estimation Methods / Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available



## Topics 12– Lab 12

### 1. The subject of the laboratory classes

Preparation and study of coagulation of sol with electrolytes

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory work aims to acquaint students with methods of obtaining, the structure of colloidal particles in liquid solutions, and the conditions of aggregative stability of ultradispersed colloidal systems. During the work, students will synthesize the sols of inorganic compounds of various nature and investigate the conditions of their coagulation under the action of electrolyte solutions with different ion charges. Based on the obtained results, the thresholds of coagulation of the studied sol for different electrolytes will be determined and conclusions will be drawn about the validity of the Schulze-Hardy empirical rule. Students will also assess the error of the conducted research. The laboratory work will end with the preparation of a report on the completion of the relevant task.

### 3. Learning outcomes

By working on this laboratory exercise, students will:

- become familiar with the methods of preparing ultrafine systems;
- gain practical skills in the synthesis of ashes of different nature;
- gain practical skills in determining the threshold of coagulation of ashes in the presence of electrolytes of different nature;
- be able to calculate the value of the coagulation threshold of sols;
- learn to estimate the error of measurements.

### 4. Necessary equipment, materials, etc

The exercise is conducted in a laboratory, which contains utensils and reagents necessary for the preparation of colloid solutions and their coagulation.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

Lab course outline:

1. Knowledge check from lecture:
  - a. A short survey of the students regarding to the methods of the production of dispersed systems, conditions of their stability, mechanism and kinetics of the coagulation of sols to make sure that ones are well prepared for laboratory work.
2. Introduction:
  - a. Familiarization with the purpose of laboratory work and discussion of individual points of the methodology of its implementation.
  - b. Discussion of the sequence of processing the obtained experimental data in accordance with the task.
3. Research:
  - a. The team will prepare an aqueous sol of the substance under study in accordance with the assigned tasks of study.
  - b. The team will study the coagulation of the obtained sol with electrolytes of different nature, which have ions of different charges in their composition.
4. Results analysis:

- a. Students will individually calculate the coagulation thresholds of the studied sol by electrolytes of different nature.
  - b. Students will individually check the validity of the Schulze-Hardy empirical rule for the studied system.
  - c. The team will present the results of their researches.
  - d. Team members will discuss and compare their results with reference (literature) data.
  - e. Students will draw conclusions about the correctness of holding experiment, the adequacy of the obtained results and, if necessary, explain the reasons for their deviation from the known table (literature) values.
5. Summary:
- a. Summarizing the results of the laboratory work in accordance with the previously set tasks.
  - b. Preparation of an individual reports by students on the performed laboratory work.

In general, the laboratory class will be divided into three parts.

The first part will include the teacher's checking of the students' theoretical knowledge on the topic of the work and evaluation of the developed theoretical introductions.

The second part involves conducting the experiment, in which each student takes an active part, and individual processing of the experimental data (graphing, calculations, formulation of conclusions). The teacher approves the research plan to make sure that the team is working towards the goal and monitors the progress of its implementation.

In the third part of the lab, the results will be discussed. Students will compare them with known data. This part will end with the independent preparation of individual reports, their submission and defense of the results in front of the teacher.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Recommended reading:

1. Chapter 13. Electrostatic and Polymer-Induced Colloid Stability / Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
2. Chapter 10. Colloid Stability – Part I: The Major Players (van der Waals and Electrical Forces) / Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

Students should prepare a theoretical introduction to the lab exercise.

## 7. Additional notes

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## 8. Optional information

Exercise manuals will be available

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**SMART CONJUGATED POLYMERS**

**Code: SCP**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### SMART CONJUGATED POLYMERS: INTRODUCTION

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Discovery of conducting polymers caused the advent of new types of electronic and optoelectronic devices. In 2000, Alan J. Heeger, Alan G. MacDiarmid, and Hideki Shirakawa were awarded the Nobel Prize for their discovery. During the lecture, the current state of organic electronics and the historical aspect of the development of the ideas about conducting polymers will be presented. Conducting polymers with conjugated  $\pi$ -electron bonds in a macromolecular chain can be classified as organic semiconductors with specific properties: increased electrical conductivity, photoconductivity, thermal stability, paramagnetism, and catalytic activity. The theory of electronic properties of conjugated polymers will be considered using polyacetylene as an example. Students will learn the chemical and electronic structure of conjugated polymers and types of polymers with alternating multiple bonds.

#### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Smart conjugated polymers, especially: fundamentals, and types.*

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *The discovery of polyacetylene film – the dawning of an era of conducting polymers.* Shirakawa H., 2001. *Curr. Appl. Phys.* 1, 281–286.
- *Semiconducting and metallic polymers: the fourth generation of polymeric materials.* Heeger A., 2001. *J. Phys. Chem. B.* 105, 36, 8475–8491.
- *Polyanilines: from solitons to polymer metal, from chemical curiosity to technology.* Epstein A.J., Mac Diarmid A.G., 1995. *Synth. Met.* 69, 179–182.
- *Focus Article: Twenty-five years of conducting polymers.* Shirakawa H., McDiarmid A., Heeger A. 2002. *Chem. Comm.* 1, 1–4.
- *Prospects of conducting polymers in molecular electronics.* Saxena V., Malhotra B.D., 2003. *Curr. Appl. Phys.* 3, 293–305.

#### 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### METHODS OF CONJUGATED POLYMERS SYNTHESIS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

When obtaining electrically conductive conjugated polymers, the main task is to create high-molecular systems with a conjugation chain capable of providing the generation of charge carriers (soliton or polaron type) with a long lifetime. The introduction of substituents into the hydrocarbon chain made it possible to obtain a class of polymers with a wide range of physicochemical properties. The lecture will present the mechanisms of basic methods of conjugated polymers synthesis:

- catalytic synthesis of polymers with an ordered structure, for example, polyacetylene, polypyrrole, polythiophene, polyparaphenylene,
- oxidative polymerization (polycondensation) of aromatic compounds (arenes), for example, aniline, using peroxide compounds as oxidants,
- electrochemical anodic (oxidative) and cathodic (reductive) polymerization, direct and indirect methods,
- photopolymerization - under the influence of UV radiation,
- thermolysis of precursors on the example of polyvinylphenylene synthesis,
- biocatalytic synthesis, for example, enzymatic.

During the lecture, students will learn methods of forming polymer films of controlled thickness on the surface of semiconductors, metals, or dielectrics using already synthesized polymer: spin-coating, Langmuir-Blodgett, layer-by-layer self-assembling, magnetron and thermovacuum sputtering.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Methods of conjugated polymers synthesis*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Conducting polymers: a comprehensive review on recent advances in synthesis, properties and applications*. Namsheer K. N., Rout C. S. 2021. RSC Advances. 11(10), 5659–5697. doi:10.1039/d0ra07800j
- *Conducting polymer nanomaterials: electrosynthesis and applications*. Li C., Bai H., Shi G. 2009. Chem. Soc. Rev. 38, 2397–2409. doi: 10.1039/b816681
- *Progress in preparation, processing and applications of polyaniline*. Bhadra S., Khastgir D., K. Singhaa N., Lee J. H., Prog. Polym. Sci. 34, 783–810. doi:10.1016/j.progpolymsci.2009.04.00



Additional, optional literature:

- *An overview on the synthesis and recent applications of conducting poly(3,4-ethylenedioxythiophene) (PEDOT) in industry and biomedicine.* Rahimzadeh Z., Naghib S. M., Zare Y., Rhee K. Y. 2020. *J. Mater. Sci.* doi:10.1007/s10853-020-04561-2.
- *Conducting electroactive polymers via photopolymerization: A review on synthesis and applications.* Heydarnezhad H. R., Pourabbas B., Tayefi M. 2017. *Polym. Plast. Technol. Eng.* 57(11), 1093–1109. doi:10.1080/03602559.2017.1370111
- *Gas sensors based on conducting polymers.* Bai H., Shi G. 2007. *Sensors.* 7(3), 267–307. doi:10.3390/s7030267

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### DOPING OF CONJUGATED POLYMERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Conjugated polymers become conductive due to doping - the addition of electrons (reduction reaction) or removal of electrons from the polymer (oxidation reaction). The process of doping of conjugated polymers can take place through the action of chemical substances – molecular dopants (iodine, sodium naphthalide), strong acids, electrochemically, by direct injection of an electron or hole into heterostructures, and by photo-doping, that is, doping under the influence of light or other radiation. The degree of doping is the number of moles (atoms) of the dopant per elementary link of the conjugated polymer. There are weakly doped  $\gamma = 0.001-1\%$ , medium doping level  $\gamma = 1-10\%$ , and highly doped polymers  $\gamma = 10-50\%$ , sometimes up to 70%. During the lecture, students will learn about the Doping mechanism of conjugated polymers; Donor and acceptor doping using chemical factors; Proton doping; Electrochemical doping of conjugated polymers (anodic and cathodic); Photodoping, and Secondary doping. The acid (proton) doping type is inherent only to conjugated polyaminoarenes, for example, polyaniline, which has an amino (imino) group in its structure. At the same time, the polymer structure rearranges from quinoid to benzoquinoid. Ultimately, the redistribution of charge and spin leads to the formation of a charge carrier – a link from two aniline fragments, which has a positive charge and an unpaired spin – a polaron. Electrochemical doping of n-type, usually with a metal ion, can be carried out using a metal as a cathode material immersed in an electrolyte containing a metal cation. As a rule, such processes take place in organic electrolytes in an inert atmosphere. Electrochemical doping of p-type (acid anions) can be carried out by anodic oxidation, immersing a film of conjugated polymer on the electrode in a dopant electrolyte and applying a positive potential. Each of the charge injection methods leads to unique phenomena. In the case of chemical and/or electrochemical doping, the induced conductivity is constant until the carriers are chemically compensated or removed by "dedoping". In the case of photoexcitation, the photoconductivity lasts only as long as the excitation lasts. If charge injection occurs at the metal-semiconductor interface, electrons are placed in the  $\pi^*$  zone and/or holes in the  $\pi$  zone only when the bias voltage is applied.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Doping of conjugated polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Conducting polymers. Handbook of polymer synthesis, characterization, and processing.* Percino M. J., Chapela V. M., 2013. 535–557. doi:10.1002/9781118480793.ch29

- *Chemical doping of organic semiconductors*. Bhagat S., Hase H., Salzmann I., 2021. *Organic Flexible Electronics*. 107–141. doi:10.1016/b978-0-12-818890-3.000
- *Processible conjugated polymers: from organic semiconductors to organic metals and superconductors*. Pron A., Rannou P., 2002. *Prog. Polym. Sci.* 27(1), 135–190. doi:10.1016/s0079-6700(01)00043-0
- *The effects of secondary doping on ink-jet printed PEDOT:PSS gas sensors for VOCs and NO<sub>2</sub> detection*. Vigna L., Verna A., Marasso S. L., et al., 2021. *Sens. Actuators: B*. 345, 130381.

## 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### MECHANISM OF CONDUCTIVITY IN CONJUGATED POLYMERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

A conjugated polymer chain can exhibit sufficient conductivity in the doped state ( $p$ - or  $n$ -doped), depending on what charge is injected, while remaining non-conductive in the undoped state. It is considered that charge transfer in conjugated polymers occurs by a jumping mechanism, which creates the movement of charge along the molecule - an electric current. The lecture will present types of charge carriers (neutral and charged solitons, charged carriers – polarons, and bipolarons). The solitons, polarons and bipolarons are mobile. Under the action of an electric field, it can move along the polymer chain by reorganization of double and single bonds in the conjugated system. During the lecture, students will learn about the conductivity mechanism of conjugated polymers; Band theory; Model of variable-range hopping (VRH); Soliton model by Su-Schrieffer-Heeger (SSH); Kivelson's model; and Domain theory of conductivity.

Known polymer semiconductors have a negative temperature coefficient of resistance, and the dependence of  $\lg \rho$  on  $1/T$  in the temperature range from 20 to 200 °C is mainly linear. So, it is possible to calculate the activation energy of conductivity. Even doped to a highly conductive state, most  $p$ -conjugated polymers behave as classic semiconductors (VRH-variable range hopping is the standard proposed mechanism). Electron tunneling through the amorphous phase can occur at a high doping level. Electron transfer in ordered crystalline materials proceeds only in the allowed zones. In contrast, there are several electron transfer channels in disordered polymer systems, namely, diffusion transfer through delocalized states and a hopping channel through localized ones.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Mechanism of conductivity in conjugated polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Conducting polymers: electrical conductivity*. Kohlman R. S., Joo J., Epstein A. J., 1996. Physical properties of polymers handbook. Mark J. E. ed.; Amer. Inst. Phys. Woodbury: New-York.
- *Systematic conductivity behavior in conducting polymers: Effects of heterogeneous disorder*. Kaiser A. B., 2001. Adv. Mater. 13, 927–941.
- *Solitons in conducting polymers*. Heeger A. J., Kivelson S., Schrieffer J. R., Su W.-P., 1988. Rev. Mod. Phys. 60(3), 782–850.
- *DC Conduction in electrochemically synthesized polypyrrole films*. Kaynak A., 1998. Tr. J. Chem. 22, 81–85.

### 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

#### FEATURES OF STRUCTURE OF CONJUGATED POLYMERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to describe the crystalline and amorphous structure of conjugated polymers. Unlike crystalline bodies with an ordered structure, polymeric materials are characterized by the absence of long-range order. Conjugated polymers in a thin layer have a globular or fibrillar structure. The supramolecular structure of conjugated polymers consists of amorphous and crystalline regions. It is considered that the islands of crystallinity are surrounded by an amorphous matrix, which creates a barrier for electron transfer. Conjugated polymers in a thin layer have a globular or fibrillar structure. Thin films up to 60-80 nm thickness consist of ordered islands (domains) with a diameter of 100-1000 nm. Each domain is an ensemble of spherical globules (grains) with a diameter of 10-30 nm. The influence of doping on the structure of polymers is explained by its different mechanisms. Protonation itself does not change the number of electrons in the polymer chain. Due to the salt formation, the level of crystallinity increases. In the case of doping with dopants of acceptor type ( $J_2$ ,  $Cl_2$ ,  $Br_2$ , etc.), or donor type (Na, Li, Ca), an electron is transferred from or to the dopant molecule. Formed charged particle plays the role of an alloying impurity ( $J^{3-}$  or  $Li^+$ ). Doping large molecules (heteropolyacids) can cause a change in the crystal structure and affect the magnetic properties.

The lecture will present features of the structure of the conjugated polymers in a thin layer. Students will learn about the influence of doping on the structure of conducting polymer, and structure research methods, namely, IR, UV, EPR, NMR spectroscopy, and X-ray phase analysis. The relationship between the structure and electronic properties of conjugated polymers, and the peculiarities of the morphology of polymer layers obtained by electrochemical polymerization in different modes, will be considered.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Structure of conjugated polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electronics of conjugated polymers (I): Polyaniline*. Molapo K. M., Ndingili P. M., Ajayi R. F., et al., 2012. Int. J. Electrochem. Sci. 7(12), 11859-11875.
- *Highly ordered conjugated polymer nanoarchitectures with three-dimensional structural control*. Vlad A., Dutu C. A., Guillet P., et al., 2009. Nano Lett. 9(8), 2838-2843.
- *Polymer nanofibers and nanotubes: Charge transport and device applications*. Aleshin A. N., 2006. Adv. Mater. 18, 17-27. doi: 10.1002/adma.200500928

- *One-Dimensional conducting polymer nanostructures: Bulk synthesis and applications*. Tran H. D., Li D., Kaner R. B., 2009. *Adv. Mater.* 21, 1487–1499. doi: 10.1002/adma.200802289
- *Structure and properties of polyaniline micro- and nano-composites with Noble metals*. Nanooptics and photonics, nanochemistry and nanobiotechnology, and their applications. Aksimentyeva O., Horbenko Yu., Demchenko P., 2020. *Springer Proceedings in Physics*. 246, 507–522. [https://doi.org/10.1007/978-3-030-51905-6\\_35](https://doi.org/10.1007/978-3-030-51905-6_35)

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### OPTICAL PROPERTIES OF CONJUGATED POLYMER SYSTEMS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Substances with a system of conjugated bonds are characterized by electronic transitions. The intensity of optical absorption increases (hyperchromic effect) as the conjugation length increases. Moreover, the absorption maximum in electronic spectra shifts toward longer wavelengths (bathochromic shift). Spectral properties of macromolecules in the optical energy range are determined by their energy structure. Conjugation lowers the energy difference between the HOMO and LUMO of the  $\pi$ -electron system. The length of the conjugated chain can be adjusted by choosing a synthesis method of conducting polymer or film formation, which is reflected in the optical properties. An essential factor determining the optical properties of conjugated polyarenes is the molecular structure of the elementary link - the nature and position of the substituents of the benzene ring, their relative arrangement, the ability to change conformation, etc. Optical absorption of carriers in conjugated polymers mainly occurs in the energy range that corresponds to the near ultraviolet (200-400 nm), visible (400-800 nm), and near-infrared (800-1100 nm) region. The chromogenic material induces a colored center capable of absorbing light in the visible part of the spectrum under external influence. The ability to generate color is determined by the energy characteristics of molecules in the base and excited states and factors characterizing the transition from one state to another.

During the lecture, students will learn about the optical properties of conjugated polymer systems; Classification of optical phenomena; Electrochromicity as a change in the optical properties of a substance when an electric field is applied; Works of Deb, Plath; Effects of Stark, Kerr; Faraday effect. The thermochromic effect is a reversible change in the absorption spectrum and, accordingly, the color of the material as a result of its heating and cooling. Electrochromicity is a change in the optical properties and, accordingly, the color of a substance when an electric field is applied.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Optical properties of conjugated polymer systems*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives*. Aksimentyeva O. I., Konopelnik O. I., Poliovyi D. O. eds.: Reshetnyak O. V., Zaikov G. E. 2017. *Computational and experimental analysis of functional materials*. Toronto: Apple Academic Press, 91-150. doi:10.1201/9781315366357

- *Conjugated amplifying Polymers for Optical Sensing Applications*. Rochat S., Swager T. M., 2013. ACS Appl. Mater. Interfaces. 5, 11, 4488–4502.
- *Exploring the origin of high optical absorption in conjugated polymers*. Vezie M. S., Few S., Meager I., et al., 2016. Nat. Mater., 15, 746–753.
- *Thermochromic effect in the films of conjugated polyaminoarenes*. Konopelnyk O. I., Aksimentyeva O. I., eds.: Reshetnyak O. V., Zaikov G. E., 2017. Computational and Experimental Analysis of Functional Materials, Toronto: Apple Academic Press, 219–242. doi:10.1201/9781315366357
- *Conjugated polymers: Optical toolbox for bioimaging and cancer therapy*. Wei J., Liu Y., Yu J., et al., 2021. Small. 17, 43. <https://doi.org/10.1002/smll.202103127>

## 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### APPLICATIONS OF CONDUCTING POLYMERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The unique electrical and optical properties and structure of conducting polymers determine their use as components of hybrid nanosystems. The lecture will present the application of conjugated conducting polymers; Light energy converters; Structure and types of electrochromic cells; Non-reflective displays; Smart windows; Mirrors with controlled reflection; During the lecture, students will learn about anotechnological approaches to improve the characteristics of optoelectronic devices.

Polymer solar cells are a type of solar cells that generate electricity from sunlight. In 1992, data on charge transfer from a semiconductor polymer to an acceptor were published for the first time. A relatively new technology is actively researched in universities, national laboratories, and several companies around the world. Prototype devices with an energy conversion efficiency of 11.5% have been demonstrated. For organic light-emitting diodes (OLEDs), polymers based on poly-para-phenylenevinylene, polycarbazole, and their derivatives have been offered. In lasers, the polymer acts as an active material capable of amplifying light and connected to the resonator. Under the action of the applied potential difference (1-5 V), the conjugated polymer is oxidized or reduced depending on the polarity of the voltage, as a result of which the electro-optical effect is induced. The chromogenic material induces a colored center capable of absorbing light in the visible part of the spectrum under external influence. Each electro-optical device consists of an electrochemical cell, which includes an ion-conducting electrolyte medium (liquid or solid) and one or more electrochromic materials whose response to an electric current causes a change in their electrical/optical properties, resulting in the generation of color.

Electronic and color transformations can be used to create non-radiative electrochromic devices - organic displays, "smart windows", indicators, sensors, optical memory devices, optical switches, etc. Examples of the application of electrochromic materials: mirrors with controlled reflection, displays on supermarket shelves, electronic books, medical tests, smart cards, bulletin boards, children's toys.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Applications of conducting polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Recent trends and developments in conducting polymer nanocomposites for multifunctional applications.* Sharma S., Sudhakara P., Omran A. A. B., Singh J., Ilyas R. A., 2021. *Polymers*. 13(17). doi:10.3390/polym13172898
- *Conducting polymer nanomaterials and their applications.* Jang J., 2006. *Adv. Polym. Sci.* 189–260. doi:10.1007/12\_075

Additional, optional literature:

- *Functionalization of conducting polymers and their applications in optoelectronics.* Khokhar D., Jadoun S., Arif R., Jabin S., 2020. *Polym-Plast. Tech. Mat.* 60(5), 465–487. doi:10.1080/25740881.2020.1819312
- *Polymer-based gas sensors to detect meat spoilage: A review.* Matindoust S., Farzi G., Nejad M. B., Shahrokhbadi M. H., 2021. *Reactive and Functional Polymers*, 104962. doi:10.1016/j.reactfunctpolym.202
- *An overview on the synthesis and recent applications of conducting poly(3,4-ethylenedioxythiophene) (PEDOT) in industry and biomedicine.* Rahimzadeh Z., Naghib S. M., Zare Y., Rhee K. Y., 2020. *J. Mater. Sci.* doi:10.1007/s10853-020-04561-2
- *E-Tongues/noses based on conducting polymers and composite materials: Expanding the possibilities in complex analytical sensing.* Sierra-Padilla A., García-Guzmán J. J., López-Iglesias D., Palacios-Santander J. M., Cubillana-Aguilera L., 2021. *Sensors*. 21(15), 4976. doi:10.3390/s21154976

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

#### OPTICAL SENSORS BASED ON CONJUGATED POLYMERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Color changes in thin layers of conductive polymers are caused by electronic transitions in the conjugated polymer chain. The rate of charge transfer and color transitions in conducting polymers depend on the structure of the polymer, the level of doping, and the composition of the liquid or gas medium. During the lecture, students will learn about the optical sensors based on conjugated polymers and composites; Types and advantages of optical sensors; Gasochromic, ionochromic and thermochromic effects in conjugated systems; Intelligent sensory environments; Basic principles of construction of optical sensors based on conjugated polymers.

The ionochromic effect can be used in optical pH sensors. The gasochromic effect in films of polyaminoarenes is used to create express indicators of product freshness. Solvatochromism is used to describe changes in optical spectra in solvents of different polarities. Indicators reveal changes in the position, intensity, and shape of the absorption band depending on the solvent nature.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Optical sensors based on conjugated polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Flexible elements of gas sensors based on conjugated polyaminoarenes*. Aksimentyeva O. I., Tsizh B. R., Horbenko Yu. Yu., et al., 2018. *Mol. Cryst. Liq. Cryst.* 670, 3–10 doi:10.1080/15421406.2018.1550546

- *Gas sensors based on conducting polymers*. Bai H., Shi G., 2007. *Sensors*. 7(3), 267–307. doi:10.3390/s7030267

Additional, optional literature:

- *Optical properties of conjugated polymer: review of its change mechanism for ionizing radiation sensor*. Isa N. M., Baharin R., Majid R. A., Rahman W. A., 2017. *Polym. Adv. Technol.* 28(12), 1559–1571. doi:10.1002/pat.4067

- *Review on the utilisation of sensing materials for intrinsic optical NH<sub>3</sub> gas sensors*. Hadi Ismail A., Sulaiman Y., 2021. *Synth. Met.* 280, 116860. doi:10.1016/j.synthmet.2021.11686

### 6. Additional notes

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## Course content – laboratory classes

### Topics 1 – Lab 1

#### 1. The subject of the laboratory classes

##### ELECTROCHEMICAL SYNTHESIS OF CONJUGATED POLYMERS

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study of the influence of the electrosynthesis mode on the formation processes and properties of conjugated polymers in a thin layer. Students will perform electrochemical synthesis of conjugated polyaminoarenes on the surface of optically transparent electrodes in the cyclic potential sweep mode and determine the thickness and morphology of the obtained films. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

#### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Electrochemical synthesis of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemical synthesis of conjugated polymers*, including critical analysis, synthesis, and conclusions.

#### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- Transmission electron microscope,
- Computer laboratory

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,



- discussion (checking students' knowledge) of methods of electrochemical synthesis of polymers, mechanism of oxidative electrochemical polymerization of anilines, methods of materials characterization, especially TEM technique,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Computational and experimental analysis of functional materials*. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. <http://www.appleacademicpress.com/computational-and-experimental-analysis-of-functional-materials-/9781771883429> – chapter 3.
- *Cyclic Voltammetry*. David K., Grosser Jk. New York: VCH Publishers, 1994.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

#### CHEMICAL SYNTHESIS OF CONJUGATED POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will perform chemical synthesis of conjugated polyaminoarenes by the method of oxidative polymerization and determine the effect of chemical doping on the structure and conductivity of samples. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Chemical synthesis of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Chemical synthesis of conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Chemical reactor,
- Magnetic stirrer,
- Water jet pump,
- Dryer,
- X-ray diffractometer,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of methods of conducting polymer synthesis,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,

- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *“Synthetic metals”: a novel role for organic polymers.* MacDiarmid A., 2001. *Curr. Appl. Phys.* 1, 269-279.
- *Conducting polymers: a comprehensive review on recent advances in synthesis, properties and applications.* Namsheer K. N., Rout C. S. 2021. *RSC Advances.* 11(10), 5659–5697. doi:10.1039/d0ra07800j
- *Conducting polymer nanomaterials: electrosynthesis and applications.* Li C., Bai H., Shi G. 2009. *Chem. Soc. Rev.* 38, 2397–2409. doi: 10.1039/b816681
- *Progress in preparation, processing and applications of polyaniline.* Bhadra S., Khastgir D., K. Singhaa N., Lee J. H., *Prog. Polym. Sci.* 34, 783–810. doi:10.1016/j.progpolymsci.2009.04.00

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

#### ELECTROCHEMICAL DOPING OF CONJUGATED POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will perform electrochemical doping of conjugated polymers during laboratory classes and determine the charge transfer parameters in obtained thin films. Students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions about the possibility of using the polymer to create electrochromic films of sufficient speed, which can be used in visualization devices, indicators, sensors, etc. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Electrochemical doping of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemical doping of conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of types of doping of conjugated polymers, possible application of conductive polymer films,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,

- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Computational and experimental analysis of functional materials*. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017.  
<http://www.appleacademicpress.com/computational-and-experimental-analysis-of-functional-materials-/9781771883429> – chapter 3.
- *“Synthetic metals”: a novel role for organic polymers*. MacDiarmid A., 2001. *Curr. Appl Phys.* 1, 269-279.
- *Halogen doped polyacetylene*. Shirakawa H., Chiang C.K., Park Y.W., Heeger A.J., Mac-Diarmid A.G., 1978. *J. Chem. Phys.* 69, 40–49.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

#### TEMPERATURE DEPENDENCE OF THE CONDUCTIVITY OF CONJUGATED POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the temperature dependence of the conductivity of conjugated polymers. Students will determine the conductivity activation parameters. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Conductivity of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Conductivity of conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Device for measuring the temperature dependence of resistance,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of types of charge carriers in conjugated polymer systems, model representations of the conduction mechanism in conjugated polymers, principle of thermocouple operation,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.



Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Low-dimensional variable range hopping in conducting polymers*. Epstein A. J., Lee W.-P., Prigodin V. N., 2001. Synth. Met. 117, 9–13.
  - *Electrical properties of polypyrrole conducting polymer at various dopant concentrations*. Othman N., Talib Z. A., Kassim A., Shaari A. H., Liew J. Y. C., 2009. J. Fundam. Sci. 5, 29–33.
  - *Conducting polymers: electrical conductivity*. Kohlman R. S., Joo J., Epstein A. J., 1996. Physical properties of polymers handbook. Mark J. E. ed.; Amer. Inst. Phys. Woodbury: New-York.
- Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### OPTICAL PROPERTIES OF CONJUGATED POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students' theoretical knowledge of UV-Vis spectroscopy technique will be verified. Students will perform measurements and analysis of transmission and absorption spectra of various polyaminoarenes on optically transparent surfaces and their application in optical pH sensors. Students will make the calibration curves based on the changes in optical density and shifts in the position of the absorption maximum. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Optical properties of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Optical properties of conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- UV-Vis spectroscopy,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,  
a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of optical phenomena in conjugated polymer systems, principles of potentiometric and optical sensors operation, UV-Vis spectroscopy,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,

- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Computational and experimental analysis of functional materials*. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. <http://www.appleacademicpress.com/computational-and-experimental-analysis-of-functional-materials-/9781771883429> – chapter 3.
- *Solvatochromic effect in polyorthotoluidine solution*. Stepura A., Aksimentyeva O., 2018. Visnyk of the Lviv University. Ser. Chem. 59, 407-413.
- *Optical properties of conjugated polymer: review of its change mechanism for ionizing radiation sensor*. Isa N. M., Baharin R., Majid R. A., Rahman W. A., 2017. Polym. Adv. Technol. 28(12), 1559–1571. doi:10.1002/pat.4067

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

#### ELECTROCHROMIC EFFECT IN CONJUGATED POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the electrochromic effect in conjugated polymers. Students will study the effect of applied potential on absorption spectra, morphology, and color of polymer films. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Electrochromic effect in conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochromic effect in conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- Optical microscope,
- UV-Vis spectroscopy,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of optical phenomena in conjugated polymers,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,

- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Polymeric electrochromics*. Sonmez G., 2005. Chem. Comm. 42, 5251. doi:10.1039/b510230h
- *New electrochromic materials*. Rowley N., Mortimer R., 2002. Sci Prog. 85(3), 243-262.
- *Colours from electroactive polymers: Electrochromic, electroluminescent and laser devices based on organic materials*. Carpi F., De Rossi D., 2006. Optics & Laser Technology. 38, 292–305.
- *Contrast limitations of dual electrochromic systems*. Padilla J., Otero T. F., 2008. Electrochem. Commun. 10, 1–6.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv



**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**ENVIRONMENTAL PROBLEMS OF MATERIALS SCIENCE**

**Code: EPMS**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### SCIENTIFIC AND TECHNICAL PROGRESS AND CURRENT TASKS OF NATURE PROTECTION

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Scientific and technical progress is closely related to the production of materials of different chemical composition and their ever-increasing use. Considering the issue of materials science, it is necessary to touch on the issues of nature protection that are relevant today.

During the lecture on the role of materials science in solving the problems of nature protection, the most important aspects of the production and use of modern materials will be presented, which indicate the need to modernize the technologies for the production of materials for various purposes. Students should systematize their knowledge of engineering and technical, socio-economic and moral and ethical aspects of environmental protection in modern materials science.

During the lecture, students will learn that despite the wide range of modern materials and their widespread use, there are a large number of questions in materials science that relate to environmental protection.

#### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to materials science and environmental pollution.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

Additional, optional literature:

- Castillo-Suárez, L.A., Sierra-Sánchez, A.G., Linares-Hernández, I. *et al.* A critical review of textile industry wastewater: green technologies for the removal of indigo dyes. *Int. J. Environ. Sci. Technol.* (2023). <https://doi.org/10.1007/s13762-023-04810-2>

## 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### BASICS OF TEACHING ABOUT THE BIOSPHERE

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The environment is a complex ecological system in which the mechanisms of material and energy chains are established. The composition of the biosphere is constantly changing. There are a large number of environmental factors that affect the environment. In the environment as a whole and its components, self-cleaning processes are constantly taking place, but their capabilities are limited. That is why environmental monitoring is carried out to assess, warn, and prevent negative impact on nature. Monitoring as a system of observing the state of the environment in order to assess its state and prevent environmental problems at various levels is especially important at the current stage of growth in the number of materials of different chemical composition and their practical use.

During the lecture, students learn about the environment as an ecosystem. They will receive information about the biosphere, its composition and structure; classification of environmental factors and their impact on biosphere components; about the protective mechanisms of the environment and the possibilities of self-cleaning of the biosphere.

During the lecture, students will also familiarize themselves with the environmental monitoring system, its levels and capabilities, methods and approaches.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to materials science and the environment.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

Additional, optional literature:

1. - Biodegradable polymer-based nanoadsorbents for environmental remediation / Sapna \*, Dinesh Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018, - P. 261-278. <https://doi.org/10.1016/B978-0-12-811033-1.00012-3>

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### ANTHROPOGENIC ENVIRONMENTAL FACTORS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

One of the important problems of today is environmental pollution. It can be caused by various factors, among which anthropogenic factors occupy a special place.

The production and use of modern materials is extremely diverse, but at the same time can be dangerous for the environment and people. The lecture will introduce the most important factors of anthropogenic impact on natural objects in relation to the synthesis and use of materials of various nature. During the lecture, students will get acquainted with the concept of an environmental pollutant, as well as priority air, water, and soil pollutants that can be formed during the production and use of various materials.

Students will also receive information on ways to reduce the negative impact on environmental pollution regarding the synthesis and use of materials for various purposes.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate it, draw conclusions, formulate and solve problems related to anthropogenic impact on the environment during the synthesis and use of materials of various nature and purpose.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

### 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### HYDROSPHERE. PROTECTION AND RATIONAL USE OF WATER

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

One of the important problems of environmental pollution at the current stage of human development concerns the pollution of water in various ways by various pollutants.

The production and use of various materials is accompanied by a negative impact on the environment, in particular, the hydrosphere. The sources and extent of pollution can be very diverse. Therefore, one of the main tasks facing humanity today is the creation of modern safe technologies for the production of materials, as well as the processing of industrial waste. The number of pollutants increases every year. Their nature and influence on the hydrosphere is changing. To solve these problems, it is also necessary to organize a rational water supply and use modern methods of water purification.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to the production and use of various materials and water pollution.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

### 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

**PROTECTION OF THE ATMOSPHERE. ENVIRONMENTAL CONSEQUENCES OF ATMOSPHERIC AIR POLLUTION**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Cleanliness and quality of atmospheric air are extremely important for human life. Today, special attention is paid to these issues, because air pollution is constantly increasing with various pollutants.

The production and use of materials is definitely associated with air pollution directly or indirectly. As a result of atmospheric pollution, its composition and properties change, and therefore the connection with the functioning of the biosphere. Therefore, one of the main tasks is to create modern productions and modern ways of using and processing materials, where this impact would be minimal.

During the lecture, students will learn about modern methods of air purification from pollutants of various nature and ways to reduce the number of pollutants.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to air pollution related to the production and use of materials.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- Lecture conducted with the use of multimedia.
- During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

### 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### ENGINEERING AND TECHNOLOGICAL ASPECTS OF ENVIRONMENTAL PROTECTION

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Issues of environmental protection are related to the choice of energy sources, raw materials, consumers, transport and other aspects.

The emergence of problems related to environmental pollution is due to the production, use and processing of materials of different nature and purpose.

At the lecture, students will be introduced to the basic economic, ecological and energy requirements for chemical production. They will try to establish a connection between the costs of energy and raw materials and, accordingly, environmental pollution. Problems related to the choice of energy carriers and raw materials in the chemical industry and in the production of various materials will be considered.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the production and use of materials and environmental pollution

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- Lecture conducted with the use of multimedia.
- During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

### 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### RADIOECOLOGY

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Radiation issues are important in addressing environmental pollution issues.

The influence of ionizing radiation is especially dangerous for living organisms, in particular, for humans. Students will be introduced to radiation doses and the corresponding radiological effect; modern methods of assessment and diagnosis of the degree of radiation contamination of the environment. A particularly important point is the classification of radioactive waste and the characteristics of their processing and disposal methods. Advantages and disadvantages of these methods.

The lecture will also consider possible environmental consequences of various man-made accidents and the use of nuclear weapons.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to threats from radioactive radiation

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Castillo-Suárez, L.A., Sierra-Sánchez, A.G., Linares-Hernández, I. *et al.* A critical review of textile industry wastewater: green technologies for the removal of indigo dyes. *Int. J. Environ. Sci. Technol.* (2023). <https://doi.org/10.1007/s13762-023-04810-2>

### 6. Additional notes

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## Course content – laboratory classes

### Lab 1

#### 1. The subject of the laboratory classes

**ANALYSIS AND PURIFICATION OF WATER FROM PRODUCTION AREAS AND PRODUCTION OF VARIOUS MATERIALS**

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of water analysis and purification will be tested. The performed experiment with samples from real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, sharing tasks and working together. They must draw up a work plan, analyze the results, and draw conclusions.

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the analysis and treatment of water of various origins and pollution  
Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. Also can prepare a theoretical introduction and description of the final results for laboratories on water analysis and treatment, including critical analysis, synthesis and conclusions.

#### 4. Necessary equipment, materials, etc

- pH meter
- spectrophotometer
- computer
- reagents and chemical utensils

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,  
a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of water analysis and purification methods,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. - P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on methods of water analysis and purification

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available



## Lab 2

### 1. The subject of the laboratory classes

#### EVALUATION OF MICROHARDNESS AND ELEMENTAL COMPOSITION OF MATERIALS OF DIFFERENT COMPOSITION AND PURPOSE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of determining microhardness and elemental analysis of various materials will be tested. The performed experiment with samples from real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, sharing tasks and working together. They must draw up a work plan, analyze the results, and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the determination of microhardness and elemental composition of materials for various purposes. Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the elemental composition of materials for various purposes, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- X-ray diffractometer
- scanning electron microscope,
- transmission electron microscope
- a device for measuring microhardness
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,  
a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining microhardness and elemental analysis,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on microhardness research and elemental analysis of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 3

### 1. The subject of the laboratory classes

#### DETERMINATION OF CHANGES IN THE DEGREE OF SWELLING AND THE DEGREE OF CROSSLINKING OF POLYMERS OF DIFFERENT COMPOSITION

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of determining the degree of swelling and the degree of polymer crosslinking will be tested. The performed experiment with samples from real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, sharing tasks and working together. They must draw up a work plan, analyze the results, and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the determination of the degree of swelling and the degree of crosslinking of polymers. Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. Also can prepare a theoretical introduction and description of the final results for the laboratories on the degree of swelling and the degree of crosslinking of polymers, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- a device for studying swelling processes
- computer
- reagents and chemical utensils.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,  
a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining the degree of swelling and the degree of crosslinking of polymers,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. - P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on the study of swelling processes of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 4

### 1. The subject of the laboratory classes

#### DETERMINATION OF THE TENSILE STRENGTH OF MATERIALS OF DIFFERENT NATURE AND PURPOSE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of studying the mechanical properties of materials of various nature and purpose will be tested. The performed experiment with samples of different nature will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, sharing tasks and working together. They must draw up a work plan, analyze the results, and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of mechanical properties of materials of various compositions

Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the study of mechanical properties of materials of different compositions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- samples of materials of different composition
- installation for studying mechanical properties
- breaking machine
- computer

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of studying the mechanical properties of materials of various nature,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on the study of mechanical properties of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv



**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**TESTING OF METALLIC AND CONVERSION CORROSION  
PROTECTION LAYERS**

**Code: TMCCPL**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### TESTING OF METALLIC AND CONVERSION CORROSION PROTECTION LAYERS: INTRODUCTION

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic, students get acquainted with the economic and social problems that arise as a result of the corrosion of various types of metal structures, cars and other types of transport and other metal inventory. Students should understand the importance of the science of corrosion of metals and alloys, the main provisions of the science of corrosion, methods of corrosion protection. In this topic, students get acquainted with a wide range of modern methods of researching the surface of metals and anti-corrosion coatings on their surface, and also learn some methods that they will use to conduct research during laboratory work.

Corrosion is defined as 'an irreversible interfacial reaction of a material (metal, ceramic, polymer) with its environment which results in consumption of the material or in dissolution into the material of a component of the environment' (IUPAC, 2012). Corrosion of metallic structures has a significant influence on the world economy. According to estimates from the World Corrosion Organization (WCO), the current worldwide cost of corrosion (COC) is larger than \$ 2.5 trillion, or around 3.4 % of the world's GDP. Corrosion costs to the US economy annually, both indirect and direct, are projected to be \$ 552 billion, or 6 % of GDP. Corrosion has a significant influence on the price of maintaining and implementing restorations on vehicles, consumer electronics, aircraft, overpasses, and industrial sites, such as those that generate and transmit energy, manufacture pharmaceuticals, desalinate water, process petrochemicals, and so forth.

Control of the quality and reliability of anti-corrosion coatings is an extremely important aspect of protecting metals from corrosion damage and destruction.

The main objectives of surface analysis and coating characteristics are as follows: measurement of surface roughness and coating thickness; surface roughness (contact method, non-contact methods); coating thickness; hardness and microhardness analysis; adhesivity testing; microstructural evaluation ((scanning tunnelling microscopy (STM) and atomic force microscopy (AFM), scanning acoustic microscopy (SAM) and scanning confocal microscopy (SKM)), chemical analysis (infra-red spectroscopy (IR-Spectroscopy), X-ray diffraction (XRD), X-ray photo-electron spectroscopy (XPS), energy dispersive X-ray analysis (EDX), auger electron spectroscopy (AES) and scanning tunnelling microscopy (STM)). Electrochemical characterization of coatings for corrosion protection: open-circuit potential (OCP); electrochemical impedance spectroscopy (EIS); potentiostatic step polarization (PSSP), galvanostatic step polarization (GSSP) and cyclic voltammetry polarization (CVAP).

In order to find ways of practical solutions to the problems arising as a result of corrosion destruction of various metal objects, knowledge and understanding of methods of protecting metals from corrosion and the ability to use modern physico-chemical methods for researching the effectiveness and reliability of various types of protective anti-corrosion coatings of metals are necessary. It is important to be able to assess environmental and socio-economic problems of ensuring the reliability of operation of potentially dangerous objects.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the results of analyzes of the state of the surface of metals and the results of studies of anti-corrosion properties using the characteristics of surface anti-corrosion coatings by modern physical and analytical methods of researching the surface, composition and structure of anti-corrosion coatings. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work based on the research findings, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *A Review of Differing Approaches Used to Estimate the Cost of Corrosion, Anti-Corrosion Method and Materials*. Bahaskaran R., Palaniswamy N., Rengaswamy N.S., Jayachandran M. 2013, J. Appl. Sci. Res. 52, 29-41
- *Characterization of surface coatings. Chapter 8*. Batchelor A.W., Loh N.L., Chandrasekaran M. // *Materials Degradation and Its Control by Surface Engineering*. 2011, 287-333. doi:10.1142/9781848165021\_0008
- *Recent Trends in the Characterization and Application Progress of Nano-Modified Coatings in Corrosion Mitigation of Metals and Alloys*. Thakur A., Kaya S., Kumar A. 2023, Appl. Sci. 13, 730. doi:10.3390/app13020730

Additional, optional literature:

- *Review–The Use of Localized Electrochemical Techniques for Corrosion Studies*. Jadhav N., Gelling V. J. 2019, J. Electrochem. Soc. 166(11), C3461-C3476. doi:10.1149/2.0541911jes
- *Passivity of Metals Studied by Surface Analytical Methods, a Review*. Strehblow H.-H. S. 2016, Electrochim. Acta, 212. doi:10.1016/j.electacta.2016.06.170
- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Characterization of coatings*. Benninghoven A. 1976, Thin Solid Films. 39, 3-23. doi:10.1016/0040-6090(76)90620-9

### 6. Additional notes

## Topics 2

### 1. The subject of the lecture

#### **CORROSION OF METALS AND ALLOYS. TYPES OF CORROSION AND THEIR DEPENDENCE ON OPERATING CONDITIONS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This topic examines types of corrosion and their dependence on operating conditions. Chemical and electrochemical corrosion of metals. Corrosion of metals in various natural conditions. Atmospheric, gas, underground, marine and biocorrosion of metals. Corrosion of metals under mechanical loads. Corrosion cracking and corrosion fatigue. The influence of various factors on the course of corrosion processes on the surface of metals. In this topic, students also study the anti-corrosion properties of natural oxide and other films on the surface of metals. Knowledge of this topic will provide an opportunity to better understand the course of both chemical and electrochemical corrosion of metals and alloys under different conditions.

According to the nature of the corrosion damage, solid and local corrosion are distinguished. Continuous corrosion can be uniform, uneven and selective. Local corrosion can spread along the boundaries of the metal grains and through them, along the welds and take the form of points, spots, cracks, shells, swelling of the surface. To assess the degree of corrosion destruction, it is customary to use the following criteria as indicators, namely: loss of mass per unit of surface area, change in geometric dimensions due to loss of mass, degree of surface damage, and others.

Effective control of corrosion damage cannot simply involve using the "right materials", as this may be practically impossible. Environmental control through inhibitors and coatings, electrochemical means such as cathodic and anodic protection, and engineering means such as structural design help effectively mitigate corrosion. Emphasis is also placed on corrosion monitoring, inspection, life prediction and proactive asset management. In all these cases, an understanding of the corrosion phenomena associated with the interaction of the metal and the environment is important.

Most metals are covered with a film of oxide or another compound when interacting with air oxygen or another oxidizing agent. Oxide films are usually a thin layer applied to the surface of a metal that has undergone an oxidation reaction by the air or moisture surrounding the material. Thin oxide films that are naturally produced from highly reactive materials from the upper part of the galvanic series play a key role in the corrosion resistance of metal and alloys. In general, the formation of oxide films on metals and alloys involves ion transport in the oxide under a strong electric field, dissolution of the oxide film at the film/solution interface, and sometimes precipitation of soluble particles from solution and/or formation of gaseous oxygen at high potentials.

### 3. Learning outcomes

Students can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to the corrosion of metals and alloys, types of corrosion and their dependence on operating conditions, as well as the impact on this of natural films on the surface of metals.

Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analysis of results and conclusions including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *Corrosion Failures: Theory, Case Studies, and Solutions*. Elayaperumal K., Raja V. S. 2015, 256 p. ISBN: 978-1-119-04327-0
- *Overview of corrosion and its control: A critical review*. Harsimran S., Santosh K., Rakesh K. 2021, Proc. Eng. Sci., 3(1), 13-24. doi: 10.24874/PES03.01.002
- *Growth of Passive Films on Valve Metals and Their Alloys*. Habazaki H. 2018, Mater. Sci. 250-258. doi:10.1016/B978-0-12-409547-2.13779-5
- *Passivity of Metals Studied by Surface Analytical Methods, a Review*. Strehblow H.-H. 2016, Electrochim. Acta, 212, 630-648. doi:10.1016/j.electacta.2016.06.170

Additional, optional literature:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Chemical corrosion of metals and alloys*. Jegdić B., Popić J., Bobić B., Stevanović M. 2016, Zastita Materijala. 57, 205-211. doi:10.5937/ZasMat1602205J
- *Corrosion of additively manufactured alloys: a review*. Sander G., Tan J., Balan P., et al. 2018, Corrosion. 74(12), 1318-1350. doi:10.5006/2926

#### 6. Additional notes

### Topics 3

#### 1. The subject of the lecture

##### PROTECTIVE ANTI-CORROSION COATINGS BASED ON NICKEL

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This topic deals with the physical and chemical properties of nickel coatings, their anti-corrosion properties, methods of application mainly on the surface of steel and products and structures based on it, as well as methods of researching the anti-corrosion properties of nickel coatings.

Nickel coatings are commonly applied to steel, zinc, and other metals to provide protection against corrosion, erosion, and abrasion. However, most nickel is consumed in decorative finishes as an interlayer for chromium coatings, while only a small percentage (less than 10%) is used in engineering applications.

Nickel coatings are commonly electrodeposited from Watts-type solutions comprised of nickel sulfate, nickel chloride, and boric acid. At normal plating current densities, about 98% of the cathodic current is consumed in the deposition of nickel, with the remainder going into discharge of protons. Nickel is also electrolessly deposited using either sodium hypophosphite or sodium borohydride type reducing agents, which give rise to nickel–phosphorus and nickel–boron alloy deposits. It is generally agreed that the corrosion resistance of the electrodeposits is typically superior to the electroless deposits, although the latter have the advantage of ease of deposit on complex shapes and internal surfaces.

Nickel coatings are corrosion-resistant to a range of chemical environments which include: the atmosphere, ammonia, coal gas, fluorine, hydrogen peroxide, mercury, alkalis, and fused magnesium fluoride, among others. Nickel is not recommended for exposure to chlorine, sulfur dioxide, nitric acid, sodium hypochlorite, and salts of silver and mercury. They are also resistant to carbon tetrachloride, oil, soaps and petrol. Nickel coating increases fatigue strength. Nickel coatings also minimize corrosion fatigue.

Nickel coatings for corrosion protection may need to be 120–130  $\mu\text{m}$  in thickness, unless machining is required, in which case it will need to be significantly thicker. Although applied for aesthetic reasons, some advantage is gained in corrosion protection by the double-layer nickel coating used in decorative applications. These coatings have a sulfur-free nickel undercoat that is cathodic to the bright nickel top-coat. Corrosive attack is then preferentially directed to the surface, and penetration to the substrate metal is delayed substantially.

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to obtaining nickel films on the surface of steel and researching their anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **protective anti-corrosion coatings based on nickel** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.



#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electroplating baths and anodes used for industrial nickel deposition. Chapter 3. || Nickel and Chromium Plating.* Dennis J.K., Such T.E. 1993, 41-65. doi:10.1533/9781845698638.41
- *Morphology, roughness and microhardness of nickel electrodeposits produced in sulfate media on 316 L SS or Ti cathodes.* Pissolati N.C., Majuste D. 2018, Hydromet. 175, 193-202. doi:10.1016/j.hydromet.2017.11.012

Additional, optional literature:

- *Nickel Plating on Steel by Chemical Reduction.* Brenner A., Riddell G.E. 1946, Mater. Sci., Chem. Eng. 37. 31-34. doi:10.6028/JRES.037019
- *Corrosion Study of Electroless Deposited Nickel-Phosphorus Solar Absorber Coatings on Carbon Steel.* Domínguez A.S., Bueno J.J.P., Torres I.Z., López M.L. 2017, Inter. J. Electrochem. Sci. 12, 2987-3000. doi:10.20964/2017.04.63

#### 6. Additional notes



## Topics 4

### 1. The subject of the lecture

#### **PROTECTIVE ANTI-CORROSION COATINGS BASED ON ZINC**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This topic deals with zinc coatings for steel, their anti-corrosion properties, methods of application mainly on the surface of steel products and structures based on it, and methods of researching their anti-corrosion properties.

Zinc plating of the surface of steel, both in the form of various rolled products and finished products, provides excellent corrosion resistance in most operating environments. In world practice, the most commonly used metal coatings are zinc. The main reasons for choosing zinc coatings for metal products are the low price of zinc and the cost of galvanizing, as well as the presence of a more electronegative stationary potential than iron when exposed to aggressive environments. The most common are zinc coatings of sheet steel, which are widely used to protect steel from corrosion in natural conditions. Metal galvanizing (galvanization) - covering the metal surface with zinc, which, due to its fragility and minimal hardness, provides reliable protection to any product. Zinc is a more active metal than iron, so it significantly slows its corrosion.

Zinc coatings for iron and steel provide excellent corrosion resistance in most atmospheres, in hard fresh waters, and in contact with many natural and synthetic substances. Zinc coatings are widely used to protect finished products ranging from structural steelwork for buildings and bridges, to nuts, bolts, strip, sheet, wire and tube. The electrochemical relationship between zinc and steel enables zinc coatings also to protect steel at cut edges and at breaks in the coating by a sacrificial action.

Zinc galvanizing can be carried out by various methods: galvanic galvanizing; thermodiffusion galvanizing, hot galvanizing; gas-thermal spraying and cold paint. Hot-dip galvanizing of metal products is considered the most effective and long-lasting method of combating corrosion. However, from an ecological point of view, this method cannot be called harmless and safe, since zinc is subject to melting, the surface of the protected metal is treated chemically. Regardless of the method of application, the zinc coating has the same corrosion rate.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the preparation of zinc films on the surface of steel and research of their anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **protective anti-corrosion coatings based on zinc** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *The metallurgy of zinc-coated steel*. Marder A.R. 2000, Prog. Mater. Sci. 45(3), 191-271. doi:10.1016/s0079-6425(98)00006-1
- *A review on recent approaches in the field of hot dip zinc galvanizing process*. Shibli S.M.A., Meena B.N., Remya R. 2015, Surf. Coat. Tech. 262, 210-215. doi:10.1016/j.surfcoat.2014.12.054
- *Corrosion mechanisms of phosphated zinc layers on steel as substrates for automotive coatings*. Amirudin A., Thierry D. 1996, Prog. Org. Coat. 28(1), 59-75. doi:10.1016/0300-9440(95)00554-4

Additional, optional literature:

- *Evolution of zinc coatings during drawing process of steel wires*. Suliga M., Wartacz R., Hawryluk M. 2023, Archiv. Civ. Mech. Eng. 23, 120. doi:10.1007/s43452-023-00669-9
- *The corrosion behavior of zinc-rich paints on steel: Influence of simulated salts deposition in an offshore atmosphere at the steel/paint interface*. Shi H., Liu F., Han E.-H. 2011, Surf. Coat. Technol. 205(19), 4532-4539. doi:10.1016/j.surfcoat.2011.03.118
- *Mechanical Behavior and Damage of Zinc Coating for Hot Dip Galvanized Steel Sheet DP600*. Li G., Long X. 2020, Coatings. 10(3), 202-221. doi:10.3390/coatings10030202

## 6. Additional notes

## Topics 5

### 1. The subject of the lecture

#### **TINNING OF THE STEEL SURFACE AS AN EFFECTIVE METHOD OF ANTI-CORROSION PROTECTION**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This topic deals with tin coatings for various metals and steel, in particular, their application, anti-corrosion properties, methods of application and methods of researching anti-corrosion properties. The question of the electrolytic method of applying tin coatings on steel, its advantages and disadvantages is considered.

Tinning is the process of applying a layer of tin to the metal surface, which has good corrosion resistance to various aggressive environments. Tin is mainly used to cover steel, as well as nickel, copper and its alloys, or aluminum, after preliminary preparation in order to protect against corrosion or apply a decorative coating. The untinned sheets employed in the manufacture are known as black plates. They are now made of steel, either Bessemer steel or open-hearth. Formerly iron was used, and was of two grades, coke iron and charcoal iron; the latter, being the better, received a heavier coating of tin, and this circumstance is the origin of the terms coke plates and charcoal plates by which the quality of tinplate is still designated, although iron is no longer used. Tinplate was consumed in enormous quantities for the manufacture of the tin cans in which preserved meat, fish, fruit, biscuits, cigarettes, and numerous other products are packed, and also for the household utensils of various kinds made by the tinsmith.

Application of tin (polud) on the surface of the product is carried out by:  
- gas thermal sputtering (metallization) and electrolytic deposition (galvanic way). Electrolytic tinning is carried out in acidic and alkaline electrolytes. In alkaline electrolytes tin is in tetravalent form, in acidic electrolytes - in divalent form.

Electrolytic tinning of steel is carried out: by depositing tin on a steel strip made of electrolyte – tinning under the action of current; immersion in molten solder – hot tinning or rubbing solder on the surface of the product – cold tinning. There are glossy and matte coatings.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the preparation of tin films on the surface of steel and methods of researching anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **tinning of the steel surface as an effective method of anti-corrosion protection** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Shreir's Corrosion || Corrosion of Tin and its Alloys*. Lyon S.B. 2010, 2068–2077. doi:10.1016/B978-044452787-5.00099-8
- *Contact tinning: A millennia-old plating technology*. Welter J.-M. 2019, *Archaeometry*. 61(4), 906-920. doi:10.1111/arcms.12454. S2CID 134869188.
- *Tin and Tin Alloys*. Hampshire W.B. 2003, *Encyclopedia of Physical Science and Technology (Third Edition)*. doi:10.1016/B0-12-227410-5/00782-1
- *Characterization of tin-plated steel*. Pandey S., Mishra K.K., Ghosh P., et al. 2023, *Front. Mater.* 10, 1113438. doi: 10.3389/fmats.2023.1113438

Additional, optional literature:

- *Electrochemical studies on the anodic behavior of tin in citrate buffer solutions*. Gervasi C.A., Palacios P.A., Fiori Bimbi M.V., Alvarez P.E. 2010, *J. Electroanal. Chem.* 639(1-2), 141-146. doi:10.1016/j.jelechem.2009.12.002
- *Study on theoretical bases of receiving composite alloy layers on surface of cast steel castings*. Gawronski J., Szajnar J., Wróbel P. 2004, *J. Mater. Proces. Technol.* 157-158, 679-682. doi:10.1016/j.jmatprotec.2004.07.153

## 6. Additional notes

## Topics 6

### 1. The subject of the lecture

#### OXIDE PROTECTIVE LAYERS ON THE ALUMINUM SURFACE

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic discusses the anodic oxide and hydroxide films on the surface of aluminum, which are very important for the protection of aluminum against corrosion, their formation and improvement of properties, applications, and anti-corrosion properties and application conditions.

Anodic oxide and hydroxide films on metals are very important for corrosion protection and they determine the electrochemical properties of electrode surfaces. For a better understanding of the leading corrosion mechanisms the chemical composition as well as the structure and electronic properties of passive layers are of decisive importance. Passive layers are usually complicated multilayer structures. Their protecting properties are determined by the chemical characteristics of the metals and their anodic oxides as well as the environmental factors as the potential and the composition of the contacting electrolyte.

Under typical atmospheric conditions, a native oxide or passive film naturally forms on aluminum. The native oxide layer is nonuniform, thin and noncoherent. Nevertheless, the native oxide film imparts a certain level of corrosion protection, provided the environment contains no unusual contaminants. Exfoliation, the formation of a network of oxide flakes or "leaves" on the aluminum surface, is an example of how corrosion of the surface can be changed through the introduction of sulfur to the environment.

Anodizing (anodic oxidation) is a process of electrolytic oxidation, in which the surface layer of a metal, such as aluminum, magnesium, zinc, and alloys based on them, is transformed into a coating (oxide film) with protective, decorative, or functional properties.

Anodizing aluminum is a sturdy fixture in the mind of the light metal industry. By capitalizing on the natural phenomenon of passive film formation on aluminum in a production environment, the anodization process has become synonymous with surface protection and durability of aluminum substrates. Anodizing can be viewed as the deliberate, controlled corrosion of the aluminum surface in sulfuric acid to yield a uniform, continuous protective oxide film.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the preparation of oxide protective layers on the aluminum surface. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **formation of oxide protective layers on the aluminum surface** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *Anticorrosive coatings: a review*. Sorensen P. A., Kiil S., Dam-Johansen K., Weinell C. E. 2009, J. Coat. Technol. Res. 6(2). 135-176. doi:10.1007/s11998-008-9144-2
- *Understanding Aluminum Anodic Oxide Film Formation*. Runge J.M., Pomis A.J. 2023, Finishing and Coating.

Additional, optional literature:

- *The Surface Treatment and Finishing of Aluminum and Its Alloys*. Wernick S., Pinner R., Sheasby P. 1990, ASM International Finishing Publication, Ltd.
- *Surface Treatment and Finishing of Aluminium Chapter 9 || Electropainting of Aluminium*. King R.G. 1988, 82-91. doi:10.1016/B978-0-08-031138-8.50015-X

## 6. Additional notes

## Topics 7

### 1. The subject of the lecture

#### CHEMICAL AND ELECTROCHEMICAL OXIDATION OF STEEL

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this lecture, students get acquainted with the problems of chemical and electrochemical oxidation of steel and the anti-corrosion properties of oxidized steel surfaces.

Oxidation (from the germ. *Oxydieren* – to oxidize) – treatment of the surface of metal or semiconductor materials by a chemical or electrochemical (anodizing) method, as a result of which a film of their oxides is formed on the surface. Such films (thickness from fractions of a micrometer to 500...600  $\mu\text{m}$ ) increase corrosion resistance, wear resistance and electrical insulating properties of products, give products an aesthetic appearance.

Oxidation of ferrous metals (iron and steel) is widely used in industry for corrosion protection and decorative treatment of precision instrument parts, optical instruments, tools, weapons, etc. However, the protective properties of films on iron and steel are small, so oxidation is used to protect steel from atmospheric corrosion only in light (indoor, workshop) operating conditions.

Oxidation of metals is of various types: - thermal oxidation; - chemical oxidation; - electrochemical oxidation; - plasma oxidation.

Oxide films on ferrous metals can be obtained by immersing samples in molten salts (for example, nitrates), heating in air or in an atmosphere of superheated water vapor. However, today steel oxidation is carried out practically only in alkaline solutions, both chemically and electrochemically.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the preparation of chemical and electrochemical oxidation films on the surface of steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **chemical and electrochemical oxidation of steel** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Anticorrosive coatings: a review*. Sorensen P. A., Kiil S., Dam-Johansen K., Weinell C. E. 2009, J. Coat. Technol. Res. 6(2), 135-176. doi:10.1007/s11998-008-9144-2
- *Role of oxidation in the mild wear of steel*. Quinn T.F.J. 1962, Brit. J. Appl. Phys. 13(1), 33-37. doi:10.1088/0508-3443/13/1/308



- *Electrochemical Science for a Sustainable Society || Passivity of Iron—A Review.* (Chapter 9), Uosaki K. 2017, 209-221. doi:10.1007/978-3-319-57310-6\_9

Additional, optional literature:

- *Review of the High-Temperature Oxidation of Iron and Carbon Steels in Air or Oxygen.* Chen R., Yeun W. 2003, *Oxid. Met.* 59, 433-468. doi:10.1023/A:1023685905159.
- *A Review of Oxidation on Steel Surfaces in the Context of Fire Investigations.* Colwell J., Babic D. 2012, *SAE Int. J. Passeng. Cars-Mech. Syst.* 5(2), 1002-1015. doi:10.4271/2012-01-0990

## 6. Additional notes

## Topics 8

### 1. The subject of the lecture

#### PHOSPHATE FILMS ON THE SURFACE OF STEEL

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic, phosphating is considered as a process of anti-corrosion protection and a method of preparing the surface of steel for the application of protective phosphate coatings. The methods of applying phosphate films to the surface of steel, as well as steel products and structures for protection against corrosion and its mitigation, are studied.

Phosphate coating is typical conversion coating widely used in various industries. Phosphating is the process of covering the metal surface with a layer of poorly soluble phosphates – salts of phosphoric acid ( $H_3PO_4$ ). As a rule, compounds with iron, zinc, and manganese are used. Carbon and low-alloy steels, cast iron, aluminum, and some alloys are most often subjected to such processing.

Metal phosphating is used to improve surface adhesion, additionally protect the product from rust, make it harder and wear-resistant. Phosphate coating is applied to already cleaned steel, cast iron and non-ferrous metal parts. This is one of the best soils for applying paint.

The main advantages of phosphating are improved quality characteristics of the obtained products: – high anti-corrosion protection; – hardness and durability; – long service life; – resistance to mechanical damage; – improvement of electrical insulating properties. Phosphated metal is not exposed to oxygen, organic oils, lubricants, benzene, toluene, all gases (except hydrogen sulfide), hot substances. In addition, due to good adhesion, the phosphate film is an excellent base for paint coatings, treatment with lubricants and passivating materials.

Products made of phosphated metal can withstand temperatures from  $-75$  to  $300^\circ C$ , and for a short time - up to  $500^\circ C$ . And in terms of corrosion resistance, they can be used in conditions of high humidity, for example, in a tropical climate.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the preparation of phosphate films on the surface of steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **preparation of phosphate films on the surface of steel** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrolytic and Chemical Conversion Coatings, A Concise Survey of Their Production, Properties and Testing.* Weber J., Biestek T. 1976, Portcullis Press. 128-224.
- *Application of magnesium phosphate coating on low carbon steel via electrochemical cathodic method and investigation of its corrosion resistance.* Dayyari M.R., Amadeh A., Sadreddini S. 2015, J. Alloy. Compd. 647, 956-958. doi:10.1016/j.jallcom.2015.06.063

Additional, optional literature:

- *Study of structure of phosphate film on carbon steel.* Zhao X., Wei G., Zhao X. H. 2008, Surf. Rev. Lett. 14(4), 577-581. doi:10.1142/S0218625X07009876

## 6. Additional notes

## COURSE CONTENT – LABORATORY CLASSES

### Topics 1

#### 1. The subject of the laboratory classes

**INTRODUCTION TO THE LABORATORY WORKSHOP FROM THE COURSE. METHODS OF TESTING ANTI-CORROSION LAYERS OF VARIOUS NATURE**

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Familiarization with the laboratory workshop from the course "Testing of metal and conversion anti-corrosion layers", instruction on safety techniques and occupational hygiene in the laboratory, instructions on the procedure for conducting and performing laboratory work, drawing up a report. Familiarization with the methods of laboratory studies of metal corrosion and the methodology of conducting laboratory work. Acquaintance with modern tests of corrosion coatings of metals and alloys, as well as with basic and auxiliary devices for electrochemical control of the condition of film coatings of metals and alloys. Acquaintance with modern methods of testing anti-corrosion layers of metals (4 hours).

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the familiarization with the methods of laboratory research of corrosion of metals and methods of conducting laboratory work. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

In addition to the basic rules of behavior in the laboratory, students at the introductory class are briefed on safety and occupational health and safety, as well as get acquainted with the scheme of drawing up reports on the performance of laboratory work on the specified topics. Important attention is paid to the description of experimental results for the preparation of conclusions. Safety and occupational health and safety instructions. Sample reports on the performance of laboratory work.

During laboratory classes, students will work in groups, get acquainted with the schematic diagrams of the main devices and methods of conducting analyzes related to corrosion processes. The acquired skills will become the basis for carrying out research on the topics of laboratory work on relevant topics.

#### 4. Necessary equipment, materials, etc

Instructions on safety and occupational health and safety in the laboratory, instructions on the procedure for carrying out and performing laboratory work, and drawing up a report.

- Potentiostatic step polarization (PSSP), - Galvanostatic step polarization (GSSP), - Cyclic voltammetry (CVA) polarization, - Potentiostat, - Electrochemical cell, - Working electrodes, - Reference electrode, - Computer laboratory

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

- a. Issues for the colloquium
- b. Exercise instruction
- c. ...

## Topics 2

### 1. The subject of the laboratory classes

#### INVESTIGATION OF THE NATURE OF CORROSION DESTRUCTION OF METALS AND ALLOYS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory lesson is related to the study of the nature of corrosion destruction of metal samples. Students will examine samples of metals damaged by corrosion (sheet and galvanized tin, aluminum and duralumin sheets, copper sheets and parts, etc.) by visual inspection, as well as inspection using a magnifying glass and an optical microscope. Based on the results of the analysis, students must determine the nature of corrosion destruction and damage and describe these processes using the appropriate chemical reactions of the metal with the reaction medium (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the nature of corrosion destruction of various samples of metals and alloys, describe these processes using equations of chemical reactions that likely caused this corrosion damage. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic.

### 4. Instructions and schematic diagrams of devices.

- Magnifiers, - Optical microscope, - Caliper, - Micrometer, - Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;

- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;

- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;



- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- Passivity of Metals Studied by Surface Analytical Methods, a Review. *Strehblow H.-H. 2016, Electrochim. Acta, 212, 630-648. doi:10.1016/j.electacta.2016.06.170*
- *Characterization of surface coatings. Chapter 8*. Batchelor A.W., Loh N.L., Chandrasekaran M. // *Materials Degradation and Its Control by Surface Engineering*. 2011, 287-333. doi:10.1142/9781848165021\_0008

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

- Issues for the colloquium
- Exercise instruction
- ...

### Topics 3

#### 1. The subject of the laboratory classes

##### **ELECTROCHEMICAL NICKEL PLATING OF STEEL**

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory session is related to the experimental study of the preparation of the surface of steel samples for/and the application of nickel coatings by electrodeposition for anti-corrosion protection of steel and the study of their physico-chemical properties and anti-corrosion properties. Based on the results of the laboratory work, it is necessary to determine: the current output, the thickness of the nickel film, and the corrosion resistance of the obtained steel samples in standard solutions. Evaluation of the topology, structure and morphology of the obtained nickel films on steel will be carried out using scanning electron microscope (SEM), X-ray (EDX) analysis, etc.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the application of nickel coatings by electrodeposition for anti-corrosion protection of steel and the study of their physico-chemical properties and anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for various multi-, micro- and nano-modified coatings for corrosion protective coatings on mild steel or copper and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

#### 4. Instructions and schematic diagrams of devices.

- DC source, - Potentiostat, - Electrochemical cell, - Steel plate, - Tin plate, - Muffle furnace, - Calipers, - Micrometer, - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - X-ray fluorescence spectroscopy (XRFS), - Contact angle (CA), Computer laboratory.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of electrolytic application of tin protective coatings on steel (or copper) and research of their physico-chemical and anti-corrosion properties;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electroplating of Nickel on Various Metal Surfaces*. Soe D.H.H., Lvin D.T.M. 2020, *Inter. J. Innovat. Sci. Res. Technol.* 5(5). 1479-1483. ISSN No:-2456-2165
- *Comparison of various electroless nickel coatings on steel: structure, hardness and abrasion resistance*. Vitry V., Sens A., Delaunois F. 2014, *Mater. Sci. Forum.* 783-786, 1405-1413. doi:10.4028/www.scientific.net/MSF.783-786.1405

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

a. Issues for the colloquium

b. Exercise instruction

c. ...

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## Topics 4

### 1. The subject of the laboratory classes

**PROTECTIVE ANTI-CORROSION COATINGS BASED ON ZINC AND THE STUDY OF THEIR ANTI-CORROSION PROPERTIES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the preparation of the surface of a steel samples for/and the application of electrolytic of zinc protective coatings on steel and research of their physico-chemical properties and comparison of the properties of the obtained surfaces and in particular, the current yield, thickness, surface topology and anti-corrosion protection of steel in standard solutions. Evaluation of the structure and morphology of the obtained zinc protective films on the steel will be carried out using a scanning electron microscope (SEM), X-ray (EDX) analysis and other.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrolytic deposition of zinc on the surface of mild steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for electrolytic zinc plating and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Instructions and schematic diagrams of devices.

- DC source, - Potentiostat, - Electrochemical cell, - Steel plate, - Zinc plate, - Ag/AgCl reference electrode, - Muffle furnace, - Drying cabinet, - Calipers, - Micrometer, - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of electrolytic application of zinc protective coatings on steel and research of their physico-chemical and anti-corrosion properties;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *The metallurgy of zinc-coated steel*. Marder A.R. 2000, Prog. Mater. Sci. 45(3), 191-271. doi:10.1016/s0079-6425(98)00006-1

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

- Issues for the colloquium
- Exercise instruction

## Topics 5

### 1. The subject of the laboratory classes

**ELECTROLITIC TINNING OF THE STEEL SURFACE AS AN EFFECTIVE METHOD OF ANTI-CORROSION PROTECTION AND THE STUDY OF THEIR ANTI-CORROSION PROPERTIES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the preparation of the surface of a steel samples for/and the application of electrolytic of tin protective coatings on steel and research of their physico-chemical properties and comparison of the properties of the obtained surfaces and in particular, the current yield, thickness, surface topology and anti-corrosion protection of steel in standard solutions. Evaluation of the structure and morphology of the obtained oxide films on the steel will be carried out using a scanning electron microscope (SEM), X-ray (EDX) analysis and other methods.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrolytic deposition of tin on the surface of mild steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for electrolytic tin plating and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Instructions and schematic diagrams of devices.

- Potentiostat, - DC source, - Electrochemical cell, - Steel plate, - Tin plate, - Drying cabinet, - Muffle furnace, - Calipers, - Micrometer, - Analytical scales (AS), - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:



- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of electrolytic application of tin protective coatings on steel and research of their physico-chemical and anti-corrosion properties;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Electrochemical studies on the anodic behavior of tin in citrate buffer solutions*. Gervasi C.A., Palacios P.A., Fiori Bimbi M.V., Alvarez P.E. 2010, J. Electroanal. Chem. 639(1-2), 141-146. doi:10.1016/j.jelechem.2009.12.002

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

- a. Issues for the colloquium
- b. Exercise instruction
- c. ...

## Topics 6

### 1. The subject of the laboratory classes

**THE FORMATION OF OXIDE PROTECTIVE LAYERS ON THE SURFACE OF ALUMINUM AND THE STUDY OF THEIR PHYSICO-CHEMICAL AND ANTI-CORROSION PROPERTIES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the electrolytic preparation of the oxide protective layers on the surface of aluminum and the study of their physico-chemical and anti-corrosion properties, research and comparison of the properties of the obtained surfaces and in particular, the current yield, thickness, surface topology and anti-corrosion protection of aluminum in standard solutions. Evaluation of the structure and morphology of the obtained oxide films on the aluminum will be carried out using a scanning electron microscope (SEM), X-ray (EDX) analysis and other methods.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to electrolytic anodization of aluminum. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on **application of protective anti-corrosion films on aluminum by anodizing method as a means of preventing corrosion and investigation of their anti-corrosion properties**, including critical analysis, synthesis and conclusions.

### 4. Instructions and schematic diagrams of devices.

- Sources of direct current, - Electrochemical cell, - Aluminum plate, - Two lead cathodes, - Calipers, - Micrometer, - Analytical scales (AS), - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of application of protective anti-corrosion films on aluminum by the method of anodization, oxidation, as a means of preventing corrosion;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Understanding Aluminum Anodic Oxide Film Formation*. Runge J.M., Pomis A.J. 2023, Finishing and Coating.
- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *The Surface Treatment and Finishing of Aluminum and Its Alloys*. Wernick S., Pinner R., Sheasby P. 1990, ASM International Finishing Publication, Ltd.

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

- a. Issues for the colloquium
- b. Exercise instruction
- c. ...

## Topics 7

### 1. The subject of the laboratory classes

#### **ELECTROCHEMICAL OXIDATION OF STEEL, RESEARCH AND COMPARISON OF THE PROPERTIES OF THE OBTAINED SURFACES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the preparation of the surface of a steel sample for/and the application electrochemical oxidation of steel, research and comparison of the properties of the obtained surfaces and in particular, the current yield, thickness, surface topology and anti-corrosion protection of steel in standard solutions. Evaluation of the structure and morphology of the obtained oxide films on the steel will be carried out using a scanning electron microscope (SEM), X-ray (EDX) analysis, and other methods.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical oxidation the surface of mild steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **electrochemical oxidation of steel, research and comparison of the properties of the obtained surfaces** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Instructions and schematic diagrams of devices.

- Sources of direct current, - Potentiostat, - Electrochemical cell, - Four steel plate, - Two lead cathodes, - Calipers, - Micrometer, - Analytical scales (AS), - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of application of protective anti-corrosion films on steel by the method of electrochemical oxidation, as a means of preventing corrosion;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Electrochemical Science for a Sustainable Society || Passivity of Iron—A Review*. (Chapter 9), Uosaki K. 2017, 209-221. doi:10.1007/978-3-319-57310-6\_9

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

- a. Issues for the colloquium
- b. Exercise instruction
- c. ...



## Topics 8

### 1. The subject of the laboratory classes

#### **CHEMICAL PHOSPHATING OF THE STEEL SURFACE AND RESEARCH ON THE PROPERTIES OF THE PHOSPHATED SURFACE**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the preparation of the surface of a steel sample for/and the chemical application of phosphate films and the study of its physicochemical properties, in particular, the current yield, thickness, surface topology and anti-corrosion protection of steel in standard solutions. Evaluation of the structure and morphology of the obtained phosphate films will be carried out using a scanning electron microscope (SEM), X-ray (EDX) analysis, etc.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical oxidation the surface of mild steel. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation for **chemical phosphating of the steel surface and research on the properties of the phosphated surface** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Instructions and schematic diagrams of devices.

Four steel plate - Calipers, - Micrometer, - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (checking students' knowledge) of methods of application of protective anti-corrosion films on steel by the method of chemical phosphating of the steel surface and research on the properties of the phosphated surface and the investigation of its physicochemical and anti-corrosion properties;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Study of structure of phosphate film on carbon steel*. Zhao X., Wei G., Zhao X.H. 2008, Surf. Rev. Lett. 14(4), 577-581. doi:10.1142/S0218625X07009876
- *A Comparative Study on Surface Structure of Thin Zinc Phosphates Layers Obtained Using Different Deposition Procedures on Steel*. Sandu A. V., Coddet C., Bejinariu C. 2012, Revista de Chimie. 63(4), 401
- *The effect of phosphate coatings on carbon steel protection from corrosion in a chloride-contaminated alkaline solution*. Girčienė O., Ramanauskas R., Gudavičiūtė L., Martušienė A. 2013, Chemija. 24(4). 251-259

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);

- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

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86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

- a. Issues for the colloquium
- b. Exercise instruction
- c. ...

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**MODERN PHYSICOCHEMICAL METHODS  
OF SURFACE ANALYSIS**

**Code: MPhChMSA**

Lecture Topics
Topics 1: Introduction to course. Electron microscopy (I): Scanning electron microscopy
Topics 2: Electron microscopy (II): Transmission electron microscopy
Topics 3: Scanning probe microscopy. Scanning tunneling microscopy (STM). Atomic force microscopy (AFM), electric force microscopy (EFM) and magnetic force microscopy (MFM)
Topic 4. Auger electron spectroscopy
Topic 5. X-ray photoelectron spectroscopy. Ultraviolet photoelectron spectroscopy
Topic 6. Fourier Transform Infrared Spectroscopy
Topic 7. Mass spectrometry. Surface plasmon resonance spectroscopy
Topic 8. X-ray methods of analysis (X-ray diffraction, X-ray absorption spectroscopy, X-ray fluorescence spectroscopy, X-ray microanalysis)
Laboratory classes Topics
Topic 1. Study of the morphology, structure, and composition of samples (polymer films deposited, metal/alloy surface, bulk material) using scanning electron microscopy (SEM) and energy dispersive X-ray microanalysis (EDX)
Topic 2. Study of morphology, determination of the size and shape of particles by scanning electron microscopy
Topic 3. FTIR studies of polymers (films deposited on substrate, bulk material)
Topic 4. X-ray fluorescence analysis of inorganic materials.
Topic 5. Qualitative analysis by X-ray fluorescence spectrometry.
Topic 6. Quantitative analysis by X-ray fluorescence spectrometry.
Topic 7. Phase analysis of materials, estimation of crystallite sizes of selected materials by X-ray phase analysis (using Scherrer's formula)
Topic 8. Atomic force microscopy analysis of surface

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### INTRODUCTION TO COURSE.

##### ELECTRON MICROSCOPY (I):- SCANNING ELECTRON MICROSCOPY (SEM)

#### 2. Thematic scope of the lecture

In this lecture, the student will learn about the concept of the term "surface", types of surfaces, surface morphology and its structure. A brief description of the physicochemical methods of surface research will be given and the interaction of radiation (electrons, X-rays, ions, etc.) with the surface will be discussed.

During this lecture, the physical basis of electron microscopy will also be presented and its comparison with light microscopy will be presented. It will be considered in detail: the basis of scanning electron microscopy (SEM), methods of signal registration and image acquisition will be considered in detail. Students will get acquainted with the areas of application of SEM.

#### 3. Learning outcomes

- Students will learn about the differences between surface and bulk material properties.
- They will have an idea about the features of the surface structure, the influence of adsorption phenomena on it.
- Students will understand the physical basis of electron microscopy methods, in particular SEM, and will familiarize themselves with the peculiarities of the structure of the microscope.
- Students will understand the principle of interaction of the electron beam with the surface, learn about the received signals, methods and modes of their registration in SEM.
- They will know the specifics of the requirements for sample preparation for SEM research.
- They will know the possibilities, shortcomings and areas of application of SEM.

#### 4. Didactic methods used

Multimedia presentation (PowerPoint presentation for discussion and examples).

Case study: presentation of specific examples.

Discussion: encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. Gatos, H.C., Structure and Properties of Solid Surfaces. In: Fréchette, V.D., LaCourse, W.C., Burdick, V.L. (Eds) Surfaces and Interfaces of Glass and Ceramics. Materials Science Research, Vol 7. Springer, Boston, MA. 1974. [https://doi.org/10.1007/978-1-4684-3144-5\\_13](https://doi.org/10.1007/978-1-4684-3144-5_13)
2. Klauber, C., & Smart, R. S. C., Solid Surfaces, Their Structure and Composition. Surface Analysis Methods in Materials Science, 2003. P. 3–69. doi:10.1007/978-3-662-05227-3
3. Klauber, C., & Smart, R. S. C. (2003). Solid Surfaces, Their Structure and Composition. Surface Analysis Methods in Materials Science, 3–69. doi:10.1007/978-3-662-05227-3



4. W. Zhou, R. Apkarian, Z. L. Wang and D. Joy, Fundamentals of Scanning Electron Microscopy (SEM), in Scanning Microscopy for Nanotechnology, Springer, 2007, pp. 1-40.

Scanning Electron Microscope A To Z

<https://admin.jeol.com.cn/admin/static/uploadfiles/20170419/680fb98a-edd2-4e2b-80a9-8dcaecbb3dde.pdf>

## 6. Additional notes

## Topics 2

### 1. The subject of the lecture

#### ELECTRON MICROSCOPY (II): TRANSMISSION ELECTRON MICROSCOPY

### 2. Thematic scope of the lecture

During the lecture, the physical basis of the transmission electron microscopy (TEM) method, the structure of the microscope and the possibilities of using TEM will be discussed in detail.

Attention will be paid to consideration of sample preparation methods for TEM.

Research methods (structural and phase) and sample preparation methods for TEM will be discussed. Let's consider the possibilities of transmission microscopy and its use in materials science. Comparative characteristics of both methods of electron microscopy will be provided.

### 3. Learning outcomes

After the lecture, students:

- will understand the physical basis of transmission electron microscopy methods (TEM).
- will know the peculiarities of the structure of microscopes and the differences in the structure of TEM and SEM devices.
- will know how an image is formed in TEM.
- will know the specifics of the requirements for sample preparation for TEM research.
- will know how to prepare samples for TEM.
- will know the possibilities, disadvantages and areas of application of TEM.
- Will get a comparative description of both methods of electron microscopy.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation (PowerPoint presentation for discussion and examples).

Case study: presentation of specific examples.

Discussion: encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. David B. Williams, C. Barry Carter, Transmission Electron Microscopy. A Textbook for Materials Science, Springer, New York, NY. 2009. – 760 p.
2. Helmut Kohl, Ludwig Reimer, Transmission Electron Microscopy, Springer-Verlag New York, 2008, 586 p.

### 6. Additional notes

## Topics 3

### 1. The subject of the lecture

#### SCANNING PROBE MICROSCOPY.

**SCANNING TUNNELING MICROSCOPY (STM). ATOMIC FORCE MICROSCOPY (AFM), ELECTRIC FORCE MICROSCOPY (EFM) AND MAGNETIC FORCE MICROSCOPY (MFM)**

### 2. Thematic scope of the lecture

This lecture will familiarize students with the general structure of a scanning probe microscope, the general principle and modes of its operation.

Students will study in detail the physical principle of the scanning tunneling microscopy (STM) method and its features. We will consider the structure of the STM microscope and its modes of operation. They learn about the requirements for samples and the procedure for their preparation. Examples and possibilities of practical application of tunneling microscopy in materials science will be given.

Part of the lecture will also be devoted to atomic force microscopy (AFM). Features of the structure and modes of operation of the AFM microscope will be presented, their advantages and disadvantages will be analyzed. Areas of application and possibilities of the method will also be presented in detail. Features of the electric force microscope (EFM), examples of its application will be discussed. An overview of magnetic force microscopy (MFM), its features and examples, spheres and prospects of practical use are provided.

### 3. Learning outcomes

After listening to the lecture, the student:

- will be familiarization with the types of scanning probe microscopes (SPM).
- will know the features of the structure of the SPM of microscopes: the role of a piezo element, a working probe, a feedback control system.
- will have knowledge of the basic principles of operation of the scanning tunneling microscope (STM), its features, shortcomings and modes of operation.
- get acquainted with the method of scanning probe lithography.
- will have an understanding of the specifics of sample preparation.
- will be able to choose the appropriate scanning mode for a specific sample surface.

### 4. Didactic methods used

Lecture conducted with the use of multimedia: (PowerPoint presentations for discussion and examples).

Case study: presentation of specific examples.

Discussion: encouraging students to participate in the discussion.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. Rebecca Howland, Lisa Benatar, A PRACTICAL GUIDE TO SCANNING PROBE MICROSCOPY, ThermoMicroscopes, 1993-2000
2. Meyers, Robert A. (2006). Encyclopedia of Analytical Chemistry (Applications, Theory and Instrumentation) || Scanning Tunneling Microscopy/Spectroscopy in Analysis of Surfaces., John Wiley & Sons, Ltd, 2006. - 10.1002/9780470027318.a2514

### 6. Additional notes

## Topics 4

### 1. The subject of the lecture

#### AUGER ELECTRON SPECTROSCOPY

### 2. Thematic scope of the lecture

Auger electron spectroscopy (OES) is a technique used to determine the atoms present on a surface and their concentration. This method also makes it possible to determine the depth of distribution of elements in the sample. The principles of obtaining Auger electrons, the understanding of the concept of the mean free path of electrons and the influence of the chemical environment on the kinetic energy and the shape of the lines in the Auger spectrum will be presented.

Features of the structure of the equipment will be considered (source of electrons, analyzers, modes of operation, methods of detection of electrons, counting of pulses).

The methods of data collection and processing, as well as the method of deep profiling, are presented. The possibilities, advantages and limitations of the OES method and its application in materials science are presented.

### 3. Learning outcomes

After the lecture, students:

- will understand the physical basis of Auger electron spectroscopy.
- will know the peculiarities of the structure of the spectrometer.
- will know methods of data collection and processing, as well as methods of deep profiling.
- will understand the advantages and limitations of the method and the possibilities of using Auger spectroscopy.
- be able to determine the chemical composition of the surface.
- will know the specifics of the requirements for sample preparation.
- will understand the advantages and limitations of the method and the possibilities of using Auger spectroscopy.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture with multimedia: (PowerPoint presentations for discussion and examples).

Case study: presentation of examples.

Discussion: encouraging students to participate in the discussion.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. D. Briggs and M. P. Seah, Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, John Wiley and Sons, New York, 1983.
2. Powell, C.J. and Seah, M.P., Precision, accuracy, and uncertainty in quantitative surface analyses by Auger-electron spectroscopy and x-ray photoelectron spectroscopy. Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films, 8(2), 1990.- pp.735-763.
3. J. C. VICKERMAN, I.S. GILMORE (Eds.), Surface Analysis – The Principal Techniques (2nd Ed.), John Wiley & Sons, Ltd., 2009. – 680p.

### 6. Additional notes

## Topics 5

### 1. The subject of the lecture

**X-RAY PHOTOELECTRON SPECTROSCOPY. ULTRAVIOLET PHOTOELECTRON SPECTROSCOPY**

### 2. Thematic scope of the lecture

The lecture will be discuss methods X-ray and ultraviolet spectroscopy (photoelectron spectroscopy) are used to study the surface of the material in order to analyze the elemental composition, chemical states, depth profile, polymers, etc.

Students will get acquainted with the physical basis of both methods - X-ray and ultraviolet spectroscopy. The peculiarities of the use of ultraviolet radiation for the study of valence levels are discussed. Let's consider what types of photons are used in photoelectron spectroscopy and the features associated with this. Attention will also be paid to the detection limit of elements in RFS.

We will analyze in detail the structure and principles of operation of spectrometers.

In this lecture, students will learn how XRF can be used to study the elemental composition and oxidation states of elements. Special attention will be paid to the use of photoelectron spectroscopy in materials science. Limitations in the use of these methods and their advantages over other methods will also be discussed.

### 3. Learning outcomes

After listening to the lecture, the student:

- will have an understanding of the concept of the photo effect.
- will study the physical principles of photoelectron spectroscopy.
- understanding the formation of the photoelectron spectrum and its use for the characterization of surface materials.
- will know the main advantages of the XPS technique for researching the chemical environment.
- familiarize yourself with the structure of a photoelectron spectrometer.
- understanding of features of photoelectron spectroscopy with angular resolution.
- acquainted with the main advantages of UVS - the study of both the electronic structure of solids and adsorption on the surface.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with a traditional board.

Lecture with the use of multimedia (PowerPoint presentation which have the schemes and spectrum samples illustrating the discussed topic are made).

Discussion with the students is expected.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. J. Moulder, W. Stickle, W. Sobol, K. D. Bomben, Handbook of X-Ray Photoelectron Spectroscopy, Perkin-Elmer Corp., 1992. – 260p.

2. Shigemasa Suga, Akira Sekiyama, Christian Tusche (eds.), Photoelectron Spectroscopy: Bulk and Surface Electronic Structures. In: Springer Series in Optical Sciences, Vol. 72, Springer International Publishing, 2021 – 511p.
3. O'Connor, D.J., Sexton, B.A., Smart, R.S.C. (eds) Surface Analysis Methods in Materials Science. Springer Series in Surface Sciences, vol 23. Springer, Berlin, Heidelberg, 1992. - .
4. María J. Hortigüela Gallo, Gonzalo Otero Irurueta, X-ray Photoelectron Spectroscopy: a Surface Characterization Technique, UA Editora Universidade de Aveiro, 2019. - 78p.
5. Lorenzo Calvo-Barrio, Gardenia Vargas, Photoelectron spectroscopy for surface analysis: X-ray and UV excitation, Centres Científics i Tecnològics. Universitat de Barcelona, 2012. -12p.

## 6. Additional notes

## Topics 6

### 1. The subject of the lecture

#### FOURIER TRANSFORM INFRARED SPECTROSCOPY

### 2. Thematic scope of the lecture

At the lecture, students will get acquainted with IR-Fourier spectroscopy: the principle of the method and the corresponding equipment. Students will study optimization of FT-IR instrument parameters for material surface analysis: identification/analysis of polymers, identification of contaminants on surfaces, identification of organic films, particles, powders, and liquids.

Students will receive detailed information about the peculiarities of the absorption of IR radiation by individual atoms and groups to obtain spectra. They will learn the interpretation of IR spectra and know the classification of IR bands.

### 3. Learning outcomes

- Familiarization with the structure and principle of operation of the FTIR spectrometer.
- Understanding the basic principle of FTIR spectroscopy.
- Understanding the importance of the Fourier transformation of interferograms into a spectrum
- Will get detailed information about the absorption of infrared radiation by the molecules of the substance.
- Learn to analyze and interpret IR spectra.
- Get acquainted with the advantages of the FTIR method.
- Knowledge of the application possibilities and limitations of the FTIR method.
- Familiarization with the possibility of identification/analysis of polymers, surface contaminants, organic films, particles, powders and liquids.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture with a traditional board and with the use of multimedia (POWERPOINT presentation with schemes, diagrams and examples of spectra).

During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. Nguyen, T. Applications of Fourier transform infrared spectroscopy in surface and interface studies // Progr. Org Coat., Vol. 13(1), 1985. 1–34. doi:10.1016/0033-0655(85)80001-7
2. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, INTRODUCTION TO SPECTROSCOPY, Gengage learning, 2013. – 786p.

### 6. Additional notes



## Topics 7

### 1. The subject of the lecture

#### MASS SPECTROMETRY. SURFACE PLASMON RESONANCE SPECTROSCOPY

### 2. Thematic scope of the lecture

During the lecture, the theoretical foundations of mass spectroscopy methods will be considered. Students will also get to know in detail the structure of the equipment and its main elements (mass analyzers and detectors). Learn about the advantages and disadvantages of different types of mass analyzers. They will get acquainted with the importance of the correct method of ionization.

They will receive information about how molecular ions and adducts are formed. get acquainted with patterns of fragmentation of functional groups. Also, the lecture will be devoted to the features of qualitative and quantitative analysis. The method of secondary ion mass spectrometry (SIMS): its fundamental principles and applications will be considered in detail. The interpretation of mass spectra (with examples given) will be considered. Also, matrix laser desorption ionization (MALDI): its principle and application, obtained images will be additionally presented.

Also, part of the lecture will be devoted to spectroscopy of surface plasmon resonance. The methodology, analytical implementations and applications of SPRS will be considered.

### 3. Learning outcomes

- Understanding the theoretical foundations of the mass spectrometry method.
- Know the basics of mass spectrometer operation, its structure and main elements (different types of mass analyzers and detectors).
- Understanding the importance of the correct ionization method.
- Understanding the formation of molecular ions and adducts.
- They will know the laws of splitting functional groups.
- Will be able to interpret mass spectra
- They will gain knowledge about qualitative and quantitative analysis by mass spectrometry.
- Understanding of secondary ion mass spectrometry (SMS): its fundamental principles and applications.
- Knowledge of the features and capabilities of the matrix laser desorption ionization (MALDI) method.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture with a traditional board and with the use of multimedia (POWERPOINT presentation with schemes, diagrams and examples of spectra).

During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. Teodor Octavian Nicolescu, Interpretation of Mass Spectra. In: Mahmood Aliofkhaezrai (Ed.) Mass Spectrometry. 2017. – 23-42 pp.
2. Edmond de Hoffmann, Vincent Stroobant, Mass Spectrometry. Principles and Applications, John Wiley & Sons Ltd, England, 2007, 502p.
3. John F Watts, John Wolstenholme, Roger Paul Webb, Secondary Ion Mass Spectrometry. In book: Characterization of Materials. 2012. – 1-33p.
4. Francisco López, Secondary Ion Mass Spectrometry (SIMS): principles and applications. In: Handbook of instrumental techniques for materials, chemical and biosciences research, Centres Científics i Tecnològics. Universitat de Barcelona, Barcelona, 2012 – 14p. Nongjian Tao, S. Boussaad, W. L. Huang, Rafael Archabaleta, J. D’Agnese, High resolution surface plasmon resonance spectroscopy // Revi. Sci. Instrum., 1999, Vol. 70(12):4656-4660
5. Richard B. M. Schasfoort (Ed.) Handbook of Surface Plasmon Resonance, Royal Society of Chemistry. 2017. – 554 p.

## 6. Additional notes

## Topics 8

### 1. The subject of the lecture

**X-RAY METHODS OF ANALYSIS (X-RAY DIFFRACTION, X-RAY ABSORPTION SPECTROSCOPY, X-RAY FLUORESCENCE SPECTROSCOPY, X-RAY MICROANALYSIS)**

### 2. Thematic scope of the lecture

This lecture will be devoted to various methods of surface analysis based on the use of X-ray radiation. During the lecture, students will get acquainted with the sources of X-ray radiation and the mechanism of interaction of X-ray radiation with matter. X-ray diffraction (XRD) methods and their principles will be presented. Students learn about Bragg's law. They learn about the study of the structure of polycrystalline materials by the Debye-Scherrer method and the structure of single-crystal materials by the Laue method.

Students will familiarize themselves with the features of small-angle X-ray scattering (SAXS) and learn about its application. For comparison, the basic principles of wide-angle X-ray scattering (WAXS) and the application of this method are presented. The structure of the devices and the features of sample preparation for the MRR and ShRR methods will be shown. Part of the lecture will be devoted to the basics of X-ray absorption spectroscopy (XAS/XANES/EXAFS). The structure of the spectrometer will be considered and various types of detectors will be presented in detail. The possibilities of using X-ray absorption spectroscopy and the peculiarities of sample preparation will also be discussed.

Special attention will be paid to X-ray fluorescence spectroscopy (XRF) and its two types - EDS, WDX. The advantages and limitations of the method and the possibilities of application will be given.

The basics of X-ray microanalysis (methods of energy dispersive and wave dispersive spectroscopy): measurements and features of application will be presented.

### 3. Learning outcomes

- Students gain knowledge about the characteristics of the most important sources of X-ray radiation.
- Students will study the principles of interaction of X-ray radiation with matter.
- Understanding the concept of X-ray diffraction.
- Understanding the operation of an X-ray diffractometer.
- Students will be exposed to the theoretical and practical aspects of X-ray microanalysis and XRF analyse.
- Familiarization with different apparatus (X-ray diffractometer, XRF spectrometr, electron probe X-ray microanalyzer).
- Students will be able to critically evaluate possibiity of electron probe x-ray microanalysis and x-ray fluorescence (XRF) analyses of materials.
- They understand the principles of X-ray absorption spectroscopy.
- They will understand what structural information can be obtained by spectroscopic methods.
- Getting to know the limitations of each methods.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture with a traditional board and with the use of multimedia (POWERPOINT presentation with schemes, diagrams and examples of spectra).

During the lecture, there is a discussion with the students.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. J. Goldstein, D. Newbury, et al. Scanning Electron Microscopy and X-ray Microanalysis. 3rd ed. Kluwer Academic/Plenum Publishers, 2003.
2. Christina Strelí, P. Wobrauschek, Peter Kregsamer, X-Ray Fluorescence Spectroscopy, Applications. In book: Encyclopedia of Spectroscopy & Spectrometry, Academia Press Ltd, London, 1999, P. 2478-2487
3. Asma Khalid, Aleena Tasneem Khan, Junaid Alam, Muhammad Sabieh Anwar, X-Ray Fluorescence (XRF) spectrometry for materials analysis and “discovering” the atomic number, 2015. – P.1-25
4. B.D. Cullity S.R. Stock, Elements of X-Ray Diffraction, Pearson Education Limited, 2014. – 654p.

#### 6. Additional notes

## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

**STUDY OF THE MORPHOLOGY, STRUCTURE, AND COMPOSITION OF SAMPLES (POLYMER FILM COATING, METAL/ALLOY SURFACE, BULK MATERIAL) USING SCANNING ELECTRON MICROSCOPY (SEM) AND ENERGY DISPERSIVE X-RAY MICROANALYSIS (EDX).**

#### 2. Thematic scope of the laboratory classes

Laboratory work involves the use of various types of samples. Therefore, before starting its implementation, it is necessary to prepare the samples (apply a polymer film coating, grinding the synthesized polymer, cleaning the surface of the metal/alloy, etc.), if necessary, apply a conductive layer on the surface sample.

Different groups of students can prepare one metal and one polymer sample for research.

The laboratory lesson aims to:

1. acquaint the student with the importance of preparing the surface of the sample for research in a scanning electron microscope.
2. show the need to consider whether the sample has electrical conductivity.
3. analyze the morphology of the selected samples and investigate the elemental composition of the selected part of the sample.

Before starting laboratory work, it is necessary:

- get acquainted with the structure of the SEM and the principle of its operation.
- know and understand the requirements for the sample (the sample must be dry, if necessary, dried and electrically conductive (if necessary, apply a conductive coating).
- clearly understand the differences and features of image acquisition in different modes (SE-, and BSE),
- to understand the essence of the EDX method for obtaining qualitative and quantitative elemental composition of the surface of the sample in SEM.
- investigate and describe the characteristics of the issued sample.

If the samples that we plan to study do not have conductivity, it is necessary to apply a conductive layer of carbon/gold to their surface.

Already prepared samples must be fixed on a conductive table (if the sample is small, it must be applied to a conductive film).

To obtain a high-quality image at different magnifications, the parameters (distance to the sample, intensity of the electron beam, voltage) are changed.

#### 3. Learning outcomes

At the end of the laboratory session, the student:

- will know the structure of a scanning electron microscope;
- will know the requirements for surface preparation of samples before examination;
- will be able to select parameters of SEM operation in image acquisition mode;

- can characterize the microstructure/morphology of the sample;
- will be able to perform qualitative and quantitative analysis by the EDX method.

#### 4. Necessary equipment, materials, etc

Samples for characterization: different types of metallic plates, polymeric powders, polymeric film coating.

Apparatus: scanning electron microscope (with EDX-analyzer), Carbon & gold sputter vacuum coaters for SEM, metal polishing machine/.

ACCESSORIES: solutions, accessories for sample preparation etc.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing laboratory work, students receive permission to perform it by answering the questions posed by the teacher (theory on the topic of the work knowledge of the methodology of the work).

During laboratory classes

- students should prepare theoretically in advance, familiarize themselves with the subject and the course of laboratory work.
- students apply the knowledge gained at lectures to understand the set goals,
- students work in groups,
- work is performed in accordance with the assigned task,
- students use necessary and available equipment, computer equipment, appropriate programs.
- analyze the obtained results,
- at the end of the completed task, formulate conclusions,
- they prepare a written report consisting of theoretical foundations, work performance methodology, necessary calculations, obtained results and conclusions.

Analyzing the obtained results, it is necessary to compare them with theoretical ones or given in the literature.

The final report is drawn up by the student in accordance with the requirements and evaluated by the teacher.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

laboratory procedure manual is available.

#### 7. Additional notes

#### 8. Optional information

## Topics 2

### 1. The subject of the laboratory classes

#### STUDY OF MORPHOLOGY, DETERMINATION OF THE SIZE AND SHAPE OF PARTICLES BY SCANNING ELECTRON MICROSCOPY

### 2. Thematic scope of the laboratory classes

The topic of the laboratory lesson is related to the assessment of morphology and analysis of the size and shape of particles (selected samples) using a scanning electron microscope. Samples must be completely dry. The particle size distribution is analyzed from the obtained SEM images.

The purpose of the classes is to evaluate the morphology of the surface of the sample/the shape of the particles, as well as to determine the size of the particles of the solid material during the laboratory work.

### 3. Learning outcomes

By the end of the laboratory session, the student:

- will know the structure of SEM microscope;
- will be able to select the parameters of SEM operation in image acquisition mode;
- can characterize the morphology and size distribution of sample particles;
- will be able to analyze dimensional characteristics;
- the student will be able to analyze the obtained results and formulate conclusions.

### 4. Necessary equipment, materials, etc

Samples for characterization;

Apparatus: scanning electron microscope (with EDX-analyzer), Carbon & gold sputter vacuum coaters for SEM.

Accessories: accessories for sample preparation etc.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory classes, the teacher evaluates the students' knowledge (theory of the topic of the work and methodology of the work).

During laboratory classes, students use the necessary research equipment and software.

During laboratory classes, students work in groups according to the assigned task

Also, students prepare samples for their characterization in accordance with the task set by the teacher.

In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

At the end of the laboratory session, students will be able to analyze the obtained results and formulate conclusions and make a final report.

The completed report of the completed laboratory work is defended by the student in front of the teacher, who evaluates the work performed and the results obtained.



**6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

laboratory procedure manual is available.

Reference list is in the syllabus.

**7. Additional notes**

**8. Optional information**

## Topics 3

### 1. The subject of the laboratory classes

#### FTIR STUDIES OF POLYMERS (FILMS DEPOSITED ON SUBSTRATE, BULK MATERIAL)

### 2. Thematic scope of the laboratory classes

The purpose of the work: familiarization with the method of infrared spectroscopy, obtaining the spectra of the studied samples.

FTIR spectroscopy is an analytical technique used to identify organic, polymeric, and sometimes inorganic materials. To study the composition of the sample, scan the sample with infrared light and observe its chemical structure of the material by studying chemical bonds and composition. The IR radiation absorbed by the sample molecules is converted into rotational or vibrational energy, and the resulting signal in the detector represents the molecular fingerprint of the sample, as each molecule or chemical structure produces a unique spectral signature. This technique takes advantage of the fact that each frequency responds differently to the material.

Analysis of the composition of the sample using FTIR is used for the following purposes:

Identification and characterization of known/unknown materials such as films, solids, powders or liquids

Identification of impurities on or in the material

To detect oxidation, segregation or non-solidification of polymers

The purpose of the laboratory work will be to investigate applied polymer films on substrates (freshly applied and those that have been exposed to atmospheric conditions for a long time), as well as loose polymer material of a similar composition. The second task will be to analyze the obtained spectra and form a conclusion about their composition based on the position of the spectral lines.

### 3. Learning outcomes

By the end of the laboratory session, the student:

- will know the structure and principle of operation of the FTIR spectrometer.
- will be able to prepare a sample for characterization of the surface of the material.
- will know the order of spectral analysis.
- will learn to decipher the range of organic compounds
- master the skills of qualitative analysis of organic compounds.
- the student will be able to analyze the obtained results and formulate conclusions.

### 4. Necessary equipment, materials, etc

FTIR spectrometer, software;

samples;

disposable rubber gloves, spatulas;

appropriate means for cleaning the surface of the crystal in FTIR;

a mortar for crushing a solid sample.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theory on the topic of the work and knowledge of the practical performance of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task
- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

Also, students must prepare samples for characterization according to the teacher's plan.

At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions, compare the obtained results with those available in the literature).

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

#### 7. Additional notes

#### 8. Optional information



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## Topics 4

### 1. The subject of the laboratory classes

#### X-RAY FLUORESCENCE ANALYSIS OF INORGANIC MATERIALS

### 2. Thematic scope of the laboratory classes

The purpose of the work: to study the technique of X-ray fluorescence spectral analysis. To acquire theoretical knowledge of the X-ray fluorescence method and practical skills in the interpretation of X-ray fluorescence spectra.

The fluorescent method is based on the analysis of the material by the spectrum of secondary radiation. The substance is placed in the path of X-ray radiation, which excites the secondary radiation of the sample under study. The energy of X-ray radiation acting on a solid body is spent on exciting the electrons of its atoms and providing them with kinetic energy. The spectrum of these electrons is discrete.

An important advantage of this method is the possibility of rapid analysis without destroying the sample.

X-ray spectral analysis can be used for qualitative and quantitative determination of elements in materials with a complex chemical composition (metals and alloys, plastics, glass, ceramics, minerals).

### 3. Learning outcomes

At the end of this lesson, students will be able to:

- know the structure and principle of operation of the XRF spectrometer;
- describe the essence of the physical process of XRF;
- students will study the purpose and main characteristics of X-ray spectroscopy;
- will be able to explain how this method can be used to obtain information about the presence of a certain element;
- will be able to distinguish between qualitative and quantitative analysis using XRF;
- will be able to apply the acquired knowledge for independent analysis;
- will be able to interpret X-ray fluorescence spectra.

### 4. Necessary equipment, materials, etc

ElvaX Pro X-ray fluorescence analyzer, computer, appropriate software.

Samples for analysis.

Disposable rubber gloves, spatulas, tweezers.

Suitable chemical solvents.

A mortar for crushing a solid sample.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theory of the topic of the work and knowledge of the practical performance of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task.
- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

Also, students must prepare samples for characterization according to the teacher's plan. At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions about the work, compare the obtained results with those available in the literature).

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

#### **7. Additional notes**

#### **8. Optional information**

## Topics 5

### 1. The subject of the laboratory classes

#### QUALITATIVE ANALYSIS BY X-RAY FLUORESCENCE SPECTROMETRY

### 2. Thematic scope of the laboratory classes

The purpose of the work: to master the technique of X-ray spectral analysis in order to conduct a qualitative analysis of selected samples and to acquire theoretical knowledge and practical skills in the interpretation of X-ray fluorescence spectra. to be able to compare qualitative data obtained by the XRF and EDS methods.

X-ray fluorescence spectrometry is a method of quantitative and qualitative assessment of characteristic X-ray radiation and scattering of photons as a result of the interaction of photons with matter.

XRF can provide both quantitative and qualitative analysis of elements. This method can analyze solids, liquids and powders. XRF gives detailed information about the chemical composition of a sample, but does not indicate which phases are present in the sample (as in the case of XRF). It can analyze elements from beryllium (Be).

The purpose of the work: to compare the qualitative composition of the surface of metal samples (for example, before and after exposure to a corrosive environment).

### 3. Learning outcomes

At the end of this lesson, students will be able to:

- know the structure and principle of operation of the XRF spectrometer;
- will be able to describe the essence of the physical process of XRF;
- will be able to explain how this method can be used to obtain qualitative information about the presence of a certain element in the sample;
- will be able to apply the acquired knowledge for independent analysis;
- will be able to compare the qualitative analysis performed using XRF and EDS (SEM).

### 4. Necessary equipment, materials, etc

Equipment (X-ray fluorescence spectrometer and scanning electron microscope), computer and appropriate software.

Samples for analysis.

Disposable rubber gloves.

Appropriate means for cleaning the surface.

Polishing machine.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theory of the topic of the work and knowledge of the practical performance of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task.



- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

Also, students must prepare samples for characterization according to the teacher's plan.

At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions about the work, compare the obtained results with those available in the literature).

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

#### **7. Additional notes**

#### **8. Optional information**

## Topic 6

### 1. The subject of the laboratory classes

#### QUANTITATIVE ANALYSIS BY X-RAY FLUORESCENCE SPECTROMETRY

### 2. Thematic scope of the laboratory classes

The purpose of the work: to study the technique of X-ray spectral analysis. To acquire theoretical knowledge of the X-ray fluorescence method and practical skills in the interpretation of X-ray fluorescence spectra. Master the performance and interpretation of quantitative analysis, be able to compare the data obtained by the XRF and EDS methods. Be able to state the advantages and disadvantages of quantitative analysis using XRF.

X-ray fluorescence is a technique that can provide rapid elemental analysis at relatively low cost. XRF measures the energy and intensity of secondary X-ray radiation. XRF is also a quantitative method because the peak height of an element is related to the concentration of that element in the sample. However, it should be remembered that there may be an overlap of peaks or the elements may interact with each other, due to which we will have a distortion of the results. In general, XRF quantification is performed using a calibration curve obtained from a large number of standards of known concentration.

Quantitative XRF is much more complex, but the accuracy is very high. The samples must be homogeneous, and the test sample and reference must be in the same state (either powder or solid material).

The purpose of the laboratory work is to compare the quantitative composition of the surface of the selected samples and to compare the obtained data with the data obtained by the EDS method

### 3. Learning outcomes

At the end of this lesson, students will be able to:

- know the structure and principle of operation of the XRF spectrometer;
- will be able to describe the essence of the physical process of XRF;
- will be able to apply the acquired knowledge for independent analysis;
- will be able to explain how this method can be used to obtain quantitative information about the composition of a sample;
- will be able to compare the quantitative analysis performed by XRF and EDS (SEM).

### 4. Necessary equipment, materials, etc

Equipment (X-ray fluorescence spectrometer and scanning electron microscope), computer and appropriate software.

Samples for analysis.

Disposable rubber gloves.

Appropriate means for cleaning the surface.

Polishing machine.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theory of the topic of the work and knowledge of the practical performance of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task.
- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

Also, students must prepare samples for characterization according to the teacher's plan.

At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions about the work, compare the obtained results with those available in the literature).

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

#### 7. Additional notes

#### 8. Optional information

## Topic 7

### 1. The subject of the laboratory classes

#### PHASE ANALYSIS OF MATERIALS, ESTIMATION OF CRYSTALLITE SIZES BY XRD METHOD (USING SCHERRER'S FORMULA).

### 2. Thematic scope of the laboratory classes

**The purpose of the work:** familiarize yourself with the operation of the X-ray diffractometer, familiarize yourself with the method of comparing the phase composition of the sample, familiarize yourself with the database, familiarize yourself with the method of deciphering diffractograms, to calculate the crystallite sizes according to Scherrer's formula.

Determining the phase composition of a substance is one of the important tasks of physicochemical analysis, since the physical properties of a substance depend on the phase composition. Phase analysis is the decomposition of the diffraction spectrum of a sample into the spectra of its phase components. In order to find the phases of the components, it is necessary to compare the already known spectra of phase standards and the spectrum of the sample under study. The process of qualitative X-ray phase analysis is facilitated by the existence of international databases.

Mechanical and physicochemical properties of crystalline substances significantly depends on the size of the crystallites. The dimensions of solid crystallites can be estimated by Scherrer's formula, which is based on the use of broadening of diffraction maxima.

The purpose of the lesson is to compare the phase composition of the selected samples, to determine the size of the crystallites.

### 3. Learning outcomes

At the end of this lesson, students will be able to:

- to know the structure and principle of operation of an X-ray diffractometer
- will be able to describe the essence of the physical process of X-ray diffraction
- will be able to apply the acquired knowledge for independent work.
- will be able to independently perform a phase analysis using an available database.
- will be able to calculate the size of crystallites using Scherrer's formula.

### 4. Necessary equipment, materials, etc

Equipment (X-ray diffractometer), computer and appropriate software.

Samples for analysis.

Disposable rubber gloves, tweezers, spatula.

Appropriate solvent (if necessary).

A mortar for grinding the sample (if necessary).

Polishing machine.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theory of the topic of the work and knowledge of the practical performance of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task.
- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

Also, students must prepare samples for characterization according to the teacher's plan.

At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions about the work, compare the obtained results with those available in the literature).

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

#### 7. Additional notes

#### 8. Optional information

## Topic 8

### 1. The subject of the laboratory classes

#### ATOMIC FORCE MICROSCOPY ANALYSIS OF SURFACE

### 2. Thematic scope of the laboratory classes

The purpose of the work: to study the theoretical foundations of atomic force scanning microscopy and to gain practical skills in working with AFM (get acquainted with the modes of conducting research and learn how to process images obtained by scanning samples with AFM).

To study the topography of the surface of materials (films, metals, alloys, ceramics, etc.), in addition to the scanning electron microscope, the atomic force microscope is widely used.

At the heart of atomic force microscopy is the phenomenon of the interaction of the working probe-needle with the atoms or molecules of the studied sample. By measuring the force (changes in the force of attraction) between the needle and the surface of the material under study, we obtain information about the topography and morphology of the surface of the sample.

The purpose of the laboratory classes: familiarization with the principle and modes of operation of AFM and learning how to process images obtained by scanning the surface of the sample under study.

### 3. Learning outcomes

At the end of this laboratory session, students will:

- will know the structure and principle of operation of an atomic force microscope.
- will be able to describe the modes of operation of AFM, their features and limitations.
- will be able to apply the acquired knowledge for independent work with a microscope.
- will be able to independently scan the surface in the selected mode and analyze the resulting images.

### 4. Necessary equipment, materials, etc

Equipment (scanning probe microscope), computer and appropriate software.

Samples for analysis.

Disposable rubber gloves, tweezers, spatula.

Appropriate solvents (if necessary).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Before performing the laboratory work, the teacher evaluates the students' knowledge through a survey (theoretical material on the subject of the work and the methodology of the work).

- During laboratory classes, students use the necessary research equipment and software.
- During laboratory classes, students work in groups according to the assigned task.
- In laboratory classes, students independently prepare samples for analysis.

- In laboratory classes, students analyze the obtained results and draw appropriate conclusions.

At the end of the laboratory session, students will be able to make a final report (analyze the obtained results and formulate appropriate conclusions regarding the completed task of this laboratory work, compare the obtained results with those available in the literature).

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Instructions for laboratory procedures are available.

The list of references is included in the course syllabus.

## 7. Additional notes

## 8. Optional information

8 Reports	32%
Tests	8%
Team project	10%
Exam	50%
Total	100%

8 reports (max. 4 points each) – max. 32 points

Tests – max. 8 points

Team project – max. 10 points

Final exam – max. 50 points

Total points – max. 100 points

Grading Scale

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**CHEMO- AND BIOSENSORS  
MATERIALS AND APPLICATIONS**

**Code: CBS**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### SENSORS AND SENSOR DEVICES

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Each of us has at least five sensors - these are our nose, tongue, ears, eyes and fingers. One of the most famous sensors used in the laboratory is litmus paper, which changes color depending on the presence of acid or alkali. The most accurate method for determining the acidity of the environment is the pH measurement. You can measure pH in different ways, for example, using special indicators that change the color of the solution or using simple pH indicator paper. However, it is best to measure pH using a pH meter - an electrochemical device that produces an electrical response of varying magnitude depending on the pH. During the lecture, as an introduction to the subject Chemo- and biosensors, the general information about sensors and current state of chemo- and biosensors will be presented. Students will learn the General characteristics and scheme of the sensor device; Sensor, transducer, actuator; Sensitive layer, active layer components; Classification of sensors and sensor devices; Principles of operation of the most common types of chemical sensors (electrochemical, electrical, optical, magnetic, gravimetric, thermometric); Selectivity of ion-selective electrodes, Nikolsky-Eisenman equation; Sensitivity (operating range, linear range and detection limit); Time characteristics (response time, regeneration time, life time); Precision, accuracy and reproducibility.

#### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to, *the general information about Chemo- and biosensors and current state of chemo- and biosensors.*

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Advanced microsystems for automotive applications*. Detlef Egbert Ricken, Wolfgang Gessner. Springer. 1999. 318 p.

#### 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### ELECTROCHEMICAL SENSORS. POTENTIOMETRIC SENSORS.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The work of potentiometric sensors is based on the use of ion-selective electrodes, which give feedback on the presence of defined ions or molecules of substances in solutions. The analytical signal in them is the potential that arises on the surface of a solid material placed in a solution containing ions that can exchange with the surface. The magnitude of the potential is related to the number of ions in the solution. It is not possible to measure the surface potential directly, but it can be measured using a suitable electrochemical cell. The selectivity of the ion-selective electrode signal is achieved by selecting a special ion-selective membrane that contains ionophores that selectively bind the ions to be determined. For example, sodium glass, which participates in the reaction with hydrogen ions, serves as such a membrane in a pH-metric electrode. The lecture will present the Potentiometric sensors: The potential of an ion-selective electrode; Designs of ion-selective electrodes; Potentiometric sensors: scheme of an electrochemical circuit; The potential of an electrochemical cell; Ion-selective membranes; Glass membranes; Membranes from insoluble inorganic salts; Polymeric membranes with an immobilized ionophore;  $\pi$ -Conjugated polymer membranes; Use of nanoscale hollow structures as a material for electrochemical sensor devices; Molecular structure of reticulated polyviologen synthesized by the method of electropolymerization anionic stamping; Dependence of the surface density of redox-active viologenic centers of GSV in a film with incorporated CPV/Cl<sup>-</sup>, CPV/Br<sup>-</sup> and CPV/I<sup>-</sup> ions when it is exposed to aqueous solutions of KCl, KBr and KI.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Potentiometric sensors*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Materials for Chemical Sensors*. Edited By Subhendu Bhandari, Arti Dinkarrao Rushi. CRC Press. 2023. 240 p. ISBN 9780367484354

- *Types of Electrochemical Sensors. Encyclopedia*. Baranwal, J.; Barse, B.; Gatto, G.; Kumar, A. Available online: <https://encyclopedia.pub/entry/33545>.

- *Potentiometric Sensing*. Elena Zdrachek and Eric Bakker. Anal. Chem. 2021. Vol. 93, Iss. 1. P. 72–102. <https://doi.org/10.1021/acs.analchem.0c04249>

- 5 - *Potentiometric sensors*. Omer Sadak. Fundamentals of Sensor Technology. Principles and Novel Designs. Woodhead Publishing Series in Electronic and Optical Materials. 2023. P. 99-121. <https://doi.org/10.1016/B978-0-323-88431-0.00009-0>

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

**ELECTROCHEMICAL SENSORS. AMPEROMETRIC, CONDUCTOMETRIC SENSORS.**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Amperometric measurements are frequently used as an analytical method of high accuracy and sensitivity in which the applied voltage serves as a driving force for electrocatalytic redox reactions that generate electrical currents proportional to the concentration of the analyte. A controlled-potential system is required for the fundamental instrumentation, and the electrochemical cell is composed of two electrodes submerged in an electrolyte of an appropriate composition. A more sophisticated and common design is the employment of a three-electrode cell, with one of the electrodes functioning as a reference electrode. The action of conductometric sensors is based on the measurement of electrical conductivity. Electrical conductivity is a generalized characteristic of an electrolyte solution, which is determined by its ionic composition. It depends on the nature and concentration of ions - charge carriers, as well as the properties of the solution as a whole - its dielectric constant, temperature, ionic strength, etc. Almost all reactions that are accompanied by a change in the number, charge or mobility of ions can be monitored by the change in conductivity. Often, the signal of conductometric sensors is formed as a result of a change in the conductivity of the surface coatings of the electrodes during the interaction of their components with the substance to be determined. The lecture will present the information about active layer components, production and properties of Amperometric and Conductometric sensors; Voltammetry with linear potential sweep; Randles-Shevchik equation; Cyclic voltammetry; Chronoamperometry; Cottrell's equation; Amperometry; The relationship between the amount of current and the amount of substance involved in the electrode process; Conductometric sensors; Conductivity; Measurement of electrical conductivity; Impedance response of the sensor; Design of conductometric cells (with immersed electrodes; with printed comb electrodes; based on a pair of planar electrodes covered with an insulating layer; with layer-by-layer arrangement of electrodes, etc;) Conductometric sensors with a solid electrolyte.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Amperometric and conductometric sensors*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Materials for Chemical Sensors*. Edited By Subhendu Bhandari, Arti Dinkarrao Rushi. CRC Press. 2023. 240 p. ISBN 9780367484354
- *Types of Electrochemical Sensors*. *Encyclopedia*. Baranwal, J.; Barse, B.; Gatto, G.; Kumar, A. Available online: <https://encyclopedia.pub/entry/33545>.
- *Hybrid Amperometric and Conductometric Chemical Sensor Based on Conducting Polymer Nanojunctions*. Erica S Forzani, Xiulan Li, Nongjian Tao. 2007. *Analytical Chemistry*. Vol. 79(14). P.5217-24. DOI:[10.1021/ac0703202](https://doi.org/10.1021/ac0703202)

## 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### OTHER TYPES OF ELECTROCHEMICAL SENSORS.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

A capacitive sensor is an electronic device that can detect solid or liquid targets without physical contact. To detect these targets, capacitive sensors emit an electrical field from the sensing end of the sensor. Any target that can disrupt this electrical field can be detected by a capacitive sensor. Some examples of the solid materials a capacitive sensor can detect are all types of metal, all types of plastic, wood, paper, glass, and cloth. Some capacitive sensors can be used to detect material inside a nonmetallic container. Coulometry determines the amount of matter transformed during an electrolysis reaction by measuring the amount of electricity (in coulombs) consumed or produced. It can be used for precision measurements of charge, and the amperes even used to have a coulometric definition. Field-Effect Transistor sensors (FET-sensors) have been receiving increasing attention for sensing over the last two decades due to their potential for ultra-high sensitivity sensing, label-free operation, cost reduction and miniaturisation. The lecture will present some types of electrochemical sensors: Electrical capacitive sensors; The influence of the amount of adsorbed component on the change in the dielectric constant; Materials of the sensitive layer and design of capacitive sensors; Materials and construction of coulometric sensors; Basic information about semiconductors; The location of the energy zones in the MDS structure at different closing voltages; Field-effect transistors: Contact of a semiconductor with a solution; Scheme and principle of operation of a field-effect transistor with an isolated gate; Scheme, principle and modes of operation of a field-effect transistor in the gate of which there is an analyte-sensitive membrane; The use of sensors based on field-effect transistors - ion-selective and enzyme field-effect transistors; New types of electrodes: modified electrodes, microelectrodes, thin film and printed electrodes.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Capacitive sensors, Coulometric sensors, Sensors based on field-effect transistors*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Materials for Chemical Sensors*. Edited By Subhendu Bhandari, Arti Dinkarrao Rushi. CRC Press. 2023. 240 p. ISBN 9780367484354

- *Types of Electrochemical Sensors. Encyclopedia.* Baranwal, J.; Barse, B.; Gatto, G.; Kumar, A. Available online: <https://encyclopedia.pub/entry/33545>.
- *Recent Advances of Capacitive Sensors: Materials, Microstructure Designs, Applications, and Opportunities.* Allen J. Cheng, Liao Wu, Zhao Sha, Wenkai Chang, Dewei Chu, Chun Hui Wang, Shuhua Peng. 2023. *Advanced Materials Technologies.* Wiley-VCH GmbH. P. 2201959 (1 -34). <https://doi.org/10.1002/admt.202201959>
- *Paper-Based Thin-Layer Coulometric Sensor for Halide Determination.* Maria Cuartero, Gastón A. Crespo, and Eric Bakker. *Anal. Chem.* 2015. Vol. 87, Iss. 3. P. 1981–1990. <https://doi.org/10.1021/ac504400w>
- Field-effect sensors – from pH sensing to biosensing: sensitivity enhancement using streptavidin–biotin as a model system. Benjamin M. Lowe, Kai Sun, Ioannis Zeimpekis, Chris-Kriton Skylaris and Nicolas G. Green. *Analyst.* 2017. Vol. 142. P. 4173-4200. <https://doi.org/10.1039/C7AN00455A>

## 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

#### OPTICAL CHEMICAL SENSORS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to describe principles of operation of optical sensors, transducer materials and methods of forming a sensitive layer. Optical sensors have a number of advantages compared to electrochemical ones. They do not require a "reference electrode", although in practice they prefer to measure the signal relative to some reference value. The optical signal is not affected by electrical interference. The immobilized reagent phase should not be in close contact with the transducer (optical fiber), so it can be easily replaced. Optical devices are safer than electrical devices, as there is no risk of electric shock. Optical sensors remain stable for a long time after calibration, especially when measuring the ratio of intensities at two different wavelengths. By immobilizing multiple reagents that signal at different wavelengths, a single sensor can be used to detect multiple analytes, such as O<sub>2</sub> and CO. Measurements at different wavelengths help to monitor the change in the state of the reagent. Optical transducers are potentially more informative than electrochemical ones because they can provide a full range of data

The lecture will present features of the Optical chemical sensors: Photometric methods; Absorption spectroscopy in the UV and visible ranges; Fluorescence spectroscopy; The Stern-Volmer equation; Chemiluminescence; Structure and design features of optical chemical sensors; Optical transducers; Light guides Snell's equation; Solid-phase sensors; Schemes of solid-phase optical sensors; Platforms for optical sensors based on  $\pi$ -conjugated polymers; Modes of operation of optical fibers in sensors; Determination of analyte in direct sensors with an immobilized reagent; Absorption spectroscopy in the visible range - measurement of pH, carbon dioxide, ammonia; Fluorescent reagents (pH-, halide-, Na<sup>+</sup>, K<sup>+</sup>, oxygen-sensitive); Indirect optical sensors; Optical sensors based on internal reflection spectroscopy; Total internal reflection is broken; Generation of an evanescent wave at the interface between two optical media; An element with multiple broken total internal reflection (BTIR); Schemes of elements with multiple BTIR; Disturbed total internal reflection with fluorescence; Fluorescent light detection schemes at right angles to the reflective surface and in the direction of the main beam; Surface plasmon resonance; Brewster's angle measurement; Generation of non-radiative plasmons in a Kretschmann prism; Optical sensors based on light scattering methods: types of light scattering; Spectroscopy of quasi-elastic light scattering; Photon correlation spectroscopy; Laser Doppler flowmetry.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Optical chemical sensors*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Optical Chemical Sensors: Design and Applications*. Roberto Pizzoferrato. *Sensors*. 2023. Vol. 23 P. 5284 (1-4). <https://doi.org/10.3390/s23115284>
- *Optical Chemical Sensors: Design and Applications [Internet]. Advances in Chemical Sensors*. Lobnik A, Turel M, Korent Spela. 2012. InTech. Available from: <http://dx.doi.org/10.5772/31534>

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### GRAVIMETRIC AND CALORIMETRIC SENSORS.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to describe gravimetric and calorimetric sensors. In some natural anisotropic crystals (for example, in crystals where there are no centers of symmetry, quartz and tourmaline crystals), which are subjected to mechanical stress, an electrical signal occurs. In such materials, the reverse effect is also revealed, namely, a change in size under the action of an electric field. When an alternating electric potential is applied to such materials, mechanical oscillations occur in them. Each crystal is characterized by its own resonant purity of vibrations, which may depend on its environment. Usually, the resonant frequencies of piezoelectric crystals lie in the radio wave region and are about 10 MHz. The natural resonance frequency depends on the mass of both the crystal itself and the material adsorbed on it. Adsorption of a substance on the crystal surface causes a change in its resonance frequency ( $\Delta f$ ), which can be measured with exceptionally high sensitivity (500-2500 Hz/ $\mu\text{g}$ ). Sensors based on this effect can be characterized by detection limits of the order of several picograms ( $10^{-12}$  g). A thermistor is a device that responds to slight changes in temperature. Its principle of operation is based on the ability of some agglomerated metal oxides to change electrical resistance when the temperature changes. Barium and calcium oxides, as well as oxides of some transition metals (Co, Ni, and Mn) have these properties. Usually, the resistance of the metal oxide changes by 4–7% when the temperature changes by 1 degree.

Thermistors are usually made in the form of small glass balls. As part of a microcalorimeter, thermistors can be used to measure a small amount of heat released during chemical and biochemical reactions. To determine the analyte in a complex mixture, the method must be selective, ensuring that the desired reaction occurs near the thermistor.

During the lecture, students will learn about Gravimetric and Calorimetric sensors: The essence of the piezoelectric effect; Types of piezoelectric materials; Change in the mass of the piezo crystal as a result of selective sorption of the substance to be determined, its relationship with the frequency of oscillations of the piezo crystal; Sauerbrey equation; Using the piezoelectric effect for gas analysis; Use of the piezoelectric effect in quartz crystal microbalances and in electrochemical quartz crystal microbalances; Piezoelectric effect and generation of acoustic waves; Propagation of acoustic waves; Volumetric acoustic waves that cause longitudinal shear; Fading waves; Lamb waves; Volumetric acoustic waves that cause transverse shear; Thermometric sensors: thermistors, design and principle of operation; Principle of operation and application of catalytic gas sensors; Non-isothermal and isothermal modes of operation of gas sensors; Pellistor construction; Scheme of using pellistors in gas sensors; Thermal conductivity meters and their use.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Gravimetric and calorimetric sensors*.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Gravimetric Dielectric And Calorimetric Methods For The Detection Of Organic Solventvapours Using Poly(etherurethane) Coatings*. R. Zhou, A. Hierlemann, U. Weimar and W. Gopel. Proceedings of the International Solid-State Sensors and Actuators Conference – TRANSDUCERS '95. Stockholm, Sweden. 1995. P. 833-836. <https://doi.org/10.1109/SENSOR.1995.721968>
- Principles of quartz crystal microbalance/heat conduction calorimetry: Measurement of the sorption enthalpy of hydrogen in palladium. Allan L. Smith, Hamid. M. Shirazi. 2005. *Thermochimica Acta*. Vol. 432, Iss. 2. P. 202-211. <https://doi.org/10.1016/j.tca.2005.03.017>

#### 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### GENERAL CHARACTERISTICS OF BIOSENSORS.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

If the structure of the sensitive layer of the sensor device contains biologically active components: enzymes, nucleic acids, yeast, liposomes, organelles, bacteria, antibodies-antigens, single-cell organisms and even whole tissues of higher organisms, then it can be designated as a biosensor. Although there are no fundamental differences between chemosensors and biosensors, biosensors differ in a much greater variety, increased selectivity and sensitivity. Mild operating conditions make them indispensable in medical and biological diagnostics, food quality analysis and environmental protection. The lecture will describe general characteristics of biosensors: Factors affecting the characteristics of biosensors - amount of enzyme, immobilization method, buffer pH; Classification of biosensors - Enzyme sensors, Substrate and inhibitor sensors, Immunosensors, DNA sensors, Biosensors based on supramolecular cell structures, Microbial biosensors; General characteristics of methods of immobilization of active biosensor components; Methods of non-covalent immobilization - Adsorption, Physical capture in a polymer matrix, Electropolymerization, Layer method, Inclusion in polyionic complexes, Lipid-membrane sensors, Langmuir-Blodgett films, Biosensors on self-assembled monomolecular layers, Photopolymerized layers, Microencapsulation, Affinity immobilization; Methods of covalent immobilization - General characteristics, Cross-linking, Molecular imprint method, Immobilization of DNA, microorganisms and supramolecular structures; Enzymatic electrodes; The working principle of the enzyme electrode; Oxireductases; Active centers in oxidases and peroxidases; Electron transfer mediators and the scheme of functioning of the mediator enzyme sensor; The Michaelis-Menten equation and its electrochemical modification; The speed of the enzymatic reaction in the kinetic and diffusion regimes; Direct electron transfer in enzyme-electrode systems; Potentiometric biosensors; Amperometric biosensors; Conductometric biosensors; Pneumatic methods in biosensory; Piezoelectric methods in biosensory; Optical methods in biosensory.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Biosensors*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.



## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Chemical Sensors and Biosensors. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- Chemical Sensors and Biosensors: Fundamentals and Applications. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Biosensors. Fundamentals, Emerging Technologies, and Applications*. Edited By Sibel A. Ozkan, Bengi Uslu, Mustafa Kemal Sezgintürk. 2022. CRC Press. 394 P. ISBN 9781032038650
- 4.2 – *Biosensors*. Akifumi Kawamura, Takashi Miyata. Biomaterials Nanoarchitectonics. 2016. P. 157-176. <https://doi.org/10.1016/B978-0-323-37127-8.00010-8>

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

#### PROSPECTS FOR THE DEVELOPMENT OF SENSOR DEVICES.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Researchers associate the further development of chemical sensors with the use of new materials and technologies to create sensors. Among the organic electrically conductive materials that began to be actively used in electroanalysis at the beginning of the third millennium, an important place belongs to electrically conductive polymer materials, which, in combination with nanomaterials and nanotechnologies, open promising prospects in the field of sensors.

During the lecture, students will learn about Prospects for the development of sensor devices; Sensor platforms from conductive polymers; Construction of sensors on a polymer-conductive platform; Sensor platforms on carbon nanotubes; Sensitive layers based on conductive polymer composites; Supramolecular strategy in chemosensory; Specialized sensor systems - pollutant biosensor systems; Specialized sensor systems - biosensor devices for the analysis of water and food products.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Prospects for the development of sensor devices*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Prospects of Biosensors Based on Functionalized and Nanostructured Solitary Materials: Detection of Viral Infections and Other Risks*. Kumar S, Sharma R, Bhawna, Gupta A, Singh P, Kalia S, Thakur P, Kumar V. ACS Omega. 2022. Vol. 7(26). P. 22073-22088. <https://doi.org/10.1021%2Facsomega.2c01033>
- *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Recent Applications and Prospects of Nanowire-Based Biosensors* Tran, Vy Anh, Giang N. L. Vo, Thu-Thao Thi Vo, Van Dat Doan, Vien Vo, and Van Thuan Le. 2023. Processes. Vol. 11, Iss. 6. P. 1739. <https://doi.org/10.3390/pr11061739>

- Material Design in Implantable Biosensors toward Future Personalized Diagnostics and Treatments. Faezeh Ghorbanizamani, Hichem Moulahoum, Emine Guler Celik, Suna Timur. 2023. Applied Sciences. Vol. 13(7). P.4630. <http://dx.doi.org/10.3390/app13074630>

## 6. Additional notes

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## Course content – laboratory classes

### Topics 1 – Lab 1

#### 1. The subject of the laboratory classes

##### A POTENTIOMETRIC CHEMOSENSOR BASED ON POLYANILINE FOR DETERMINING THE PH OF AQUEOUS SOLUTIONS

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the electrochemical synthesis of polyaniline on a platinum electrode and testing its operation as a working electrode of a pH meter. Students will carry out the process of modifying the electrode with a conductive polymer (polyaniline doped with sulfuric acid or polyaniline doped with naphthalene sulfonic acid), investigate its potentiometric response to the concentration of hydrogen ions in aqueous solutions, based on the obtained data, determine the sensitivity of the constructed chemosensor and study the limits of measuring the pH of aqueous solutions. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

#### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Potentiometric chemosensors, pH-sensors, application of electroactive polymers in sensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Potentiometric chemosensor based on polyaniline for determining the pH of aqueous solutions*, including critical analysis, synthesis, and conclusions.

#### 4. Necessary equipment, materials, etc

- electrochemical cell,
- potentiostat (three-electrode measuring system for the synthesis of polyaniline and two-electrode for potentiometric pH determinations),
- working and auxiliary Pt electrodes,
- silver chloride reference electrode,
- computer laboratory

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of the potential of an ion-selective electrode; Designs of ion-selective electrodes; Potentiometric sensors: scheme of an electrochemical circuit; The potential of an electrochemical cell; Ion-selective membranes; Glass membranes; Membranes from insoluble inorganic salts; Polymeric membranes with an immobilized ionophore;  $\pi$ -Conjugated polymer membranes; Use of nanoscale hollow structures as a material for electrochemical sensor devices; Use of conductive polymers for the manufacture of sensors,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Chemical Sensors and Biosensors: Fundamentals and Applications. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Advanced microsystems for automotive applications*. Detlef Egbert Ricken, Wolfgang Gessner. Springer. 1999. 318 p.
- *Chapter 7. Polyaniline in Chemo-and Biosensorics: Overview* Kovalyshyn Ya.S., Reshetnyak O.V. // *Computational and Experimental Analysis of Functional Materials* / O.V. Reshetnyak, G. E. Zaikov (Eds.) [Series: AAP Research Notes on Polymer Engineering Science and Technology]. Toronto, New Jersey: Apple Academic Press, CRC Press (Taylor@ Francis Group). 2017. – 571 p.
- *Potentiometric Sensing*. Elena Zdrachek and Eric Bakker. Anal. Chem. 2021. Vol. 93, Iss. 1. P. 72–102. <https://doi.org/10.1021/acs.analchem.0c04249>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

#### ELECTROCHEMICAL UREA BIOSENSOR BASED ON POLYLUMINOL

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will synthesize an electroactive polymer on a platinum electrode in potentiostatic, galvanostatic, or potentiodynamic modes; immobilize urease on the surface of an electroactive polymer; investigate the dependence of conductivity (or response current) on the concentration of urea in the solution; determine the sensitivity of the sensor and the working range of substrate concentrations by the tangent of the angle of inclination and the limits of linearity of the obtained dependence. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Conductometric biosensors, application of electroactive polymers in sensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemical urea biosensor based on polyluminol*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- electrochemical cell,
- urease,
- potentiostat (three-electrode measuring system for the synthesis of polyluminol and two-electrode for conductometric urea determinations),
- working and auxiliary Pt electrodes,
- silver chloride reference electrode,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.



Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of Conductometric sensors; Conductivity; Measurement of electrical conductivity; Impedance response of the sensor; Design of conductometric cells (with immersed electrodes; with printed comb electrodes; based on a pair of planar electrodes covered with an insulating layer; with layer-by-layer arrangement of electrodes, etc;) Conductometric sensors with a solid electrolyte; Factors affecting the characteristics of biosensors; Classification of biosensors; General characteristics of methods of immobilization of active biosensor components; The working principle of the enzyme electrode; Electron transfer mediators,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Types of Electrochemical Sensors. Encyclopedia.* Baranwal, J.; Barse, B.; Gatto, G.; Kumar, A. Available online: <https://encyclopedia.pub/entry/33545>.
- *Hybrid Amperometric and Conductometric Chemical Sensor Based on Conducting Polymer Nanojunctions.* Erica S Forzani, Xiulan Li, Nongjian Tao. 2007. Analytical Chemistry. Vol. 79(14). P.5217-24. DOI:[10.1021/ac0703202](https://doi.org/10.1021/ac0703202)- *Biosensors. Fundamentals, Emerging Technologies, and Applications.* Edited By Sibel A. Ozkan, Bengi Uslu, Mustafa Kemal Sezgintürk. 2022. CRC Press. 394 P. ISBN 9781032038650
- 4.2 – *Biosensors.* Akifumi Kawamura, Takashi Miyata. Biomaterials Nanoarchitectonics. 2016. P. 157-176. <https://doi.org/10.1016/B978-0-323-37127-8.00010-8>
- *A Novel Conductometric Urea Biosensor with Improved Analytical Characteristic Based on Recombinant Urease Adsorbed on Nanoparticle of Silicalite.* Velychko, T.P., Soldatkin, O.O., Melnyk, V.G. et al. 2016. Nanoscale Res. Lett. Vol. 11. P. 106 (1-6). <https://doi.org/10.1186/s11671-016-1310-3>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

**ELECTROCHEMILUMINESCENT CHEMOSENSOR FOR DETERMINATION OF PERSULFATE IONS.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will investigate the dependence of the intensity of electrochemiluminescence radiation depending on the material of the electrode and the concentration of  $K_2S_2O_8$  solutions in water; construct the dependence of radiation intensity on concentration; use the straight-line plot as a calibration graph to determine the concentration of the persulfate solutions under study. Students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *optical sensors, construction and work of electrochemiluminescent chemosensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemiluminescent chemosensor for determination of persulfate ions*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- electrochemical cell,
- photomultiplier,
- diffraction monochromator,
- potentiostat (three-electrode measuring system),
- working (Cu, Zn, Al, Mg, Pt, In) and auxiliary (Pt) electrodes,
- silver chloride reference electrode,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of features of the Optical chemical sensors; Chemiluminescence; Electrochemiluminescence; Luminescent light detection scheme,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Optical Chemical Sensors: Design and Applications*. Roberto Pizzoferrato. *Sensors*. 2023. Vol. 23 P. 5284 (1-4). <https://doi.org/10.3390/s23115284>
- *Electrochemiluminescent Chemosensors for Clinical Applications: A Review*. Truong, C.K.P., Nguyen, T.D.D. & Shin, I.S. 2019. *BioChip. J.* Vol. 13. P. 203-216. <https://doi.org/10.1007/s13206-019-3301-9>
- *Multifunctional solid-state electrochemiluminescent chemosensors and aptasensor with free-standing active sites based on task-specific pyrene-terminated polymers via RAFT polymerization*. Yuanhong Xu, Tao Chen, Jing Sun, Jingquan Liu. 2018. *Analytica Chimica Acta*. Vol. 1039. P. 31-40. <https://doi.org/10.1016/j.aca.2018.07.046>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

#### QUARTZ MICROBALANCE AMMONIA SENSOR

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the gravimetric sensors. Students will make a piezoelectric sensor for determining ammonia in an aqueous solution by modifying the surface of a quartz crystal with an electrically conductive polymer (polyaniline); determine the dependence of the frequency on the content of ammonia in an aqueous solution using the quartz crystal microbalance method; investigate the change in sensor sensitivity when modifying a polyaniline film with metal nanoparticles. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Gravimetric sensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Quartz microbalance ammonia sensor*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- electrochemical cell,
- AT-cut quartz crystals of mass production,
- frequency meter,
- potentiostat (three-electrode measuring system),
- silver chloride reference electrode,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of the essence of the Piezoelectric effect; Types of piezoelectric materials; Change in the mass of the piezo crystal as a result of selective sorption of the substance to be determined, its relationship with the frequency of oscillations of the piezo crystal; Sauerbrey equation; Using the piezoelectric effect for gas analysis; Use of the piezoelectric effect in quartz crystal microbalances and in electrochemical quartz crystal microbalances; Piezoelectric effect and generation of acoustic waves; propagation of acoustic waves; Volumetric acoustic waves that cause longitudinal shear; Fading waves; Lamb waves; Volumetric acoustic waves that cause transverse shear,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- *Recent Advances in Quartz Crystal Microbalance-Based Sensors*. Sandeep Kumar Vashist, Priya Vashist. 2011. Journal of Sensors. Vol. 2011, Article ID 571405, 13 pages, <https://doi.org/10.1155/2011/571405>
- *Polymer coated quartz crystal microbalance sensors for detection of volatile organic compounds in gas mixtures*. Pengchao Si, John Mortensen, Alexei Komolov, Jens Denborg, Preben Juul Møller. 2007. Analytica Chimica Acta. Vol. 597, Iss. 2. P. 223-230. <https://doi.org/10.1016/j.aca.2007.06.050>
- *Quartz microbalance sensors for gas detection*. R. Lucklum, B. Henning, P. Hauptmann, K.D. Schierbaum, S. Vaihinger, W. Göpel. 1991. Sensors and Actuators A: Physical. Vol. 27, Iss. 1-3. P. 705-710. [https://doi.org/10.1016/0924-4247\(91\)87074-D](https://doi.org/10.1016/0924-4247(91)87074-D)

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),



- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### OPTICAL CHEMOSENSOR BASED ON POLYANILINE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will make a sensitive sensor element by applying a conductive polyaniline film on a transparent substrate; investigate and construct a calibration curve of the dependence of the optical density of the polyaniline film on the ammonia content in the gas mixture (nitrogen+ammonia); calculate the analytical characteristics of the constructed sensor. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Optical chemical sensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Optical chemosensor based on polyaniline*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- transparent substrate or ITO (Indium Tin Oxide) Electrode,
- spectrophotometer,
- potentiostat (three-electrode measuring system),
- electrochemical cell,
- silver chloride reference electrode,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of features of the Optical chemical sensors: Photometric methods; Structure and design features of optical chemical sensors; Optical transducers; Light guides Snell's equation; Solid-phase sensors; Schemes of solid-phase optical sensors; Platforms for optical sensors based on  $\pi$ -conjugated polymers; Modes of operation of optical fibers in sensors; Determination of analyte in direct sensors with an immobilized reagent; Absorption spectroscopy in the visible range - measurement of pH, carbon dioxide, ammonia,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- *Optical Chemical Sensors: Design and Applications*. Roberto Pizzoferrato. Sensors. 2023. Vol. 23 P. 5284 (1-4). <https://doi.org/10.3390/s23115284>
- *Optical Chemical Sensors: Design and Applications [Internet]. Advances in Chemical Sensors*. Lobnik A, Turel M, Korent Spela. 2012. InTech. Available from: <http://dx.doi.org/10.5772/31534>
- *Synthesis and optical characterization of benzene sulfonic acid doped polyaniline*. N. Karaođlan, Cuma Bindal. 2018. Engineering Science and Technology, an International Journal. Vol. 21, Iss. 6. P. 1152-1158. <https://doi.org/10.1016/j.jestch.2018.09.010>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

#### GLUCOSE OXIDASE AMPEROMETRIC BIOSENSOR

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the amperometric sensors and the basic principles of its fabrication methods and operation principles. Students will electrochemically synthesize an electroactive polymer on a platinum electrode; immobilize glucose oxidase enzyme on an electrode; investigate the dependence of the response current of the sensor on the concentration of glucose in the solution; determine the sensitivity of the sensor and the working range of substrate concentrations based on the obtained dependence; students will calculate the kinetic parameters of the enzymatic reaction. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Amperometric biosensors*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Glucose oxidase amperometric biosensor*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- electrochemical cell,
- glucose oxidase,
- potentiostat (three-electrode measuring system for the synthesis of electroactive polymer and amperometric glucose determinations),
- working and auxiliary Pt electrodes,
- silver chloride reference electrode,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of general characteristics of biosensors: Factors affecting the characteristics of biosensors; Classification of biosensors; General characteristics of methods of immobilization of active biosensor components; Enzymatic electrodes; The working principle of the enzyme electrode; Electron transfer mediators and the scheme of functioning of the mediator enzyme sensor,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Chemical Sensors and Biosensors. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
- Chemical Sensors and Biosensors: Fundamentals and Applications. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
- Design of an amperometric biosensor using polypyrrole-microgel composites containing glucose oxidase. J. Rubio Retama, E. López Cabarcos, D. Mecerreyes, B. López-Ruiz. 2004. Biosensors and Bioelectronics. Vol. 20, Iss. 6. P. 1111-1117. <https://doi.org/10.1016/j.bios.2004.05.018>
- *Glucose Oxidase Captured into Electropolymerized p-Coumaric Acid towards the Development of a Glucose Biosensor*. Valdés-Ramírez, G.; Galicia, L. 2023. Chemosensors Vol. 11. P. 345. <https://doi.org/10.3390/chemosensors11060345>
- *An Amperometric Glucose Biosensor Composed of Prussian Blue, Nafion, and Glucose Oxidase Studied by Flow Injection Analysis*. Steven M. Drew and Tristan Belzer. 2023. J. Chem. Educ. Vol. 100, Iss. 2. P. 760–766. <https://doi.org/10.1021/acs.jchemed.2c00534>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),

- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**MEMBRANE PROCESSES**  
**MATERIALS, PROPERTIES AND APPLICATIONS**

**Code: MP**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### THEORETICAL FOUNDATIONS OF MASS TRANSFER.

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The main force of membrane technology is the fact that it works without the addition of chemicals, with a relatively low energy use and easy and well-arranged process conduction. Membrane technology is a generic term for a number of different, very characteristic separation processes. During the lecture, the current state of membranes and membrane processes will be presented. Students will learn the Basics of mass transfer theory; Kinetics and thermodynamics of mass transfer; Physical modeling of membrane processes; Membrane equilibrium, Donnan equilibrium; Diffusion of electrolytes; Membrane potential; The influence of the processes of adsorption, polarization, complexation and gelation on the separation of components; Influence of pressure and temperature on the process of membrane separation.

#### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Membrane processes: materials, properties and applications, especially: fundamentals, and theoretical foundations of mass transfer.*

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**  
a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Nanocomposite Membranes for Water and Gas Separation. A volume in Micro and Nano Technologies Chapter 1 - Overview of membrane technology.* Asad Asad, Dan Sameoto, Mohtada Sadrzadeh. 2020. Micro and Nano Technologies. P. 1-28.  
<https://doi.org/10.1016/B978-0-12-816710-6.00001-8>

- *Science and Technology of Separation Membranes.* Tadashi Uragami. Wiley. 2017. 848 p. ISBN: 978-1-118-93256-8.

- *Membrane processes.* Katarzyna Staszak. 2017. Phys. Sci. Rev. <https://doi.org/10.1515/psr-2017-0142>

- *The Future of Membrane Separation Processes: A Prospective Analysis.* Eric Favre. 2022. Front. Chem. Eng., Sec. Separation Processes. Vol. 4. <https://doi.org/10.3389/fceng.2022.916054>

#### 6. Additional notes

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### Topics 2

## 1. The subject of the lecture

### TRANSFER PHENOMENA IN POROUS BODIES.

## 2. Thematic scope of the lecture (abstract, maximum 500 words)

Porous bodies can be represented as reversible suspensions or powders, and powders and concentrated suspensions, in turn, can be represented as porous bodies. This lecture discusses the movement of liquids and gases in pores and capillary porous bodies. Most of the regularities of such movement are also characteristic of powders, sediments, and other dispersed systems. The lecture will present the basic laws of fluid flow in porous bodies; Stokes' law for liquid flow in a capillary; maximum and average speed of fluid movement; Hagen-Poiseuille equation; peculiarities of laminar and turbulent liquid flow in a capillary; Darcy's Law; the coefficient of permeability of a porous body; Determination of pore sizes by filtration method; capillary impregnation; capillary pressure; rate of capillary impregnation, Washburn equation; elementary transfer mechanisms, driving forces; Hydrodynamic mode of transfer of gases and components of solutions; Diffusion mode of substance transfer; Fick's law; diffusion coefficient; diffusion transfer of gas when the condition of medium integrity is not met; Knudsen's gas; effusion; activated diffusion in micropores, enthalpy of activation; surface diffusion; the total flow of matter with the simultaneous implementation of various types of diffusion.

## 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Transfer Phenomena In Porous Bodies*.

## 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Science and Technology of Separation Membranes*. Tadashi Uragami. Wiley. 2017. 848 p. ISBN: 978-1-118-93256-8.

- *Transport Phenomena in Porous Media II. 1st Edition*. I. Pop, Derek B Ingham. Pergamon. 2002. 468 p. Hardback ISBN: 9780080439655, eBook ISBN: 9780080543178

- *Liquid and Vapour Flows in Porous Bodies: Surface Phenomena (Topics in Chemical Engineering) 1st Edition*. N.V. Churaev. CRC Press. 2000. 338 p.

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### GENERAL CHARACTERISTICS, CLASSIFICATION, PRODUCTION AND PROPERTIES OF MEMBRANES.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The initial sections of the lecture describe membrane classifications in different categories based on porosity and morphology. Further, the membrane properties are categorized based upon their pore size and applications. Thereafter, different membrane materials and fabrication processes are discussed. The lecture will present the classification of membranes according to their chemical structure, polymer membranes, rigid membranes, metal, ceramic, diffusion, dynamic, ion exchange, symmetric and asymmetric, liquid membranes; membranes based on cellulose and its derivatives, membranes made of polyamide, polysulfone, polyimide and other polymers; composite polymer membranes; membrane formation processes and basic requirements for them; general principles of production of polymer membranes; methods of modification of polymer membranes (polymer analogue transformations, graft polymerization); chemical composition and structure of modified membranes; methods of studying the structure and separation properties of polymer membranes; methods of determining porosity and permeability; adsorption studies in the process of membrane separation.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *General characteristics, classification, production and properties of membranes*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Inorganic Membranes Synthesis, Characteristics and Applications*. R. Bhawe. 2012. Springer Science & Business Media. 336 p.

- *Handbook of Industrial Membranes*. K. Scott. 1995. Elsevier. 904 p.

### 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### MEMBRANE STRUCTURE

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The membranes used in the various applications differ widely in their structure and function and the way they are operated in the various membrane processes. The preparation and characterization of porous symmetric, asymmetric and composite membranes made from polymers or inorganic materials to be used in the different membrane processes and applications are described. The preparation of ion-exchange membranes and supported and unsupported liquid membranes containing specific carrier components and other special property membranes is also discussed. The lecture will present structural design of membranes; chemical design of membrane materials; physical construction of separation membranes; symmetric non-porous and porous membranes; asymmetric and composite membranes; relation between structure and preparation condition of membrane; kind of polymer material; polymer concentration in casting solution; casting solvent; combination of casting solvent; addition of additive in casting solution; temperature of casting solution; casting condition; temperature and humidity during casting; gelation condition; gelation period and temperature; the kind of gelation medium; method of heat treatment; temperature and period of heat treatment; pressure treatment; elongation treatment; post-solvent treatment; structure of liquid membranes; bulk liquid membrane; emulsion liquid membrane; supported liquid membrane; thin-porous-film-supported liquid membrane; hollow-fibre-supported liquid membrane; structure of inorganic membranes.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Membrane structure*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Membrane structure and its correlation with membrane permeability*. W. Pusch, A. Walch. 1982. Journal of Membrane Science. Vol. 10, Iss. 2-3, P. 325-360. [https://doi.org/10.1016/S0376-7388\(00\)81417-9](https://doi.org/10.1016/S0376-7388(00)81417-9)
- *Polymer membrane formation through the thermal-inversion process. 1. Experimental study of membrane structure formation*. Gerard T. Caneba and David S. Soong. 1985. Macromolecules. 18, 12. P. 2538-2545. <https://doi.org/10.1021/ma00154a031>

- *Effects of membrane structure and operational variables on membrane distillation performance.* Vasiliki Karanikola, Andrea F. Corral, Hua Jiang, A. Eduardo Sáez, Wendell P. Ela, Robert G. Arnold. 2017. Journal of Membrane Science. Vol. 524. P. 87-96.  
<https://doi.org/10.1016/j.memsci.2016.11.038>

## 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

**MEMBRANE METHODS OF SEPARATION OF MIXTURES. DIALYSIS AND REVERSE OSMOSIS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to describe dialysis and reverse osmosis. Separations of liquids and gases are commonly accomplished using membrane separation methods which include dialysis, reverse osmosis, ultrafiltration and microfiltration. Reverse osmosis and normal osmosis (dialysis) are directly related processes. In simple terms, if a permselective membrane (i.e. a membrane freely permeable to water, but much less permeable to salt) is used to separate a salt solution from pure water, water will pass through the membrane from the pure-water side of the membrane into the side less concentrated in water (salt side). This process is called normal osmosis. If a hydrostatic pressure is applied to the salt side of the membrane, the flow of water can be retarded and, when the applied pressure is sufficient, the flow ceases. In selective examples the application of the mature membrane processes such as reverse osmosis and dialysis in water desalination and purification and in the chemical industry or food and drug production are described and energy requirements and process costs of a given plant capacity are estimated.

The lecture will present features of the dialysis and reverse osmosis; principle of diffusion dialysis; membranes for diffusion dialysis; membranes and technology of donnan dialysis; neutralization dialysis; piezodialysis; membranes for piezodialysis; principle of reverse osmosis; materials and structures of reverse osmosis membranes; concentration polarization and fouling; membrane cleaning.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *membrane methods of separation of mixtures such as dialysis and reverse osmosis*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Membrane separations. Rate controlled separation processes*. Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.
- *Membrane separation technologies: current developments*. Kamallesh K. Sirkar. 1996. Chemical Engineering Communications. Vol. 157, Iss. 1. P. 145-184. <https://doi.org/10.1080/00986449708936687>

- *Membrane Separation Technology for Wastewater Treatment and its Study Progress and Development Trend*. Jianwen Gao. 2016. 4th International Conference on Mechanical Materials and Manufacturing Engineering (MMME 2016). 4 p.
- *Membrane Separation Technology: An Overview*. Zhongde Deng. 2023. Journal of Membrane Science & Technology. Vol. 12, Iss. 6. 12:283.
- *Short Review of Salt Recovery from Reverse Osmosis Rejects*. Boopathy Ramasamy. From the edited volume Salt in the Earth. Edited by Mualla Cengiz Çinku and Savas Karabulut 2019. DOI: 10.5772/intechopen.88716

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### MEMBRANE METHODS OF SEPARATION OF MIXTURES. ULTRAFILTRATION AND MICROFILTRATION.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to describe ultrafiltration and microfiltration. Separations of liquids and gases are commonly accomplished using membrane separation methods which include dialysis, reverse osmosis, ultrafiltration and microfiltration. Microfiltration and ultrafiltration are both processes by which a contaminated liquid is passed through a semipermeable membrane that removes solids too large to fit through the membrane's pore size, yielding a purified liquid stream. To what degree the stream is purified depends on the contaminants present and the pore size of the membrane. Ultrafiltration and microfiltration are generally used for pretreating industrial process streams prior to further separation, purifying various types of streams for potable water generation, treating waste to meet effluent regulations, and performing other applicable separation processes, such as refining oil and concentrating proteins like whey. These membrane filtration units come in various configurations and materials.

The lecture will present features of the ultrafiltration; fundamental analysis of ultrafiltration; phenomenological treatment of membrane permeation; pore model; rejection rate and concentration polarization; concentration magnification and rejection rate; molecular weight cut-off; batch-style concentration; membranes for ultrafiltration; ultrafiltration modes; batch concentration; multistage continuous concentration; batch diafiltration; continuous diafiltration; concentration polarization in ultrafiltration; fouling in ultrafiltration; ultrafiltration technology; modules of ultrafiltration; ultrafiltration applications; drinking water; protein concentration; wastewater; recycling of water; oil and gas wastewater treatment; chemical solutions; wine production; principle of microfiltration; fundamental analysis of microfiltration; dead-end filtration; crossflow filtration; membranes for microfiltration; membrane materials; polymer membranes; inorganic membranes; fouling in microfiltration; module of microfiltration; plate-and-frame module; spiral-wound module; microfiltration technology; water treatment; dairy industry; sterilization; virus removal; oil refining.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *membrane methods of separation of mixtures such as ultrafiltration and microfiltration*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Membrane separations. Rate controlled separation processes.* Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.
- *Membrane separation technologies: current developments.* Kamalesh K. Sirkar. 1996. Chemical Engineering Communications. Vol. 157, Iss. 1. P. 145-184. <https://doi.org/10.1080/00986449708936687>
- *Membrane Separation Technology for Wastewater Treatment and its Study Progress and Development Trend.* Jianwen Gao. 2016. 4th International Conference on Mechanical Materials and Manufacturing Engineering (MMME 2016). 4 p.
- *Ultrafiltration and Microfiltration Handbook.* Munir Cheryan. 1998. CRC Press. 552 p.
- *Physicochemical aspects of polymer selection for ultrafiltration and microfiltration membranes.* E.R. Cornelissen, Th. van den Boomgaard, H. Strathmann. 1998. Colloids and Surfaces A: Physicochemical and Engineering Aspects. Vol. 138, Iss. 2–3. P. 283-289. [https://doi.org/10.1016/S0927-7757\(96\)03862-9](https://doi.org/10.1016/S0927-7757(96)03862-9)

## 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### ION EXCHANGE MEMBRANE PROCESSES. ELECTRODIALYSIS.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will describe electromembrane processes and how to model them in a basic way. Electrodialysis is taken as the starting point. Electrodialysis is a complex process in terms of modeling, since three different driving forces are intrinsically present in the system: the electrical potential, which is the applied driving force, but due to the concentration changes related to the separation itself, concentration differences and (osmotic) pressure differences also occur as driving forces for transport through membranes. In electrodialysis, simple cation and anion exchange membranes are sandwiched between two electrodes, and spacers are used to separate different chambers. Under the application of an electrical field, the ions pass from the membranes and move towards opposite electrodes. Aspects of ion permeation, water transport, and permselectivity are considered, as well as the efficiency of the process in terms of electrical energy use. The focus in this lecture is on macroscopic modeling, that is, understanding the process performance from an overall perspective.

Various related processes and materials are also described: transport through ion exchange membranes; chemistry of ion exchange membranes; homogeneous membranes; heterogeneous membranes; concentration polarization and limiting current density; current efficiency and power consumption; system design; electrodialysis applications; brackish water desalination; salt recovery from seawater; other electrodialysis separation applications; continuous electrodeionization and ultrapure water; bipolar membranes; fuel cells; membranes in chlor-alkali processes.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *ion exchange membrane processes and electrodialysis*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Ion Exchange Membranes: Fundamentals and Applications*. Yoshinobu Tanaka. 2015. Elsevier. 522 p.

- *Membrane separations. Rate controlled separation processes*. Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.

- *Membrane separation technologies: current developments*. Kamalesh K. Sirkar. 1996. *Chemical Engineering Communications*. Vol. 157, Iss. 1. P. 145-184. <https://doi.org/10.1080/00986449708936687>
- *Membrane Separation Technology for Wastewater Treatment and its Study Progress and Development Trend*. Jianwen Gao. 2016. 4th International Conference on Mechanical Materials and Manufacturing Engineering (MMME 2016). 4 p.
- *Chapter 7 - Ion-exchange membrane systems—Electrodialysis and other electromembrane processes*. Bart Van der Bruggen. *Fundamental Modelling of Membrane Systems. Membrane and Process Performance*. 2018. P. 251-300. <https://doi.org/10.1016/B978-0-12-813483-2.00007-1>
- *Recent developments on ion-exchange membranes and electro-membrane processes*. R.K. Nagarale, G.S. Gohil, Vinod K. Shahi. 2006. *Advances in Colloid and Interface Science*. Vol. 119, Iss. 2–3. P. 97-130. <https://doi.org/10.1016/j.cis.2005.09.005>
- *Electrodialytic Membrane Processes and their Practical Application*. H. Strathmann. 1994. *Studies in Environmental Science*. Vol. 59. P. 495-533. [https://doi.org/10.1016/S0166-1116\(08\)70563-6](https://doi.org/10.1016/S0166-1116(08)70563-6)

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

#### MEMBRANE REACTOR

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

A membrane reactor is a physical device that combines chemical conversion and membrane separation processes to add reactants or remove reaction products. Chemical reactors that use membranes are commonly referred to as membrane reactors. Membranes can be used for a variety of tasks. Separation; Selective extraction of products; Catalyst retention; Reactant dispensing/dosing; Catalyst support (often combined with reactant distribution). Membrane reactors are an example of combining two unit operations in one step (eg membrane filtration with chemical reaction). By integrating the reaction section and selective extraction of the reactants, conversion rates can be improved compared to equilibrium values. This property makes membrane reactors suitable for carrying out equilibrium-limited endothermic reactions. During the lecture, students will learn about the concept of membrane reactors; membranes for membrane reactors; inorganic membranes; metal membranes; ceramic membranes; zeolite membranes; carbon membranes; polymer membranes; technology of membrane reactors; catalytic membrane reactors; biocatalyst-immobilized polymer membranes; technology of biocatalyst-immobilized polymer membranes in membrane reactors; polymer-metal complex membranes; polymer catalysis membranes; ion-exchange resins and ion-exchange membranes in membrane reactor; metal membranes; ceramic membranes; polymer-metal composite membranes; membrane reactor with pervaporation and evaporation.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Membrane reactor*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chapter 13 - Membrane Reactor*. Endre Nagy. Basic Equations of Mass Transport Through a Membrane Layer (Second Edition). 2019. P. 369-380. <https://doi.org/10.1016/B978-0-12-813722-2.00013-3>
- *Catalytic Membrane Reactors: The Industrial Applications Perspective*. Catia Algeri, Gerardo Coppola, Debolina Mukherjee et al. 2021. Catalysts. Vol. 11, Iss. 6. P. 691; <https://doi.org/10.3390/catal11060691>



- *The Principle of Membrane Reactors*. Giorno, L. In: Encyclopedia of Membranes. Drioli, E., Giorno, L. (eds) 2015. Springer, Berlin, Heidelberg. [https://doi.org/10.1007/978-3-642-40872-4\\_2232-1](https://doi.org/10.1007/978-3-642-40872-4_2232-1)
- *Handbook of Membrane Reactors. Reactor Types and Industrial Applications*. Edited by: Angelo Basile. 2013. Woodhead Publishing. 937 p. ISBN 978-0-85709-415-5
- *Chapter 6 - Performance of Reactors with PMs*. Mohammad R. Rahimpour, Leila Mahmoodi. Current Trends and Future Developments on (Bio-) Membranes. Photocatalytic Membranes and Photocatalytic Membrane Reactors. 2018. P. 173-188. <https://doi.org/10.1016/B978-0-12-813549-5.00006-2>

## 6. Additional notes

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## Course content – laboratory classes

### Topics 1 – Lab 1

#### 1. The subject of the laboratory classes

##### STUDY OF THE MICROFILTRATION PROCESS

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study of the influence of the filtration condition and membrane properties on the process kinetic parameters. Students will perform the suspension filtration process at given pressure drop values on both sides of the filter partition or different suspension concentrations, calculate the parameters of the filtering process: speed, constants of the filtering process, specific filter performance, specific resistance of the sediment, resistance of the filter partition. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

#### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Principle of Microfiltration; Membranes for Microfiltration; Membrane Materials; Microfiltration Technology*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Principle of Microfiltration; Membranes for Microfiltration; Membrane Materials; Microfiltration Technology*, including critical analysis, synthesis, and conclusions.

#### 4. Necessary equipment, materials, etc

- membranes,
- installation for microfiltration,
- vacuum pump,
- finely dispersed powders for preparation of suspensions,
- magnetic stirrer,
- computer laboratory

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of principle of microfiltration; fundamental analysis of microfiltration; dead-end filtration; crossflow filtration; membranes for microfiltration; membrane materials; polymer membranes; inorganic membranes; fouling in microfiltration; module of microfiltration; plate-and-frame module; spiral-wound module; microfiltration technology,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- 3 – *Microfiltration*. Catherine Charcosset. Membrane Processes in Biotechnology and Pharmaceutics. 2012. P. 101-141. <https://doi.org/10.1016/B978-0-444-56334-7.00003-4>
- *Membrane separations. Rate controlled separation processes*. Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.
- *Ultrafiltration and Microfiltration Handbook*. Munir Cheryan. 1998. CRC Press. 552 p.
- *Physicochemical aspects of polymer selection for ultrafiltration and microfiltration membranes*. E.R. Cornelissen, Th. van den Boomgaard, H. Strathmann. 1998. Colloids and Surfaces A: Physicochemical and Engineering Aspects. Vol. 138, Iss. 2–3. P. 283-289. [https://doi.org/10.1016/S0927-7757\(96\)03862-9](https://doi.org/10.1016/S0927-7757(96)03862-9)

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),

- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

#### ANALYSIS OF POROUS GRANULAR MATERIAL

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will analyze of porous granular material, determinate of bulk, imaginary and true density of bulk material, calculate of porosity of granular material, manufacture membrane by pressing the granular material, determination of its characteristics by the filtering method. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Analysis properties of porous material*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Analysis properties of porous material*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- graduated glass test tube with grinding,
- water jet pump,
- dryer,
- magnetic stirrer,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,

- discussion (checking students' knowledge) of methods of porous bodies investigation; determination of pore sizes by filtration method; capillary impregnation; mechanism of transfer of gases and components of solutions in porous bodies,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Pore classification in the characterization of porous materials: A perspective*. Borislav D. Zdravkov, Jiri J. Cermak, Martin Sefara, Josef Janku. 2007. Central European Journal of Chemistry. Vol. 5, Iss. 2. P. 385–395. DOI: 10.2478/s11532-007-0017-9
- *Quantifying three-dimensional bodies and throats of particulate system pore space*. Nimisha Roy, J. David Frost, M. Mahdi Roozbahani. 2023. Powder Technology. Vol. 415. 118160. <https://doi.org/10.1016/j.powtec.2022.118160>
- *Drying and Wetting of Capillary Porous Materials: Insights from Imaging and Physics-based Modeling*. Habilitationsschrift. Abdolreza Kharaghani. 1980. 154 p. [https://opendata.uni-halle.de/bitstream/1981185920/32881/1/Kharaghani\\_Abdolreza\\_Habil\\_2020.pdf](https://opendata.uni-halle.de/bitstream/1981185920/32881/1/Kharaghani_Abdolreza_Habil_2020.pdf)
- *Adsorption and capillary condensation in porous media: Liquid retention and interfacial configurations in angular pores*. Markus Tuller, Dani Or, and Lynn M. Dudley. 1999. Water Resources Research. Vol. 35, No. 7. P. 1949-1964. <https://agupubs.onlinelibrary.wiley.com/doi/epdf/10.1029/1999WR900098>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

**ULTRAFILTRATION STUDY OF THE PERMEABILITY OF CELLULOSE ACETATE MEMBRANES.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will investigate the permeability of cellulose acetate membranes by the method of ultrafiltration under different pressure drops and different concentrations of water-soluble polymers, calculate the parameters of the ultrafiltration process. Students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions about the possibility of using the polymer to change of membranes properties. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Ultrafiltration process*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Ultrafiltration process*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- membranes
- installation for ultrafiltration,
- vacuum pump,
- water-soluble polymers,
- magnetic stirrer,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of features of the ultrafiltration; phenomenological treatment of membrane permeation; pore model; rejection rate and concentration polarization; membranes for ultrafiltration; concentration polarization and fouling in ultrafiltration; ultrafiltration technology,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Membrane separations. Rate controlled separation processes.* Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.
- *Membrane separation technologies: current developments.* Kamallesh K. Sirkar. 1996. Chemical Engineering Communications. Vol. 157, Iss. 1. P. 145-184. <https://doi.org/10.1080/00986449708936687>
- *Ultrafiltration and Microfiltration Handbook.* Munir Cheryan. 1998. CRC Press. 552 p.
- *Physicochemical aspects of polymer selection for ultrafiltration and microfiltration membranes.* E.R. Cornelissen, Th. van den Boomgaard, H. Strathmann. 1998. Colloids and Surfaces A: Physicochemical and Engineering Aspects. Vol. 138, Iss. 2–3. P. 283-289. [https://doi.org/10.1016/S0927-7757\(96\)03862-9](https://doi.org/10.1016/S0927-7757(96)03862-9)
- *Ultrafiltration membranes — characterization methods.* G. Capannelli, F. Vigo, S. Munari. 1983. Journal of Membrane Science. Vol. 15, Iss. 3. P. 289-313. [https://doi.org/10.1016/S0376-7388\(00\)82305-4](https://doi.org/10.1016/S0376-7388(00)82305-4)

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

#### STUDY OF THE MEMBRANE APPARATUS OPERATION

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the membrane apparatus operation. Students will investigate the operation of the membrane apparatus, the structure of the membrane apparatus, the flat-chamber ultrafiltration module, the influence of the concentration of surface-active substances on the process parameters. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Membrane apparatus and ultrafiltration*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Membrane apparatus and ultrafiltration*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- membrane apparatus with the flat-chamber ultrafiltration module,
- membranes,
- solutions of surface-active substances,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,

- discussion (checking students' knowledge) of theoretical foundations of mass transfer; physical modeling of membrane processes; the influence of the processes of adsorption, polarization, complexation and gelation on the membrane's properties; influence of pressure on the process of membrane separation; structure of the membrane apparatus; ultrafiltration,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Nanocomposite Membranes for Water and Gas Separation. A volume in Micro and Nano Technologies Chapter 1 - Overview of membrane technology.* Asad Asad, Dan Sameoto, Mohtada Sadrzadeh. 2020. Micro and Nano Technologies. P. 1-28. <https://doi.org/10.1016/B978-0-12-816710-6.00001-8>
- *Science and Technology of Separation Membranes.* Tadashi Uragami. Wiley. 2017. 848 p. ISBN: 978-1-118-93256-8.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

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## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### SOLS PURIFICATION BY DIALYSIS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will learn in practice physico-chemical basics of dialysis and ultradialysis. Students will make polymer membranes, purify the sols of gelatin, starch, and iron hydroxide by dialysis and ultradialysis methods, determine the diffusion rates of low molecular weight impurities through the membrane. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Dialysis and ultradialysis*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Sols purification by dialysis*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- polymer for membranes preparing,
- installation for dialysis,
- sols of gelatin, starch, or iron hydroxide,
- magnetic stirrer,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:



- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of features of the dialysis and ultradialysis methods; principle of diffusion dialysis; membranes for diffusion dialysis,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Membrane separations. Rate controlled separation processes.* Marco Mazzotti, Matteo Gazzani, Federico Milella, Paolo Gabrielli. 2016. ETH ZURICH — HS. Note for students. 86 p.
- *Membrane separation technologies: current developments.* Kamallesh K. Sirkar. 1996. Chemical Engineering Communications. Vol. 157, Iss. 1. P. 145-184. <https://doi.org/10.1080/00986449708936687>
- *Handbook of Dialysis.* John T. Daugirdas, Peter G. Blake, Todd S. Ing. 2012. Lippincott Williams & Wilkins. 800 p.
- *Dialysis Membranes Today.* Bowry S.K. 2002. The International Journal of Artificial Organs. Vol.25, Iss.5. P. 447-460. doi:[10.1177/039139880202500516](https://doi.org/10.1177/039139880202500516)

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+

71 - 80 points = C  
66 - 70 points = D+  
61 - 65 points = D  
0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

#### ELECTRODIALYSIS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the ion exchange membrane processes and the basic principles of the electrodialysis method, anion- and cation-selective membranes. Students will study the scheme of the electrodialyzer, calculate of concentration distribution in the deionization section, manufacture of anion- and cation-selective membranes, determine of the ion-exchange capacity of a membrane. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. The completed experiment will be the basis for developing a report on the exercises.

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *ion exchange membrane processes*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrodialysis*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- anion- and cation-selective membranes,
- installation for electrodialysis,
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,

- discussion (checking students' knowledge) of ion exchange membranes; chemistry of ion exchange membranes; homogeneous membranes; heterogeneous membranes; concentration polarization and limiting current density; system design; electro dialysis applications; brackish water desalination; other electro dialysis separation applications,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Ion Exchange Membranes: Fundamentals and Applications*. Yoshinobu Tanaka. 2015. Elsevier. 522 p.
- *Chapter 7 - Ion-exchange membrane systems—Electrodialysis and other electromembrane processes*. Bart Van der Bruggen. *Fundamental Modelling of Membrane Systems. Membrane and Process Performance*. 2018. P. 251-300. <https://doi.org/10.1016/B978-0-12-813483-2.00007-1>
- *Recent developments on ion-exchange membranes and electro-membrane processes*. R.K. Nagarale, G.S. Gohil, Vinod K. Shahi. 2006. *Advances in Colloid and Interface Science*. Vol. 119, Iss. 2–3. P. 97-130. <https://doi.org/10.1016/j.cis.2005.09.005>
- *Electrodialytic Membrane Processes and their Practical Application*. H. Strathmann. 1994. *Studies in Environmental Science*. Vol. 59. P. 495-533. [https://doi.org/10.1016/S0166-1116\(08\)70563-6](https://doi.org/10.1016/S0166-1116(08)70563-6)

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**NANOMATERIALS AND NANOTECHNOLOGIES IN ECOLOGY**

**Code: NNE**



## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### NANOMATERIALS AND NANOTECHNOLOGY

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Nanomaterials and nanotechnologies are increasingly used in all fields at the current stage of development of human society. Therefore, the amount of information about the benefits and at the same time the harmfulness of such implementations and the production itself is increasing.

During the lecture on nanomaterials and nanotechnologies, modern aspects of the production and use of nanomaterials will be presented, which indicate the need to modernize the technologies for the production of such materials, as well as the need for their use for the purification of air, water and soil resources. Students must systematize their knowledge of the physical and chemical properties of nanomaterials and their importance in environmental protection at the current stage.

During the lecture, students will learn that in connection with the wide use of nanomaterials and nanotechnologies at the current stage of the development of civilization, there are a large number of issues related to environmental protection.

#### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to nanomaterials, nanotechnology and environmental pollution.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. H. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter 2, Wiley, 2017, pp. 21–146, [https://doi.org/ 10.1002/9783527698158](https://doi.org/10.1002/9783527698158).

2. M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.

Additional, optional literature:

1. S. Lu, L. Liu, H. Demissie, G. An, D. Wang, Design and application of metal-organic frameworks and derivatives as heterogeneous Fenton-like catalysts for organic wastewater treatment: a review, *Environ. Int.* 146 (2021), <https://doi.org/10.1016/j.envint.2020.106273>.
2. M. Suh, S. Weon, R. Li, P. Wang, J. Kim, Enhanced pollutant adsorption and regeneration of layered double hydroxide-based photoregenerable adsorbent, *Environ. Sci. Technol.* 54 (2020) 9106–9115.
3. A. Belgada, B. Achiou, S. Alami Younssi, F.Z. Charik, M. Ouammou, J.A. Cody, R. Benhida, K. Khaless, Low-cost ceramic microfiltration membrane made from natural phosphate for pretreatment of raw seawater for desalination, *J. Eur. Ceram. Soc.* 41 (2021) 1613–1621.
4. M. Nasrollahzadeh, M. Sajjadi, S. Irvani, R.S. Varma, Carbon-based sustainable nanomaterials for water treatment: state-of-art and future perspectives, *Chemosphere* 263 (2021) 128005, <https://doi.org/10.1016/j.chemosphere.2020.128005> (Internet).

## 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### NANOMATERIALS BASED ON METALS AND METAL OXIDES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

With the expansion of the use of nanomaterials and nanotechnologies, it is important to make maximum use of various materials and their physical and chemical properties.

Nanomaterials are modern materials of different nature, with different properties and different areas of application. A separate large group consists of nanomaterials based on metals or their oxides. It is important to modernize the processes of obtaining such materials, as well as to expand their practical use in relation to the problems of environmental pollution.

During the lecture, students will learn about methods of obtaining nanomaterials based on metals and their oxides. They will receive information about the special properties of such materials, as well as the impact of the technologies of their production and use on the components of the biosphere.

During the lecture, students will also learn about the methods and approaches of using nanomaterials based on metals and their oxides to solve environmental pollution issues.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to methods of preparation, properties and use of nanomaterials based on metals and their oxides.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. H. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter 2, Wiley, 2017, pp. 21–146, <https://doi.org/10.1002/9783527698158>.
2. M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.

3. - Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

Additional, optional literature:

1. C. Zhang, B. Xie, Y. Zou, D. Zhu, L. Lei, D. Zhao, H. Nie, Zero dimensional, one-dimensional, two-dimensional and three dimensional biomaterials for cell fate regulation, *Adv. Drug Deliv. Rev.* (2018), <https://doi.org/10.1016/j.addr.2018.06.020>.

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### THE MAIN AREAS OF APPLICATION OF NANOMATERIALS AND NANOTECHNOLOGIES IN ECOLOGY

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Scientific and technological progress led to the aggravation of problems related to environmental pollution. This is the pollution of water, air, and soil resources. Undoubtedly, these problems are caused by the expansion of production of various materials.

The production and use of nanomaterials is extremely diverse and is expanding every time. At the same time, it can be dangerous for the environment and people. At the lecture, students will be introduced to the main methods of obtaining and analyzing nanomaterials of various nature and purpose. During the lecture, the audience will get acquainted with the features of metal-organic materials, double hydroxides, membranes, modified nanoparticles and the possibility of their use for air, water and soil purification.

Students will also receive information about ways to reduce the negative impact on environmental pollution regarding the use of nanomaterials and nanotechnologies for various purposes.

### 3. Learning outcomes

Able to use information from lectures, literature and other available sources, interpret and critically evaluate it, draw conclusions, formulate and solve problems related to anthropogenic impact on the environment during the synthesis and use of nanomaterials of various nature and purpose.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. E. Gulcay, I. Erucar, Metal-organic frameworks for biomedical applications, in: Two-Dimensional Nanostructures for Biomedical Technology, Elsevier, 2020, pp. 173–210, <https://doi.org/10.1016/C2018-0-00949-4>.

2. M. Suh, S. Weon, R. Li, P. Wang, J. Kim, Enhanced pollutant adsorption and regeneration of layered double hydroxide-based photoregenerable adsorbent, *Environ. Sci. Technol.* 54 (2020) 9106–9115.
3. K. Muramatsu, S. Hayashi, Y. Kuroda, Y. Oka, H. Wada, A. Shimojima, K. Kuroda, Selective covalent modification of layered double hydroxide nanoparticles with tripodal ligands on outer and interlayer surfaces, *Inorg. Chem.* 59 (9) (2020) 6110–6119, <https://doi.org/10.1021/acs.inorgchem.0c00192>.
4. G.S. dos Reis, B.G. Cazacliu, A. Cothenet, P. Poullain, M. Wilhelm, C.H. Sampaio, E.C. Lima, W. Ambros, J.-M. Torrenti, Fabrication, microstructure, and properties of fired clay bricks using construction and demolition waste sludge as the main additive, *J. Clean. Prod.* 258 (2020) 120733.

## 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### USE OF NANOTECHNOLOGIES IN SOIL RESTORATION PROCESSES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The problems of soil pollution are among the global ones at the current stage of the development of civilization. Along with the improvement of cleaning methods, it is important to use the capabilities of nanotechnology for this purpose.

The production and use of various nanomaterials is accompanied by a negative impact on the environment, in particular, soils. Sources and scales of pollution can be very diverse. Therefore, one of the main tasks facing humanity today is the creation of modern safe technologies for the production of nanomaterials, as well as their use. The number of pollutants increases every year. Their nature and influence on the lithosphere is changing. Modern nanotechnology and nanomaterials can also be used to solve these problems. This applies, in particular, to the use of nanocomposites based on graphene and others.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the production and use of various nanomaterials and soil pollution.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. J.V.F.L. Cavalcanti, T.J.M. Fraga, V.F. de Lima, D.F. Dos Santos e Silva, M.D.A. Loureiro Leite, C.W.A. do Nascimento, et al., Advanced oxidation of polycyclic aromatic hydrocarbons in soils contaminated with diesel oil at pilot-scale, Chem. Eng. Technol. (3) (2021). ceat.202000244 (Internet]). Available from: <https://onlinelibrary.wiley.com/doi/10.1002/ceat.202000244>.
2. J.V.F.L. Cavalcanti, T.J.M. Fraga, M.D.A. Loureiro Leite, D.F. dos Santos e Silva, V.F. de Lima, A.R.P. Schuler, et al., In-depth investigation of sodium percarbonate as oxidant of PAHs from soil contaminated with diesel oil, Environ. Pollut. 268 (2021), 115832.



3. A.U. Siddiqui, M.K. Jain, R.E. Mastro, Pollution evaluation, spatial distribution, and source apportionment of trace metals around coal mines soil: the case study of eastern India, Environ. Sci. Pollut. Res. 27 (10) (2020) 10822–10834. (Internet). Available from: <http://link.springer.com/10.1007/s11356-019-06915-z>.

## 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

#### APPLICATION OF NANOTECHNOLOGIES TO RESTORE THE STATE OF NATURAL WATERS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The quality of water resources is very harmful for the life of living organisms, first of all, and then for industrial production and agriculture. Therefore, it is important to use modern technologies for wastewater treatment. In this aspect, it will be interesting to use the achievements of nanotechnology.

The use of nanotechnologies and nanomaterials at the current stage is directly or indirectly related to the pollution of water resources. As a result of pollution of the hydrosphere, its composition and properties change, and therefore, the connection with the functioning of the biosphere. Therefore, one of the main tasks is to create modern productions and modern ways of using nanomaterials and nanotechnologies, where this impact would be minimal.

During the lecture, students will learn about modern methods of water purification from pollutants of various nature using modern nanomaterials, in particular, polymer nanocomposites and modified membranes, as well as nanostructured amorphous alloys.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the pollution of water resources due to the production and use of nanomaterials. And also to propose the use, in particular, of polymer nanocomposites or modified membranes for wastewater treatment.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Belgada, B. Achiou, S. Alami Younssi, F.Z. Charik, M. Ouammou, J.A. Cody, R. Benhida, K. Khaless, Low-cost ceramic microfiltration membrane made from natural phosphate for pretreatment of raw seawater for desalination, *J. Eur. Ceram. Soc.* 41 (2021) 1613–1621.
2. R. Mouratib, B. Achiou, M.E. Krati, S.A. Younssi, S. Tahiri, Low-cost ceramic membrane made from alumina and silica-rich water treatment sludge and its application to wastewater filtration, *J. Eur. Ceram. Soc.* 40 (2020) 5942–5950.
3. L. Xiao, J. Liua, J. Ge, Dynamic game in agriculture and industry cross-sectoral water pollution governance in developing countries, *Agric Water Manage* 243 (2021), <https://doi.org/10.1016/j.agwat.2020.106417>, 106417.

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### APPLICATION OF NANOTECHNOLOGIES AND NANOMATERIALS FOR CLEANING POLLUTED ATMOSPHERIC AIR

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In connection with the growing variety of environmental pollutants, in particular, atmospheric air, it is important to constantly develop and improve methods of air purification. This can be done using nanotechnology.

At the current stage of development, civilization has faced global problems related to air pollution. The emergence of these problems is caused by the production and use of nanomaterials of various nature and purpose, as well as nanotechnologies. The number and variety of environmental pollutants is constantly increasing. However, nanomaterials and nanotechnologies can also be used to clean the air from pollutants of various nature. In particular, organic metal complexes are used for this.

At the lecture, students will get acquainted with the basic environmental requirements for nanochemical production. Problems related to the improvement of nanomaterial synthesis methods and nanotechnologies will be considered. As well as expanding their practical use for air purification.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the production and use of nanomaterials and atmospheric air pollution, as well as methods of its purification.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. H. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter 2, Wiley, 2017, pp. 21–146, <https://doi.org/10.1002/9783527698158>.
3. M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.

## 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### PROBLEMS OF ENVIRONMENTAL POLLUTION ASSOCIATED WITH THE SPREAD OF NANOPARTICLES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Today, the use of nanoparticles in all areas of human activity is becoming more and more widespread. Therefore, it is important to assess the benefits and harms of such innovations. At the current stage of development of human society, environmental pollution is partly related to nanomaterials and nanotechnologies, the spread of nanoparticles. The sources and ways of getting engineered nanoparticles into the environment are constantly expanding and becoming more diverse. It is important to predict the possibilities of accumulation and transformation of nanoparticles in the atmosphere, water and soil, to evaluate the physico-chemical and biological transformations of nanoparticles, as well as to know the level of toxicity caused by nanoparticles.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the entry of nanoparticles into the environment, their accumulation and transformation.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.
2. -Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

#### PROBLEMS OF ENVIRONMENTAL POLLUTION ASSOCIATED WITH THE USE OF NANOTECHNOLOGY AND THE CREATION OF NANOMATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Environmental pollution is becoming more and more diverse both in qualitative and quantitative format. But the sizes of individual pollutants themselves change, in particular, to the size of nanoparticles.

Nanotechnology, as a collection of various methods and techniques, provides the possibility of manipulating matter on the atomic scale of distances and controllable creation and modification of objects smaller than 100 nm, at least in one measurement. As a result, you can get fundamentally new qualities. Nanotechnology is being developed in various fields of science and technology and is one of the main directions of the new stage in the development of human civilization. However, most of the problems of environmental pollution are related to the use of nanotechnology and the creation of nanomaterials of various nature and uses. At the same time, nanomaterials can be actively used in environmental analysis.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the use of nanomaterials for various purposes.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. H. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter 2, Wiley, 2017, pp. 21–146, [https://doi.org/ 10.1002/9783527698158](https://doi.org/10.1002/9783527698158).
2. M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.

3. -Green Nanomaterials, Processing, Properties, and Applications. Edited by Shakeel Ahmed, Wazed Ali, Springer Nature Singapore Pte Ltd. 2020, <https://doi.org/10.1007/978-981-15-3560-4>

## 6. Additional notes

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## Course content – laboratory classes

### Lab 1

#### 1. The subject of the laboratory classes

##### EVALUATION OF MICROHARDNESS AND ELEMENTAL COMPOSITION OF INITIAL AND NANOSTRUCTURED AMORPHOUS ALLOYS BASED ON FE, CO AND AL

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern materials research methods will be tested, in particular, structure determination, determination of microhardness and elemental composition of various samples. The conducted experiment with samples of real objects, in particular amorphous initial and nanostructured alloys, will become the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the determination of microhardness and elemental composition of materials for various purposes, in particular, amorphous metal alloys.

Students can work in groups, assigning tasks and together make a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of final results for laboratories on the elemental composition of materials for various purposes, including critical analysis, synthesis and conclusions.

#### 4. Necessary equipment, materials, etc

- X-ray diffractometer
- scanning electron microscope,
- transmission electron microscope
- a device for measuring microhardness
- computer laboratory

## 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining structure, microhardness and elemental analysis,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. H. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter 2, Wiley, 2017, pp. 21–146, <https://doi.org/10.1002/9783527698158>.

2. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on the study of structure, microhardness and elemental analysis of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 2

### 1. The subject of the laboratory classes

#### STUDY OF THE PHYSICAL AND CHEMICAL PROPERTIES OF MODIFIED POLYMERS OF DIFFERENT COMPOSITION

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of researching the physicochemical properties of polymers and composites will be tested. The conducted experiment with samples of real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to determining the strength, conductivity, degree of swelling of modified composites.

Students can work in groups, assigning tasks and together make a work plan, analyze the results and draw conclusions. May also prepare a theoretical introduction and description of final results for laboratories on the physicochemical properties of composites, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- a device for researching swelling processes
- a device for testing the strength of samples
- a device for studying the conductivity of samples
- a computer
- reagents and chemical utensils.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - reading,

a set of practical methods - a laboratory exercise/experiment; observation

a. Laboratory classes are conducted using special research equipment and specialized software.

b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.

in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining the strength and conductivity of composites, the degree of swelling,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals for studying the physical and chemical properties of composites

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A



91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 3

### 1. The subject of the laboratory classes

#### DETERMINATION OF THE LIMIT OF STRENGTH OF MATERIALS OF DIFFERENT NATURE AND PURPOSE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of studying the mechanical properties of materials of various nature and purpose will be tested. The performed experiment with samples of different nature will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, sharing tasks and working together. They must draw up a work plan, analyze the results, and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of mechanical properties of materials of various compositions

Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the study of mechanical properties of materials of different compositions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- samples of materials of different composition
- installation for studying mechanical properties
- tearing machine
- a computer

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of studying the mechanical properties of materials of various nature,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. - Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>

Additional, optional literature:

- any textbooks or manuals on the study of mechanical properties of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 4

### 1. The subject of the laboratory classes

#### ELECTROCHEMICAL STUDIES OF HYDROGEN RELEASE PROCESSES ON NANOSTRUCTURED AMORPHOUS ALLOYS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern electrochemical methods of materials research will be tested, in particular, in the processes of hydrogen release from alkaline solutions. The conducted experiment with samples of real objects, in particular amorphous initial and nanostructured alloys, will become the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of electrochemical properties of materials for various purposes, in particular, amorphous metal alloys.

Students can work in groups, setting tasks and drawing up a work plan together, analyzing the results and drawing conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the electrochemical parameters of electrodes of different compositions in alkaline solutions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat-galvanostat
- pH meter
- a device for measuring the volume of released gas
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **a laboratory exercise/experiment; observation**

a. Laboratory classes are conducted using special research equipment and specialized software.

b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.

in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of electrochemical research of materials of different composition and purpose,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. <https://www.sciencedirect.com/topics/materials-science/electrochemical-property>
2. Maksym Nizameiev, Oksana Hertsyk, Lidiya Boichyshyn, Physicochemical properties of amorphous and nanocrystalline alloys: Structure, physical-mechanical and corrosion properties of amorphous and nanocrystalline iron-based alloys. – LAP Lambert Academic Publishing, 2022. – 292 p. (ISBN: 978-620-5-52884-6)
3. Nanoobjects & Nanostructuring. Volume I / Edited by Lidiya M. Boichyshyn and Oleksandr. V. Reshetnyak. – Mississauga, Ontario: Nova Printing Inc., 2022. – 160 + xviii p. (ISBN: 978-617-7546-09-1).

Additional, optional literature:

- any textbooks or manuals for the study of electrochemical properties of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),

- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available



## Lab 5

### 1. The subject of the laboratory classes

**WASTEWATER TREATMENT USING NANOSTRUCTURED AMORPHOUS IRON-BASED ALLOYS.  
OBTAINING EDH SPECTRA AND ELECTRONIC MAPS OF SAMPLE SURFACES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of water analysis and purification will be tested. The conducted experiment with samples of nanostructured amorphous alloys of different composition will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the analysis and treatment of water of various origins and pollution

Students can work in a group, dividing the tasks and working together to create a work plan, analyze the results and draw conclusions. Also can prepare a theoretical introduction and description of the final results for laboratories on water analysis and treatment, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- pH meter
- spectrophotometer
- scanning electron microscope,
- transmission electron microscope
- computer
- reagents and chemical utensils

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of water analysis and purification methods,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. <https://sensorex.com/water-purification-methods/>

Additional, optional literature:

- any textbooks or manuals on methods of water analysis and purification

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 6

### 1. The subject of the laboratory classes

#### ELECTROCHEMICAL STUDIES OF INITIAL AND NANOSTRUCTURED AMORPHOUS ALLOYS IN ALKALINE AND ACIDIC SOLUTIONS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern electrochemical methods of materials research, in particular amorphous metal alloys in solutions of various nature, will be tested. The conducted experiment with samples of real objects, in particular amorphous initial and nanostructured alloys, will become the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of electrochemical properties of materials for various purposes, in particular, amorphous metal alloys.

Students can work in groups, together setting tasks and making a work plan, analyzing the results and drawing conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the electrochemical parameters of electrodes of different compositions in alkaline and acidic solutions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat-galvanostat
- pH meter
- scanning electron microscope,
- transmission electron microscope
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **a laboratory exercise/experiment; observation**

- a. Laboratory classes are conducted using special research equipment and specialized software.
- b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.
- in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of electrochemical research of materials of different composition and purpose,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. <https://www.sciencedirect.com/topics/materials-science/electrochemical-property>
2. Electrochemical properties of ternary amorphous alloys based on iron and cobalt in alkali solutions / L.M. Boichyshyn, O.M. Hertsyk, M.M. Lopachak and all. // Mat. Sci. – 2020. – Vol. 55, Is. 5. – P. 703-709. (<https://doi.org/10.1007/s11003-020-00361-w>)
3. Maksym Nizameiev, Oksana Hertsyk, Lidiya Boichyshyn, Physicochemical properties of amorphous and nanocrystalline alloys: Structure, physical-mechanical and corrosion properties of amorphous and nanocrystalline iron-based alloys. – LAP Lambert Academic Publishing, 2022. – 292 p. (ISBN: 978-620-5-52884-6)
4. Nanoobjects & Nanostructuring. Volume I / Edited by Lidiya M. Boichyshyn and Oleksandr. V. Reshetnyak. – Mississauga, Ontario: Nova Printing Inc., 2022. – 160 + xviii p. (ISBN: 978-617-7546-09-1).

Additional, optional literature:

- any textbooks or manuals for the study of electrochemical properties of materials

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 7

### 1. The subject of the laboratory classes

#### ANALYSIS AND PURIFICATION OF WASTEWATER USING ZEOLITE-BASED COMPOSITES FROM CHROMIUM COMPOUNDS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of water analysis and purification using adsorbents of various nature, in particular, celite-based composites, will be tested. Particular attention should be paid to the methods of purification from chromium compounds. The conducted experiment with samples of real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the analysis and purification of water from chromium compounds.

Students can work in groups, assigning tasks and together make a work plan, analyze the results and draw conclusions. May also prepare theoretical introduction and description of final results for water analysis and treatment laboratories, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- pH meter
- spectrophotometer
- scanning electron microscope,
- transmission electron microscope
- computer
- reagents and chemical utensils

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods of analysis and purification of water from chromium compounds,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Zeolite/polyaniline composite: synthesis and adsorptive properties regarding Cr(VI) from aqueous solutions / MS Sydorko, MM Yatsyshyn, IY Marchuk, AA Zelynskii, Polymer Journal 41 (1), 69-78. <https://doi.org/10.15407/polymerj.45.01.069>
2. Nasar A., Mashkoo F. Application of polyaniline-based adsorbents for dye removal from water and wastewater – a review. Environ. Sci. Pollut. Res., 2019, 26: 5333–5356. <https://doi.org/10.1007/s11356-018-3990-y>.
3. Adam M.R., Salleh N.M., Othman M.H.D., Dzarfan M.H., Takeshi M., Hafizi A.M., Hafiz P.M., Ismail A.F., Rahman M.A., Juhana J. The adsorptive removal of chromium (VI) in aqueous solution by novel natural zeolite based hollow fibre ceramic membrane. J. Environ. Manage., 2018, 224: P. 252–262. <https://doi.org/10.1016/j.jenvman.2018.07.043>.

Additional, optional literature:

- any textbooks or manuals on methods of water analysis and purification

Students should prepare a theoretical introduction to the laboratories.



## 7. Additional notes

### - ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Lab 8

### 1. The subject of the laboratory classes

#### ANALYSIS AND PURIFICATION OF WASTEWATER USING POLYMER NANOCOMPOSITES FROM AZO DYES

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of water purification from dyes of various nature will be tested. Particular attention should be paid to methods of cleaning from azo dyes using composites. The conducted experiment with samples of real objects will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the analysis and purification of water from dyes of various nature.

Students can work in groups, setting tasks and drawing up a work plan together, analyzing the results and drawing conclusions. May also prepare theoretical introduction and description of final results for water analysis and treatment laboratories, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- pH meter
- spectrophotometer
- scanning electron microscope,
- transmission electron microscope
- computer
- reagents and chemical utensils

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods of analysis and purification of water from azo dyes,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. King-Thom Chung, Azo dyes and human health: A review // Journal of Environmental Science and Health, Part C . Volume 34, 2016 - Issue 4, P. 233-261.
2. Nasar A., Mashkoo F. Application of polyaniline-based adsorbents for dye removal from water and wastewater – a review. Environ. Sci. Pollut. Res., 2019, 26: 5333–5356. <https://doi.org/10.1007/s11356-018-3990-y>.
3. Mossvi S, Kher X, Madamar D. Isolation, characterization and decoloration of textile dyes by a mixed bacterial consortium. *Dyes and Pigm.* 2007;7(3):723–729. DOI:[10.1016/j.dyepig.2006.05.005](https://doi.org/10.1016/j.dyepig.2006.05.005)

Additional, optional literature:

- any textbooks or manuals on methods of water analysis and purification

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**TESTING OF POLYMERIC CORROSION  
PROTECTION LAYERS**

**Code: TPCPL**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

##### TESTING OF POLYMERIC CORROSION PROTECTION LAYERS: INTRODUCTION

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture, as an introduction to the issue of testing of polymeric corrosion protection layers. In this topic, students get acquainted with the economic and social problems that arise as a result of the corrosion of various types of metal structures, cars and other types of transport, as well as other metal inventory. Students should understand the importance of corrosion science, corrosion mechanisms, modern methods that are actively used to protect against corrosion of metals and alloys, as well as methods of researching the properties of anti-corrosion polymer and similar coatings.

Corrosion is an expensive and potentially dangerous problem in many industries. Corrosion is defined as “an irreversible interfacial reaction of a material (metal, ceramic, polymer) with the environment, resulting in the consumption of the material or the dissolution of a component of the environment in the material” (IUPAC, 2012). Corrosion of metal structures has a significant impact on the global economy and causes significant damage to society as it spoils structural innovations and engineering materials. In the United States alone, costs incurred due to corrosion are estimated to exceed \$500 billion each year. Meanwhile, a study by NACE International estimates that global corrosion costs are estimated at \$2.5 trillion, or 3.4% of global GDP in 2013. In addition, the cost of corrosion control is also very high, with costs in the \$. 276 billion per year.

The term "corrosion control" is used in construction, industry and other industries where the materials used are constantly exposed to chemicals or sea water. The main criterion for using any corrosion control technique is the balance between durability and cost. However, the effectiveness of mechanical methods is limited, since the effectiveness of their prevention depends on the effectiveness of the covering materials and the cost of protecting the structures. To achieve the best possible balance between durability and cost, the following methods are used separately or in combination with each other: - surface coating; - chemical inhibitors; - modified building material.

Knowledge and understanding of the course of corrosion processes, methods of protecting metals from corrosion, and the ability to use modern physico-chemical methods of researching the effectiveness and reliability of various types of protective anti-corrosion coatings of metals and alloys are necessary for the practical solution of problems arising from the corrosion destruction of various metal products and structures.

#### 3. Learning outcomes

Students can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to **the testing of polymeric corrosion protection layers**.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *A Review of Differing Approaches Used to Estimate the Cost of Corrosion, Anti-Corrosion Method and Materials*. Bahaskaran R., Palaniswamy N., Rengaswamy N.S., Jayachandran M. 2005, J. Appl. Sci. Res. 52, 29-41. doi:10.1108/00035590510574899

Additional, optional literature:

- *A review on the assessment of polymeric materials used as corrosion inhibitor of metals and alloys*. Arthur D.E., Jonathan A., Ameh P.O., Anya C. 2013, Int. J. Ind. Chem. 4(2). 1-9. doi:10.1186/2228-5547-4-2
- *Recent Trends in the Characterization and Application Progress of Nano-Modified Coatings in Corrosion Mitigation of Metals and Alloys*. Thakur A., Kaya S., Kumar A. 2023, Appl. Sci. 13, 730. doi:10.3390/app13020730

#### 6. Additional notes



## Topics 2

### 1. The subject of the lecture

**CORROSION OF METALS AND ALLOYS. TYPES OF CORROSION AND THEIR DEPENDENCE ON OPERATING CONDITIONS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic examines types of corrosion and their dependence on operating conditions. Types of corrosion and their dependence on operating conditions. Chemical and electrochemical corrosion of metals. Corrosion of metals in various natural conditions. Atmospheric, gas, underground, marine and biocorrosion of metals. Corrosion of metals when mechanical loads are applied. Corrosion cracking and corrosion fatigue. The influence of various factors on the course of corrosion processes on the surface of metals.

Most corrosion processes are electrochemical. The two primary ubiquitous reactions that keep a corrosion process continuing are hydrogen evolution (prevalent in acidic media) and oxygen reduction (prevalent in neutral or alkaline environments). Corrosion is caused by a variety of factors, the most prevalent of those are the metal's composition, atomic structure, micro, and macroscopic imperfections, and stress response (tensile, compressive, and cyclic); the environment and its chemical nature, quality, and quantity of reactive species, pressure, temperature, the metal-environment interface, metal oxidation, and dissolution kinetics in solution.

For the corrosion of metals and alloys, a different nature of corrosion damage and destruction is possible, depending on many factors. To assess the degree of corrosion destruction, it is customary to use various criteria as indicators.

Corrosion of metals and alloys is a primary concern for engineers. Effective control of corrosion failures cannot involve just using the "right materials", as that may not be practically possible. Taming of environments through inhibitors and application of coatings, electrochemical means such as cathodic and anodic protection, and engineering means like structural design help to mitigate corrosion effectively.

The lecture also pays attention to monitoring corrosion, investigating the nature of corrosion damage to protective coatings of devices and structures, and predicting the service life after eliminating the manifestations of corrosion damage. In all these cases, it is important to understand the phenomena that caused the corrosion damage associated with the interaction of the metal and the environment.

### 3. Learning outcomes

Students can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to corrosion and the nature of corrosion damage to protective coatings of devices and structures, predict service life after elimination of manifestations corrosion damage to metals and alloys.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Engineering Principles and Solved Problems*. Popov B. N. Elsevier 2015, 774 p. doi:10.1016/C2012-0-03070-0
- *Corrosion Failures: Theory, Case Studies, and Solutions*. Elayaperumal K., Raja V. S. 2015, 256 p. ISBN: 978-1-119-04327-0
- *Corrosion inhibitors*. In: Singh A, editor. *Corrosion Inhibitors*. Palanisamy G. [Internet]. London: IntechOpen; 2019 [cited 2022 Dec 29]. Available from:  
- <https://www.intechopen.com/chapters/64392>. doi: 10.5772/intechopen.80542

Additional, optional literature:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Overview of corrosion and its control: A critical review*. Harsimran S., Santosh K., Rakesh K. 2021, Proc. Eng. Sci., 3(1), 13-24. doi: 10.24874/PES03.01.002\i
- *Corrosion of additively manufactured alloys: a review*. Sander G., Tan J., Balan P., et al. 2018, Corrosion. 74(12), 1318-1350. doi:10.5006/2926

#### 6. Additional notes

## Topics 3

### 1. The subject of the lecture

**CHARACTERISTICS OF SURFACE ANTICORROSION COATINGS. MODERN PHYSICAL AND ANALYTICAL METHODS OF STUDYING THE SURFACE, COMPOSITION AND STRUCTURE OF ANTICORROSION COATINGS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topics students get acquainted with a wide range of modern physico-chemical methods of researching the surface of metals and anticorrosion coatings on their surfaces, and also learn some methods that they will use to conduct research during laboratory work.

Control of the quality and reliability of anticorrosion coatings is an extremely important aspect of protecting metals from corrosion damage and destruction. The composition and structure of coatings are established using various physical and analytical methods. Methods range from the use of rudimentary tools such as optical inspection to X-ray analysis.

The composition and structure of the coatings are established by using various physical and analytical techniques. The special features of surface coatings as opposed to bulk materials have led to the modification of some analytical techniques or the development of special analytical techniques. The main objectives of surface analysis and coating characteristics are as follows: measurement coating thickness; surface roughness (contact method, non-contact methods), hardness and microhardness analysis; adhesivity testing; water absorption tests (WAT); contact angle test (CAT); microstructural evaluation (scanning tunnelling microscopy (STM) and atomic force microscopy (AFM); chemical analysis (infra-red spectroscopy (FT-IR-Spectroscopy), X-ray diffraction (XRD), X-ray photo-electron spectroscopy (XPS), energy dispersive X-ray analysis (EDX). Electrochemical characterization of coatings for corrosion protection: open-circuit potential (OCP); electrochemical impedance spectroscopy (EIS); potentiostatic step polarization (PSSP), galvanostatic step polarization (GSSP), cyclic voltammetry (CVA), electrical conductivity (EC).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the results of analyzes of the state of the surface of metals and the results of studies of anti-corrosion properties using the **characteristics of surface anticorrosion coatings by modern physical and analytical methods of researching the surface, composition and structure of protective coatings**. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and description of the final results for the laboratory work based on the research findings, including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description  
a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Characterization of coatings*. Benninghoven A. 1976, Thin Solid Films. 39, 3-23. doi:10.1016/0040-6090(76)90620-9
- *Characterization of surface coatings. Chapter 8*. Batchelor A.W., Loh N.L., Chandrasekaran M. // *Materials Degradation and Its Control by Surface Engineering*. 2011, 287-333. doi:10.1142/9781848165021\_0008

Additional, optional literature:

- *Passivity of Metals Studied by Surface Analytical Methods, a Review*. Strehblow H.-H. S. 2016, *Electrochim. Acta*, 212. doi:10.1016/j.electacta.2016.06.170
- *Review–The Use of Localized Electrochemical Techniques for Corrosion Studies*. Jadhav N., Gelling V. J. 2019, *J. Electrochem. Soc.* 166(11), C3461-C3476. doi:10.1149/2.0541911jes
- *Corrosion of additively manufactured alloys: a review*. Sander G., Tan J., Balan P., et al. 2018, *Corrosion*. 74(12), 1318-1350. doi:10.5006/2926

#### 6. Additional notes

## Topics 4

### 1. The subject of the lecture

#### ELECTROCHEMICAL APPLICATION OF PROTECTIVE POLYMER COATINGS ON STEEL SURFACES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this lecture, students study the methods of electrochemical application of non conductive polymer (polyvinyl acetate, polyacrylamide and other) coatings on the surface of steel and the properties of polymer coatings on the surface of steel.

Structural metals include a wide range of steels: carbon steel (CS), low-carbon steel (LCS), mild steel (MS), low-alloy steel (LAS), stainless steel (SS) and other grades of steel that, depending on the operating conditions, must be selected from corrosion

The application of electrochemical polymerization mechanism, nanostructured coatings, applying organic or inorganic coatings, and cathodic and anodic protection are methods for decreasing corrosion on metallic materials. Polymer coatings of steel devices and structures are the most common type of protection of metals against corrosion. They are mostly used to protect metal parts, structures and buildings from atmospheric corrosion, as well as to protect metals from underground corrosion (pipelines) or from corrosion in electrolytes (ship hulls).

The main role of such coatings as a means of protecting metals from corrosion is to isolate the metal surface from the external environment. The bulk of protective polymer coatings (paint coatings) are applied mechanically, however, the electrochemical method of their application, when polymer coatings are formed on an electrode from initial monomers, is of increasing interest.

The advantage of the electrochemical method lies in the possibility of forming a coating immediately from monomers, as a result of which the polymerization process becomes more economical and makes it possible to easily change the nature and composition of the coating of steel. The active centers responsible for initiating polymerization are formed as a result of the electrode process, so it is very easy to adjust the rate of polymerization by changing the current density. This creates conditions for obtaining polymers with a fairly narrow molecular weight distribution.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical application of protective polymer coatings on steel surfaces. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **electrochemical application of protective polymer coatings on steel surfaces** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Acrylic polymers. Chapter-15.* Umoren S.A., Solomon M.M., Saji V.S. 2022, Polymeric Materials in Corrosion Inhibition. Fundamentals and Applications. 343-372. doi:10.1016/B978-0-12-823854-7.00015-1
- *Vinyl polymers. Chapter-16.* Umoren S.A., Solomon M.M., Saji V.S. 2022, Polymeric Materials in Corrosion Inhibition. Fundamentals and Applications. 373-398. doi:10.1016/B978-0-12-823854-7.00003-5

Additional, optional literature:

- *Anticorrosive coatings: a review.* Sorensen P.A., Kiil S., Dam-Johansen K., Weinell C.E. 2009, J. Coat. Technol. Res. 6(2), 135-176. doi:10.1007/s11998-008-9144-2
- *Electrochemical Characterization of Polymeric Coatings for Corrosion Protection: A Review of Advances and Perspectives.* Trentin A., Pakseresht A., Duran A., et al. 2022, Polymers. 14, 2306. doi:10.3390/polym14122306
- *Corrosion protection by organic coatings: Electrochemical mechanism and novel methods of investigation.* Grundmeier G., Schmidt W., Stratmann M. 2000, Electrochim. Acta. 45, 2515-2533. doi:10.1016/S0013-4686(00)00348-0

#### 6. Additional notes

## Topics 5

### 1. The subject of the lecture

#### ELECTROCHEMICAL APPLICATION OF PROTECTIVE CONDUCTING POLYMER COATINGS ON STEEL SURFACES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

At this topic, students get acquainted with a new class of polymers that have electrical conductivity, study methods of electrochemical coating of conductive polymer on the surface of steel and testing their physico-chemical and anticorrosion properties.

Intrinsically conductive polymer (CP) coatings may be the most common method of corrosion protection for metals. Electrodeposition of CP on the surface of a metal electrode has been a very active area of research in electrochemistry for the past two decades. The advantage of CPs and their composites over other coatings such as paints is that they do not contain toxic substances harmful to the environment. In addition, CP act as both a physical and an electronic barrier, improving the protection provided by other materials that act only as physical barriers. Polymers have a long chain of carbon bonds, therefore, upon adsorption, they are able to block large areas of metal surfaces subject to corrosion.

CP films are applied to the surface of metals by electrochemical methods, namely cyclic voltammetry, chronopotentiometry, chronoamperometry. Electropolymerization application of CP films can be an inexpensive alternative to electrophoretic deposition of protective coatings on the surface of metals. Obtaining good protective layers requires, first of all, the correct passivation of the protected metal and the appropriate choice of electrolyte in terms of its nature and concentration.

Since 1984, CPs have attracted considerable interest as components of corrosion-resistant coatings of various metals and alloys. Electrochemically deposited PAN has been found (DeBerry) to protect stainless steel (SS) with anodic protection. Passivation of SS is usually achieved by chemical or electrochemical coating of the surface with such EPPs. The polymer film passivates the electrode by keeping the potential in the passive region. CPs cause oxide formation on the metal surface, repairing the chemical degradation of the metal/oxide interface. To date, two forms of PAN have been most thoroughly investigated in anticorrosive coatings: the non-conductive emeraldine base (EB, half-oxidized form) and the electrically conductive emeraldine salt (ES, half-oxidized and protonated form), respectively. Emerald salt is the most stable form of PAN, which is obtained by chemical or electrochemical polymerization of aniline in mainly aqueous solutions of strong inorganic and organic acids, buffer solutions, namely acetate (pH 3.5–5) and phosphate (pH 5). The specific dopant will also affect the synthesis process and the internal molecular properties of the polyaniline.

The results of many studies of the protective properties of PAN coatings have shown that such coatings can have different protection mechanisms depending on the metal used, the synthesis method, corrosive environments and the method of preparation of the coating.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the



electrochemical application of protective conducting polymer (polyaniline) coatings on mild steel surfaces. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **electrochemical application of protective conducting polymer (polyaniline) coatings on steel surfaces** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Corrosion Protection of Metals by Intrinsically Conducting Polymer*. Deshpande P. P., Sazou D. 2016, Taylor & Francis Group, LLC. 224. International Standard Book Number-13: 978-1-4987-0693-3 (eBook - PDF)
- *Coatings based on electronic conducting polymers for corrosion protection of metals*. Baldissera A.F., Ferreira C.A. 2012, Prog. Org. Coat. 75(3), 241-247. doi:10.1016/j.porgcoat.2012.05.004
- *A Review on Conducting Polymer Coatings for Corrosion Protection*. Ates M. 2016, J. Adhes. Sci. Technol. 30, 1510-1536. doi:10.1080/01694243.2016.1150662

Additional, optional literature:

- *Electrochemical Characterization of Polymeric Coatings for Corrosion Protection: A Review of Advances and Perspectives*. Trentin A., Pakseresht A., Duran A., et al. 2022, Polymers. 14, 2306. doi:10.3390/polym14122306
- *Comparison study for passivation of stainless steel by coating with polyaniline from two different acids*. Ganash A.A., Al-Nowaiser F.M., Al-Thabaiti S.A., Hermas A.A. 2011, Prog. Org. Coat. 72(3), 480-485. doi:10.1016/j.porgcoat.2011.06.006
- *Corrosion of mild steel with composite polyaniline coatings using different formulations*. Grgur B.N., Elkais A.R., Gvozdenović M.M., et al. 2015, Prog. Org. Coat. 79, 17-24. doi:10.1016/j.porgcoat.2014.10.013

#### 6. Additional notes



## Topics 6

### 1. The subject of the lecture

#### PROTECTIVE CONDUCTING POLYMER COATINGS OF ALUMINUM SURFACES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic, students get acquainted with a new class of polymers that have electrical conductivity, study methods of electrochemical coating of intrinsically conductive polymers (CPs) on the surface of aluminum and study their physico-chemical and anticorrosion properties.

Approximately 50 years ago, the discovery of a new polymer family, the CPs, motivated the scientific community because of its enormous potential for application. These new materials, also called synthetic metals, can reach high electrical conductivity, very close to the value of some metals. In recent years, a wide variety of CPs have been tested as corrosion inhibitors or coatings; they are usually deposited chemically or electrochemically in their pure form on the metal. These polymers in the undoped (nonconductive) and doped (conductive) states are able to protect metals and alloys from corrosion through various mechanisms, and they are also able to regenerate the metal and the oxide layer if the coating is broken.

CPs and in particular polyaniline (PAn) and polypyrrole (PPI) can be an effective alternative to phosphate-chromate pretreatment of aluminum, which is hazardous due to toxic hexavalent chromium. Aluminum alloys (AA) are widely used in the aerospace industry for airframes and structural materials due to their superior mechanical properties such as, e.g. high strength at low density. However, these alloys are very sensitive to local corrosion and therefore there is an urgent need to prevent their environmental degradation. Moreover, improved environmental performance can be achieved by using nanostructured particles in the coating and eliminating the need for toxic solvents.

Among these CPs, polyaniline is considered one of the best anti-corrosion materials not only because of its environmental resistance, unique ability to control the redox process, simple acid-base doping-dedoping process, rapid transition from one state to another, but also due to the passivation of the metal surface an oxide layer is formed under the coating, which protects the metal from further corrosion.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the protective conducting polymers (polyaniline and polypyrrole) coatings of aluminum surfaces. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and a description of the final results for laboratory work on the preparation of aluminum samples for the **electrochemical deposition of films of polyaniline and polypyrrole and carry out coating of aluminum surfaces**, investigate their physicochemical and anticorrosive properties, including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *A Review on Conducting Polymer Coatings for Corrosion Protection*. Ates M. 2016, J. Adhes. Sci. Technol. 30, 1510-1536. doi:10.1080/01694243.2016.1150662
- *Corrosion Protection of Aluminum and Al-Based Alloys by Polyaniline and Its Composites. Chapter 8*. Reshetnyak O.V., Yatsyshyn M.M. 2017. Computational and Experimental Analysis of Functional Materials. / Oleksandr V. Reshetnyak, Gennady E. Zaikov (Eds.) [Series: AAP Research Notes on Polymer Engineering Science and Technology]. Toronto, New Jersey: Apple Academic Press, CRC Press (Taylor & Francis Group). 287-329

Additional, optional literature:

- *The electrochemical deposition of polyaniline at pure aluminium: electrochemical activity and corrosion protection properties*. Conroy K.G., Breslin C.B. 2003, Electrochim. Acta 48(6), 721-732. doi:10.1016/S0013-4686(02)00741-7
- *Computational and experimental analysis of functional materials*. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. <http://www.appleacademicpress.com/computational-and-experimental-analysis-of-functional-materials-/9781771883429> – chapter

#### 6. Additional notes

## Topics 7

### 1. The subject of the lecture

**POLYANILINE FOR SMART-RESPONSIVE AND SELF-HEALING COATINGS FOR METALS AND THEIR ALLOYS FOR CORROSION PROTECTION**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic deals with smart-responsive and self-healing anti-corrosion coatings of metals and alloys based on conductive polymers and polyaniline (PAn) in particular and study these coatings on the surface of steel and study their physico-chemical and anti-corrosion properties.

Recently, intrinsically conductive polymers (CPs) were investigated and proposed for a wide range of advanced and emerging technological applications. The novel and tremendous applications of CPs originated from (1) the vast synthetic routes that provide fast and scalable synthesis with controlled hierarchical microstructures and nanostructures, and (2) CPs can be practically applied, alone or as nanocomposites, as coatings to create multifunctional smart conductive surfaces or devices, or they can be prepared as standalone smart, thin films.

Among all the polyaniline is one of the most vividly researched one, due to its low-cost monomer, ease of synthesis, environmental stability, unique redox properties, and different oxidation states along with the wide range of applicability.

Recent trends in the production of anticorrosion coatings are based on smart-responsive and self-healing polymers coatings with autonomous self-healing functionality through various mechanisms such as UV radiation and thermal or mechanical loads, or external sensitive mechanisms such as pH, temperature, redox or light. Polyaniline exhibits three different oxidation states: the partially oxidized form emeraldine base (EB) is conductive, while the oxidized base pernigraniline (PB) and the fully reduced leucoemeraldine base (LB) are nonconductive. Due to the presence of these form-states, PAn can be used as an intelligent coating with redox function. In addition, PAn exhibits pH sensitivity during the dedoping process, and the conformation of the polymer chains changes when the environment changes from acidic to alkaline or vice versa.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical application of protective polyaniline coatings on mild steel surfaces. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples **polyaniline for smart-responsive and self-healing coatings for steel corrosion protection** and the investigation of its physicochemical and anticorrosion properties, including critical analysis, synthesis and conclusions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrically conducting polyaniline smart coatings and thin films for industrial applications Chapter-22 Advances in Smart Coatings and Thin Films for Future Industrial and Biomedical Engineering Applications.* Abu-Thabit N. Y. 2020, 585-617. doi:10.1016/B978-0-12-849870-5.00026-4
- *Potential use of smart coatings for corrosion protection of metals and alloys: a review.* Nazeer A.A., Madkour M. 2018, J. Mol. Liq. 253, 11-22. doi:10.1016/j.molliq.2018.01.027
- *Development of nanostructured polyaniline dispersed smart anticorrosive composite coatings.* Alam J., Riaz U., Ahmad S. 2008, Polym. Adv. Technol., 19(7), 882-888. doi:10.1002/pat.1054
- *High Performance Self-Healing Epoxy/Polyamide Protective Coating Containing Epoxy Microcapsules and Polyaniline Nanofibers for Mild Carbon Steel.* Zhang H., Wang J., Liu X., et al. 2013, Ind. Eng. Chem. Res. 52(30), 10172-10180. doi:10.1021/ie400666a

Additional, optional literature:

- *Fundamentals of corrosion inhibition. Chapter-4 Polymeric Materials in Corrosion Inhibition. Fundamentals and Applications.* Umoren S. A., Solomon M. M., Saji V. S. 2022. 103-127. doi:10.1016/B978-0-12-823854-7.00026-6
- *Advances in corrosion protection by organic coatings: What we know and what we would like to know.* Lyon S. B., Bingham R., Mills D. J. 2017. Progr. Org. Coat. 102(A). 2-7. doi:10.1016/j.porgcoat.2016.04.030

## 6. Additional notes

## Topics 8

### 1. The subject of the lecture

**NANOCOMPOSITE ORGANIC-INORGANIC COATINGS FOR CORROSION PROTECTION OF METALS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this topic, students get acquainted with a type of protective anticorrosion coatings - nanocomposite organic-inorganic coatings of the metals, study these coatings on the surface of steel and study their physico-chemical and anticorrosion properties.

In recent decades, nanocomposite organic-inorganic coatings have been widely used to protect metals from corrosion. Conjugated polymer systems (CPs), including polyaniline (PAn), polypyrrole (PPi), etc., are used as organic components of such anti-corrosion coatings. Various oxides, mineral clays, etc. serve as inorganic materials. The most common inorganic components of such protective coatings are montmorillonite (MMT), smectite, halloysite, etc. Clays are the most common inexpensive natural material with high chemical resistance, which allows to increase the barrier properties of polymer coatings.

Research on composites/blends containing PAn has attracted numerous scientists and engineers due to their excellent adhesion and anticorrosive properties. Nano-structured PAn composites and matrix resins play a key role in physical and anticorrosive performance.

Conductive polymers are excellently combined with various materials, including clay, by a fairly simple method, such as the chemical oxidative polymerization of aniline in situ in the presence of clay in the reaction mixture. Due to the layered structure of clays, in particular MMT, in the initial stages, aniline is intercalated in the interlayer areas of organophilic clays, followed by one-stage oxidative polymerization.

Various composite materials, which include organic and inorganic substances, enhance the anticorrosion properties of conductive polymers and PAn, in particular. Thus, the study of anti-corrosion composites/mixtures containing nanostructured PAn is of significant technical and scientific interest.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the nanocomposite organic-inorganic coatings for corrosion protection the surface of metals. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for **nanocomposite organic-inorganic coatings for corrosion protection of steel** and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - informative lecture, monographic lecture, description

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Nanocomposite organic coatings for corrosion protection of metals: a review of recent advances*. Nazari M.H., Zhang Y., Mahmoodi A., et al. 2022, Prog. Org. Coat. 162, 106573. doi:10.1016/j.porgcoat.2021.106573
- *Polymer nanocomposites in corrosion control*. Weng, C.-J., Chang C.-H., Yeh J.-M 2012, Corrosion Protection and Control Using Nanomaterials. 330-356. doi:10.1533/9780857095800.2.330
- *The potential of nanocomposite-based coatings for corrosion protection of metals: A review*. Randis R., Darmadi D.B., Gapsari F., et al. 2023, J. Mol. Liq. 390(A), 123067. doi:10.1016/j.molliq.2023.123067
- *Nanocomposite Coatings for Anti-Corrosion Properties of Metallic Substrates*. Muresan L.M. 2023, Materials. 16, 5092. doi:10.3390/ma16145092

Additional, optional literature:

- *Composite Coatings with Polyaniline Doped with Different Organic Acids on the Corrosion of Mild Steel*. Grgur B. N., Popović A., Ayad M. 2023, Metals. 13, 1364. doi:10.3390/met13081364
- *Synthesis and characterization of polyaniline-based polymer nanocomposites as anti-corrosion coatings*. Rangel-Olivares F.R., Arce-Estrada E.M., Cabrera-Sierra R. 2021, Coatings. 11(6), 653. doi:10.3390/coatings11060653

#### 6. Additional notes



## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

##### INTRODUCTION TO THE LABORATORY WORKSHOP FROM THE COURSE

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Introduction to the laboratory workshop from the course "Testing of polymeric corrosion protection layers" instruction on the procedure for conducting and performing laboratory work and occupational health and safety. Familiarization with the methods of laboratory research of corrosion of metals and methods of conducting laboratory work. Acquaintance with modern test tests of corrosion coatings of metals and alloys. Acquaintance with basic and auxiliary devices for electrochemical control of the condition of film coatings of metals and alloys. Detailed explanation of corrosion measurement procedures (4 hours).

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the familiarization with the methods of laboratory research of corrosion of metals and methods of conducting laboratory work. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

In addition to the basic rules of behavior in the laboratory, students at the introductory class are briefed on safety and occupational health and safety, as well as get acquainted with the scheme of drawing up reports on the performance of laboratory work on the specified topics. Important attention is paid to the description of experimental results for the preparation of conclusions.

Safety and occupational health and safety instructions. Sample reports on the performance of laboratory work.

#### 4. Necessary equipment, materials, etc

- Scanning electron microscopy (SEM), - energy dispersive X-ray (EDX) microanalysis, - X-ray fluorescence spectroscopy (XRF), - FTIR spectroscopy (FTIR-S), - Potentiostatic step polarization (PSSP), - Galvanostatic step polarization (GSSP), - Cyclic voltammetry (CVA) polarization, - Potentiostat, - Electrochemical cell (EC), - Working electrodes (WE), - Reference electrode (RE), - Contact angle (CA) - Computer laboratory.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods.* Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5
- *Passivity of Metals Studied by Surface Analytical Methods, a Review.* Strehblow H.-H. 2016, *Electrochim. Acta*, 212, 630-648. doi:10.1016/j.electacta.2016.06.170

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information



## Topics 2

### 1. The subject of the laboratory classes

**STUDY OF THE NATURE OF DAMAGE TO POLYMER PROTECTIVE COATINGS OF METALS AND ALLOYS CAUSED BY METAL CORROSION**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory lesson is related to the study of the nature of damage to protective coatings of metals and alloys. Students can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to corrosion and the nature of corrosion damage to protective coatings of devices and structures, predict service life after elimination of manifestations corrosion damage to metals and alloys. Students analyze samples of various protective coatings of metals and alloys damaged by corrosion, propose possible mechanisms and chemical reactions that caused the corrosion damage present on the samples. Based on the results of the analysis, students must draw appropriate conclusions about the causes of damage to the protective coatings of the studied samples (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the nature of corrosion and the nature of corrosion damage to protective coatings of devices and structures, predict service life after elimination of manifestations corrosion damage to metals and alloys. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic.

### 4. Necessary equipment, materials, etc

- Magnifiers, - Optical microscope, - Caliper, - Micrometer, - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *A Review of Differing Approaches Used to Estimate the Cost of Corrosion, Anti-Corrosion Method and Materials*. Bahaskaran R., Palaniswamy N., Rengaswamy N.S., Jayachandran M. 2005, J. Appl. Sci. Res. 52, 29-41. doi:10.1108/00035590510574899
- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods*. Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

## Topics 3

### 1. The subject of the laboratory classes

#### METHODS OF TESTING ANTICORROSION LAYERS OF VARIOUS NATURE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory lesson is related to familiarization and study of generally accepted methods of researching the properties of anti-corrosion polymer protective coatings of metals and alloys.

Students learn to work and carry out research with the help of methods of physical and chemical analysis, which will be used in the process of performing laboratory work. To analyze the surface of metals and anti-corrosion coatings, students will use: chemical methods for determining the thickness of the coating; microhardness; microstructural assessment using scanning electron microscopy (SEM); X-ray diffraction (XRD); energy dispersive analysis X-ray analysis (EDX); X-ray fluorescence analysis (XRF); analysis of the composition and structure of metal surfaces and anti-corrosion coatings (infrared spectroscopy (FTIR spectroscopy); potentiostatic step polarization (PSSP); galvanostatic step polarization (GSSP); chronopotentiometry (SPM); cyclic voltammetry (CVA) and etc. (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the methods of analyzing the composition and structure of coatings vary from the use of elementary tools, such as optical inspection, X-ray analysis, electrochemical analysis, etc. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions.

During laboratory classes, students will work in groups, get acquainted with the schematic diagrams of the main devices and methods of conducting analyzes related to corrosion processes. The acquired skills will become the basis for carrying out research on the topics of laboratory work on relevant topics.

### 4. Necessary equipment, materials, etc

- Scanning electron microscopy (SEM), - energy dispersive X-ray (EDX) microanalysis, - FTIR spectroscopy (FTIR-S), - Potentiostatic step polarization (PSSP), - Galvanostatic step polarization (GSSP), - Cyclic voltammetry (CVA) polarization, - Potentiostat, - Electrochemical cell (EC), - Working electrodes (WE), - Reference electrode (RE), - Contact angle (CA), - Höppler-Konsistometer (HK), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Characterization of surface coatings. Chapter 8.* Batchelor A.W., Loh N.L., Chandrasekaran M. // *Materials Degradation and Its Control by Surface Engineering.* 2011, 287-333. doi:10.1142/9781848165021\_0008
- *Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods.* Schweitzer P.A. 2009, CRC Press, York. 416 s. ISBN 978-1-4200-6770-5

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

## Topics 4

### 1. The subject of the laboratory classes

#### **ELECTROCHEMICAL APPLICATION OF PROTECTIVE POLYMER COATINGS ON STEEL SURFACES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory session is related to the experimental study of the preparation of the surface on steel samples for/and the electrochemical application of protective nonconductive polymer coatings on steel surfaces and the study of their physico-chemical, in particular, thickness, surface topology, structure, and morphology of films on steel. Evaluation of properties will be carried out using SEM, EDX, XRF, FTIR, CA and other methods, as well as anticorrosion protection of steel in standard solutions (3% NaCl).

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical application of protective nonconductive polymer coatings on steel surfaces and the study of its physico-chemical and anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for polyaniline coating on steel surfaces laboratories, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat, - Electrochemical cell, - Steel-electrode, - Pt counter electrode, - Ag/AgCl reference electrode, - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;

- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *The effect of electrolytes on the coating of polyaniline on mild steel by electrochemical methods and its corrosion behavior.* Gupta D.K., Neupane S., Singh S., et al. 2021, Prog Org. Coat. 152. 106127. doi:10.1016/j.porgcoat.2020.106127
- *A study on corrosion protection of different polyaniline coatings for mild steel.* Zhang Y. Shao Y., Liu X., et al. 2017, Prog. Org. Coat. 111, 240-247. doi:10.1016/j.porgcoat.2017.06.015
- *Inhibition of steel corrosion by polyaniline coatings.* Kraljić M., Mandić Z., Duić L. 2003, Corr. Sci. 45. 181-198.
- *Corrosion protection of mild steel by coatings containing polyaniline.* Lu W.-K., Elsenbaumer R.L., Wessling B. 1995, Synth. Met. 71(1-3), 0–2166. doi:10.1016/0379-6779(94)03204-j

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information



## Topics 5

### 1. The subject of the laboratory classes

**ELECTROCHEMICAL APPLICATION OF PROTECTIVE POLYANILINE COATINGS ON STEEL SURFACES**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory session is related to the experimental study of the preparation of the surface on steel samples for/and the electrochemical application of protective conductive polyaniline coatings on steel surfaces and the study of their physico-chemical, in particular, thickness, surface topology, structure, and morphology of films on steel. Evaluation of properties will be carried out using SEM, EDX, XRF, FTIR, CA and other methods, as well as anticorrosion protection of steel in standard solutions (3% NaCl).

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical application of protective conductive polyaniline coatings on steel surfaces and the study of its physico-chemical and anti-corrosion properties. Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for polyaniline coating on steel surfaces laboratories, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat, - Electrochemical cell, - Steel-electrode, - Pt counter electrode, - Ag/AgCl reference electrode, - Scanning electron microscopy (SEM), energy dispersive X-ray (EDX) microanalysis, - FTIR spectroscopy (FTIR-S), - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *The effect of electrolytes on the coating of polyaniline on mild steel by electrochemical methods and its corrosion behavior.* Gupta D.K., Neupane S., Singh S., et al. 2021, Prog Org. Coat. 152. 106127. doi:10.1016/j.porgcoat.2020.106127
- *A study on corrosion protection of different polyaniline coatings for mild steel.* Zhang Y., Shao Y., Liu X., et al. 2017, Prog. Org. Coat. 111, 240-247. doi:10.1016/j.porgcoat.2017.06.015
- *Inhibition of steel corrosion by polyaniline coatings.* Kraljić M., Mandić Z., Duić L. 2003, Corr. Sci. 45. 181-198.
- *Corrosion protection of mild steel by coatings containing polyaniline.* Lu W.-K., Elsenbaumer R.L., Wessling B. 1995, Synth. Met. 71(1-3), 0–2166. doi:10.1016/0379-6779(94)03204-j

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information



## Topics 6

### 1. The subject of the laboratory classes

#### PROTECTIVE CONDUCTING POLYANILINE/POLYPIRROLE COATINGS OF ALUMINUM SURFACES

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory session is related to the experimental study of the preparation of the surface of aluminum samples for/and the electrochemical application of protective conductive polyaniline/polypyrrole coatings on aluminum surfaces and the study of their physico-chemical, in particular, thickness, surface topology, structure, and morphology of films on aluminum. Evaluation of properties will be carried out using SEM, EDX, XRFs, FTIR, CA and other methods, as well as anticorrosion protection of aluminum in standard solutions.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the electrochemical (potentiodynamic) application of protective conductive polyaniline/polypyrrole coatings on aluminum surfaces.

Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of aluminum samples for/and the electrochemical application of protective anti-corrosion polyaniline/polypyrrole coatings on aluminum surfaces and the study of its physico-chemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat, - Electrochemical cell, - Aluminum plate (electrode), - Pt plate, - Ag/AgCl reference electrode, - Calipers, - Micrometer, - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - FTIR spectroscopy (FTIR-S), - Contact angle (CA), Höppler-Konsistometer (HK), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Polyaniline coatings on aluminium alloy 6061-T6: Electrosynthesis and characterization.* Martins N.C.T., Moura e Silva T., Montemor M.F., et al. 2010, *Electrochim. Acta.* 55(10), 3580-3588. doi:10.1016/j.electacta.2009.12.007
- *Synthesis of conductive polymeric composite coatings for corrosion protection applications.* Tsirimpis A., Kartsonakis I., Danilidis I., et al. 2010, *Prog. Org. Coat.* 67(4), 389-397. doi:10.1016/j.porgcoat.2009.12.010
- *Electropolymerized polyaniline coatings on aluminum alloy 3004 and their corrosion protection performance.* Shabani-Nooshabadi M., Ghoreishi S.M., Behpour M. 2009, *Electrochim. Acta*, 54(27), 6989–6995. doi:10.1016/j.electacta.2009.07.017
- *Influence of the thickness and roughness of polyaniline coatings on corrosion protection of AA7075 aluminum alloy.* Bandeira R.M., van Drunen J., Garcia A. C., Tremiliosi-Filho G. 2017, *Electrochim. Acta*, 240, 215-224. doi:10.1016/j.electacta.2017.04.083

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+

71 - 80 points = C  
66 - 70 points = D+  
61 - 65 points = D  
0 - 60 points = F

## 8. Optional information

## Topics 7

### 1. The subject of the laboratory classes

**POLYANILINE FOR SMART-RESPONSIVE AND SELF-HEALING COATINGS FOR METALS AND THEIR ALLOYS CORROSION PROTECTION**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory session is related to the experimental study of surface preparation of steel samples for/and the use of polyaniline for intelligent-responsive and self-healing coatings for corrosion protection and the study of their physicochemical characteristics (thickness, surface topology, composition, morphology, microhardness and anti-corrosion protection of steel in standard solutions).

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the PAN for intelligent-responsive and self-healing coatings for corrosion protection mild steel.

Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on the preparation of steel samples for of polyaniline for intelligent and self-healing coatings for corrosion protection and the investigation of its physicochemical and anti-corrosion properties, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat, - Electrochemical cell, - Steels plate, - Muffle furnace, - Calipers, - Micrometer, - Analytical scales (AS), - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - FTIR spectroscopy (FTIR-S), - Contact angle (CA), - Höppler-Konsistometer (HK), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Development of nanostructured polyaniline dispersed smart anticorrosive composite coatings.* Alam J., Riaz U., Ahmad S. 2008, Polym. Adv. Technol., 19(7), 882-888. doi:10.1002/pat.1054
- *A long-term stable and environmental friendly self-healing coating with polyaniline/sodium alginate microcapsule structure for corrosion protection of water-delivery pipelines.* Cui J., Li X., Pei Z., Pei Y. 2019, Chem. Eng. J. 358, 379-388. doi.10.1016/j.cej.2018.10.062

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

## Topics 8

### 1. The subject of the laboratory classes

#### THE FORMATION OF NANOCOMPOSITE ORGANIC-INORGANIC COATINGS FOR CORROSION PROTECTION OF STEEL

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory class is related to the experimental study of the formation of nanocomposite polyaniline-montmorillonite (or glauconite) coatings for corrosion protection of steel and the study of their physico-chemical and anticorrosion properties, research and comparison of the properties of the obtained surfaces and in particular, the current yield, thickness, surface topology and anticorrosion protection of steel in standard solution.

During the laboratory classes, students will work in groups, assigning tasks and with joint efforts draw up a work plan, perform an experiment, analyze its results and draw conclusions. The conducted experiment will be the basis for preparing a report on the performance of laboratory work on the specified topic (4 hours).

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve formation of nanocomposite polyaniline-montmorillonite (or glauconite) coatings for corrosion protection of steel.

Students are able to work in a group, distributing tasks and working together on drawing up a work plan, analyzing results and conclusions. They can prepare a theoretical introduction and description of the final results for the laboratory work on formation of nanocomposite polyaniline-montmorillonite (or glauconite) coatings for corrosion protection of steel and investigation of their anticorrosion properties, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Steel plate, - Muffle furnace, - Calipers, - Micrometer, - Analytical scales (AS), - Potentiostat, - Electrochemical cell (EC), - Scanning electron microscopy (SEM), - Energy dispersive X-ray (EDX) microanalysis, - FTIR spectroscopy (FTIR-S), - Höppler-Konsistometer (HK), - Contact angle (CA), - Computer laboratory.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - laboratory exercise/experiment; observation

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations;
- discussion (testing of students' knowledge) of methods of the nature of corrosion damage to various metals in operating conditions;
- getting acquainted with the research equipment in the laboratory, - students in groups, students carry out a selected experiment;
- during the experiment, students make observations, record comments and the results of the experiment;
- completion of the experiment and formulation of preliminary conclusions. Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Polyaniline-clay composite-containing epoxy coating with enhanced corrosion protection and mechanical properties*. Motlatle A.M., Ray S.S., Scriba M. 2018, Synth. Met. 245, 102-110. doi:10.1016/j.synthmet.2018.07.012
- *Investigation of corrosion protection performance of epoxy coatings modified by polyaniline/clay nanocomposites on steel surfaces*. Navarchian A. H., Joulazadeh M., Karimi F. 2014, Progr. Org. Coat. 77. 347-353. doi:10.1016/j.porgcoat.2013.10.
- *Polymer nanocomposites in corrosion control*. Weng, C.-J., Chang C.-H., Yeh J.-M. 2012, Corrosion Protection and Control Using Nanomaterials. 330-356. doi:10.1533/9780857095800.2.330

## 7. Additional notes

### ASSESSMENT

They will be assessed:

- substantive preparation (20%);
- the ability to properly plan and execute an experiment (20%);
- the ability to observe, analyze the results and draw appropriate conclusions (20%);
- activity (20%);
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**NEW ELECTROCHROMIC MATERIALS**

**Code: NEMD**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

**INTRODUCTION. ACTUAL STATE OF ORGANIC ELECTRONICS. HISTORICAL ASPECTS OF IDEAS IN ELECTROCHROMIC MATERIALS AND DEVICES**

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Functional nano- and microelectronics today develop in the area of organic electronics. It refers to the branch of electronics that studies, develops, and manufactures electronic devices (as well as their functional elements) based on organic chemistry materials: organic macromolecules or polymers. It is related to physics, chemistry, biology, medicine, and information technologies. The lecture will present the current state and the historical development of the ideas about electrochromic materials and devices. Electrochromic phenomena as changes in the optical properties of a substance under an applied electric field. The electrochromic effect is defined as visible and reversible changes in optical properties, namely, transmission (absorption) or reflection of light, which occurs under electrochemical oxidation/reduction of an electroactive substance. As a result of the modification of the electronic properties of the material (in particular, the width of the band gap), there is a change in its optical properties - the position and intensity of the absorption bands.

The first description of electrochromism is considered to be Deb's work in 1969 [USA Patent 3,500,392, 1970], devoted to  $WO_3$ , where the electrochromic effect of inorganic materials was observed for the first time. The study of electrochromism of organic substances was carried out early by Plath back in 1961. The development of the ideas leads to the electro-optic Kerr phenomenon – the orientation of molecules under the action of a constant electric field, and Faraday's magneto-optical phenomena. The discovery of conducting polymers caused the advent of new types of electronic and optoelectronic devices. In 2000, Alan J. Heeger, Alan G. MacDiarmid, and Hideki Shirakawa were awarded the Nobel Prize for their discovery. This discovery and the results of other studies of the electrical properties of organic materials opened the way to new electronics based on new organic electrochromic materials.

#### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *New electrochromic materials and devices, especially: fundamentals, and peculiarities.*

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrochromic materials and devices*. Ed. Mortimer R. J., Rosseinsky D. R., [Monk P. M. S.](#), 2015. <https://www.wiley.com/en-us/Electrochromic+Materials+and+Devices-p-9783527679874>
- *Prospects of conducting polymers in molecular electronics*. Saxena V., Malhotra B. D., 2003. *Curr. Appl. Phys.* 3, 293–305. [https://doi.org/10.1016/S1567-1739\(02\)00217-1](https://doi.org/10.1016/S1567-1739(02)00217-1)
- M. H. Chua, T. Tang, K. H. Ong, W. T. Neo, and J. W. Xu, in *Electrochromic Smart Materials: Fabrication and Applications*, ed. J. W. Xu, M. H. Chua, and K. W. Shah, The Royal Society of Chemistry, 2019, ch. 1, pp. 1-21. <https://doi.org/10.1039/9781788016667-00001>
- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives*. Aksimentyeva O. I., Konopelnik O. I., Poliovyi D. O. in *Computational and experimental analysis of functional materials*. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. 91–150. <https://doi.org/10.1201/9781315366357>

Additional, optional literature:

- *Physical, chemical, theoretical aspects of conducting polymer electro-chromics in the visible, IR and microwave regions*. Chandrasekhar P., Zay B. J., McQueeney T., et al., 2005. *Synth. Met.* 155, 623–627. <https://doi.org/10.1016/j.synthmet.2005.08.015>
- *A Novel Electrophotographic System*. Deb S. K., 1969. *Appl. Opt.* 8, 192–195. <https://doi.org/10.1364/AO.8.S1.000192>
- *Optical and photoelectric properties and colour centres in thin films of tungsten oxide*. Deb S. K., 1973. *Philos. Mag.* 27, 801–822. <https://doi.org/10.1080/14786437308227562>

## 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### METHODS OF SYNTHESIS AND PRODUCTION OF ELECTROCHROMIC MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The advantages of organic electronics are the ability to create ultra-thin and ultra-light devices on a flexible base, compatibility with inkjet and electronic printing technologies, access to new markets, and cheaper production technologies. The lecture will present the types of electrochromic materials and their chemical and electronic structure. Color changes in thin layers of conductive polymers are caused by electronic transitions in the conjugated polymer chain. The rate of charge transfer and color transitions in conducting polymers depends on the polymer structure and the level of doping.

The electrochromic layer may be formed from presynthesized electrochromic substances or by the „in situ“ synthesis of electrochromic substances on the conductive surface. For the production of the electrochromic layer on the conductive transparent surfaces, methods are used: electrochemical polymerization, photopolymerization - under the influence of UV radiation, thermolysis of precursors on the example of polyvinylphenylene synthesis. The product of the reaction is an electroactive film on the surface of the electrode, which has high electrical conductivity. The method allows obtaining a film of the required mass and thickness. The properties of the polymer film can be controlled during its synthesis.

During the lecture, students will learn methods of forming polymer films of controlled thickness on the surface of semiconductors, metals, or dielectrics using already synthesized polymer: spin coating, dip coating, Langmuir-Blodgett films, layer-by-layer self-assembling, magnetron and thermovacuum sputtering, thermo-vacuum deposition, sol-gel deposition, 3D printing.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Methods of electrochromic materials synthesis and thin layer formation*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrochromic materials and devices*. Ed. Mortimer R. J., Rosseinsky D. R., Monk P. M. S., 2015. <https://www.wiley.com/en-us/Electrochromic+Materials+and+Devices-p-9783527679874>

- *Solution-processable electrochromic materials and devices: roadblocks and strategies towards large-scale applications.* Li X., Perera K., He J., et al., 2019. *J. Mat. Chem. C.* 41, 12761–12789. <https://doi.org/10.1039/C9TC02861G>
- *Conducting polymers: a comprehensive review on recent advances in synthesis, properties and applications.* Namsheer K. N., Rout C. S., 2021. *RSC Advances.* 11(10), 5659–5697. <https://doi.org/10.1039/d0ra07800j>
- *Electrochromic nanostructured Tungsten oxide films by sol-gel: Structure and intercalation properties.* Deepa M., Joshi A. G., Srivastava A. K., Shivaprasad S. M., Agnihotry S. A., 2006. *J. Electrochem. Soc.* 153 (5), C365. <https://doi.org/10.1149/1.2184072>

Additional, optional literature:

- *Conducting electroactive polymers via photopolymerization: A review on synthesis and applications.* Heydarnezhad H. R., Pourabbas B., Tayefi M. 2017. *Polym. Plast. Technol. Eng.* 57(11), 1093–1109. <https://doi.org/10.1080/03602559.2017.1370111>
- *An overview on the synthesis and recent applications of conducting poly(3,4-ethylenedioxythiophene) (PEDOT) in industry and biomedicine.* Rahimzadeh Z., Naghib S. M., Zare Y., Rhee K. Y. 2020. *J. Mater. Sci.* <https://doi.org/10.1007/s10853-020-04561-2>
- *Processible conjugated polymers: from organic semiconductors to organic metals and superconductors.* Pron A., Rannou P., 2002. *Prog. Polym. Sci.* 27(1), 135–190. [https://doi.org/10.1016/s0079-6700\(01\)00043-0](https://doi.org/10.1016/s0079-6700(01)00043-0)
- *Thermo-vacuum deposition and electrooptical properties of polyaniline thin films.* Aksimentyeva O. I., Beluh V. M., Poliovyi D. O., 2007. *Mol. Cryst. Liq. Cryst.* 467, 143–152. <https://doi.org/10.1080/15421400701221336>
- *Inkjet-printed electrochromic devices utilizing polyaniline-silica and poly(3,4-ethylene dioxythiophene)-silica colloidal composite particles.* Shim G. H., Han M. G., Sharp-Norton J. S., et al., 2008. *J. of Mater. Chem.* 18, 594–601. <https://doi.org/10.1039/B712766A>

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### OPTICAL PROPERTIES AND DOPING OF ELECTROCHROMIC MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Optical absorption of the electrochromic materials in the visible part of the spectrum and in the near UV region can be used to create electro-optical devices for various purposes, such as light valves, color indicators, sensors, etc. Both linear and nonlinear optical properties of polymers, their ability to change the spectrum under the influence of external factors (electrochromicity), radiation under the influence of an electromagnetic field, and the presence of a photocurrent are important. The size of the energy gap between the valence band or the highest  $p$ -electron occupied band (HOMO) and the conduction band as the lowest unoccupied band – (LUMO) is responsible for the optical properties of the material, and, accordingly, for its color. For most electrochromic materials, the value of the band gap (or the difference between LUMO–HOMO) is  $E_g = 1.3\text{--}3.2$  eV. Optical absorption mainly occurs in the energy range corresponding to the near ultraviolet (UV) region (200–400 nm), visible (400–800 nm), and near-infrared (IR) region (800–1100 nm) of the spectrum. However, the positions of the maxima of the absorption bands and their intensity differ markedly, depending on the conditions of the synthesis of the electrochromic compounds and their doping. Doping mechanism of electrochromic materials directly connects with color change. Redox potential is applied to the electrode with an electrochromic film during electrochemical doping. At the same time, an electron is ejected (supply) or extracted (injection) from the conjugated (conjugated) polymer. Ions diffuse from the background electrolyte into the layer to maintain electroneutrality. The doping takes place through the action of chemical substances – molecular dopants, strong acids, by direct injection of an electron or hole into heterostructures, and by photo-doping under the influence of light or other radiation.

The acid (proton) doping type is inherent only to conjugated polyaminoarenes, for example, polyaniline, which has an amino (imino) group in its structure. In the case of chemical and/or electrochemical doping, the induced conductivity is constant until the carriers are chemically compensated or removed by "dedoping". In the case of photoexcitation, the photoconductivity lasts only as long as the excitation lasts. If charge injection occurs at the metal-semiconductor interface, electrons are placed in the  $\pi^*$  zone and/or holes in the  $\pi$  zone only when the bias voltage is applied. Students will learn about secondary doping of electrochromic films.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Optical properties and doping of electrochromic materials*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.



## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrochromic materials: Microstructure, electronic bands, and optical properties*. Granqvist C. G., 1993. Appl. Phys. 57, 3–12. <https://doi.org/10.1007/BF00331209>
- *Chemical doping of organic semiconductors*. Bhagat S., Hase H., Salzmann I., 2021. Organic Flexible Electronics. 107–141. <https://doi.org/10.1016/b978-0-12-818890-3.000>
- *The effects of secondary doping on ink-jet printed PEDOT:PSS gas sensors for VOCs and NO<sub>2</sub> detection*. Vigna L., Verna A., Marasso S. L., et al., 2021. Sens. Actuators B. 345, 130381. <https://doi.org/10.1016/j.snb.2021.130381>
- *Conducting polymer nanomaterials: electrosynthesis and applications*. Li C., Bai H., Shi G., 2009. Chem. Soc. Rev. 38, 2397–2409. <https://doi.org/10.1039/b816681>
- *Spectral and optical performance of electrochromic poly(3,4-ethylenedioxythiophene) (PEDOT) deposited on transparent conducting oxide coated glass and polymer substrates*. Sindhu S., Rao K. N., Ahuja S., et al., 2006. Mater. Sci. Eng. B. 132, 39–42. <https://doi.org/10.1016/j.mseb.2006.02.030>
- *Progress in preparation, processing and applications of polyaniline*. Bhadra S., Khastgir D., Singhaa N. K., Lee J. H., 2009. Prog. Polym. Sci. 34, 783–810. <https://doi.org/10.1016/j.progpolymsci.2009.04.003>

## 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### CHARACTERIZATION OF ELECTROCHROMIC SYSTEMS AND DEVICES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The electrochromic devices may have different architectures with light transmission, light absorption, light reflection and dual devices, and microencapsulated electrophoretic displays. Each device consists of an electrochemical cell that includes an ionically conductive electrolyte medium (liquid or solid) and one or more electrochromic materials whose response to an electric current causes a change in their electrical/optical properties, resulting in the generation of color. By controlling the conditions of formation, it is possible to obtain polymer layers with specified optical properties – absorption in a definite range of electromagnetic radiation, changes in the contour of the absorption spectrum under the influence of physical and chemical factors, etc. The advantage of electrochromic devices is the absence of radiation and unrequired special processing of the light signal, as opposed to liquid crystal devices working only in polarized light.

The experimental study of electrochromicity includes measuring the relative change in the light intensity that has passed through a substance when a constant electric field is applied. The electrochromic system is characterized by electrochromic efficiency and speed of electrochromic effect. Since the basis of the phenomenon is the reversible injection (extraction) of ions and electrons, their number is proportional to the charge  $\Delta Q$ , which determines the value of the given optical density. Contrast (CR) is defined as the ratio of transmittance (T) or light reflection by the film in the colorless state to the same characteristic in the colored state.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Characterization of electrochromic systems and devices*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Encyclopedia of smart materials*. Bell J. M., Skryabin I. L., Matthews J. P., 2002. New-York: Wiley-Interscience Publication. <https://doi.org/10.1002/0471216275>

- *Contrast limitations of dual electrochromic systems*. Padilla J., Otero T. F., 2008. *Electrochem. Commun.* 10, 1–6. <https://doi.org/10.1016/j.elecom.2007.10.004>

- *Faradaic charge corrected colouration efficiency measurements for electrochromic devices.*  
Fabretto M., Vaithianathan T., Hall C., 2008. *Electrochim. Acta.* 53, 2250–2257.  
<https://doi.org/10.1016/j.electacta.2007.09.054>

Additional, optimal literature:

*Dual-polymer electrochromic film characterization using bipotentiostatic control* / Unur E., Jung J.-H., Mortimer R. J., et al., 2008. *Chem. Mater.* 20, 2328–2334.  
<https://doi.org/10.1021/cm703354q>

## 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

#### MAIN CLASSES OF ELECTROCHROMIC MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

A large number of chemical compounds of both organic and inorganic nature exhibit electrochromic properties, including:

- Metal oxide films ( $\text{WO}_3$ ,  $\text{IrO}_2$ ,  $\text{TiO}_2$ ,  $\text{Nb}_2\text{O}_5$ ,  $\text{MoO}_2$ ,  $\text{V}_2\text{O}_5$ );
- Ferrum hexacyanoferrate salts with anion  $[\text{Fe}^{\text{III}}\text{Fe}^{\text{II}}(\text{CN})_6]$ ;
- Polypyridine complexes of transition metals;
- Metal coordination complexes, Metallo-phthalocyanines;
- Viologens (4,4'-bipyridinium salts; in solution and as polymer films);
- Redox dyes;
- Liquefied crystals;
- Conductive conjugated polymers.

Polymer electrolytes for electrochromic devices may be liquid, gel or solid film between two electrodes.

Cluster-type and columnar microstructures based on the  $\text{MeO}_6$  units exist in electrochromic films. The coordination of the ions leads to schematic electronic band structures that, at least for the (defect) perovskite and rutile lattices, can explain the presence or absence of cathodic and anodic electrochromism. Weak polaron absorption prevails in disordered oxides, while crystalline tungsten oxide can show free-electron effects. Under the action of the applied potential difference (1–5 V), the organic electrochromic compound is oxidized or reduced depending on the polarity of the voltage. Under external influence, the chromogenic material induces a colored center capable of absorbing light in the visible part of the spectrum.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Main classes of electrochromic materials*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

- a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrochromic materials and devices*. Ed. Mortimer R. J., Rosseinsky D. R., Monk P. M. S., 2015. <https://www.wiley.com/en-us/Electrochromic+Materials+and+Devices-p-9783527679874>

- *Metal-oxide films for electrochromic applications: present technology and future directions.* Gillaspie D. T., Tenent R. C., Dillon A. C., 2010. *J. Mater. Chem.* 20 (43): 9585–9592. <https://doi.org/10.1039/C0JM00604A>
- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives.* Aksimentyeva O. I., Konopelnik O. I., Poliovyi D. O. in *Computational and experimental analysis of functional materials.* eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. 91–150. <https://doi.org/10.1201/9781315366357>
- *Origin of electrochromism in high-performing nanocomposite Nickel oxide.* Lin F., Nordlund D., Weng T.-C., et al., 2013. *ACS Appl. Mater. Interfaces.* 5 (9), 3643–3649. <https://doi.org/10.1021/am400105y>

Additional, optimal literature:

- *Electrochromism and Electrochromic Devices.* Monk P. M. S., Mortimer R. J., Rosseinsky D. R., 2007. Cambridge University Press. <https://doi.org/10.1017/CBO9780511550959>
- *Electrochromic nanostructured Tungsten oxide films by sol-gel: Structure and intercalation properties.* Deepa M., Joshi A. G., Srivastava A. K., Shivaprasad S. M., Agnihotry S. A., 2006. *J. Electrochem. Soc.* 153 (5), C365. <https://doi.org/10.1149/1.2184072>
- *Viologens: a versatile organic molecule for energy storage applications.* Murugavel K., Bebin A., Natarajan A., Deepa M. E., Dhavamani S., Arul Manuel S., 2021. *J. Mater. Chem. A.* 9 (48): 27215–27233. <https://doi.org/10.1039/D1TA07201C>
- *Polymer electrolytes for electrochromic devices.* X.Fu., 2010. *Polymer Electrolytes. Fundamentals and Applications.* 471–523. <https://doi.org/10.1533/9781845699772.2.471>

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### INVESTIGATION OF THE STRUCTURE AND PROPERTIES OF ELECTROCHROMIC MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Electrochromic materials of inorganic and organic nature have crystalline, amorphous, or amorphous-crystalline structures. Organic and polymeric materials are characterized by the absence of long-range order, unlike crystalline bodies with an ordered structure. Electrochromic polymers in a thin layer have a globular or fibrillar structure. The supramolecular structure of conjugated polymers consists of amorphous and crystalline regions. It is considered that the islands of crystallinity are surrounded by an amorphous matrix, which creates a barrier for electron transfer. During the lecture, students will learn methods of structure investigation of the electrochromic materials in a thin layer: Infra-red (IR, FTIR) molecular spectroscopy; UV-viz-NIR electron spectroscopy; NMR spectroscopy; transmissive and scanning electron microscopy, atom force microscopy, X-ray phase analysis, optical microscopy.

The electrochemical methods - cyclic voltammetry, chronoamperometry, and potentiometry are used to study the electrochromic properties of materials. The lecture will present the electrochemical kinetics of electrochromic systems. Important and unique are spectroelectrochemical experiments because the optical spectrum and coloration of the film impedance spectroscopy allow to determine the connection between structure and electronic and optical properties of electrochromic materials.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Investigation of the structure and properties of electrochromic materials*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Highly ordered conjugated polymer nanoarchitectures with three-dimensional structural control*. Vlad A., Dutu C. A., Guillet P., et al., 2009. Nano Lett. 9(8), 2838–2843. <https://doi.org/10.1021/nl9008937>
- *Atomic force microscope*. Binnig G., Quate C. F., Gerber Ch., 1986. Phys. Rev. Lett. 56(9), 930–933. <https://doi.org/10.1103/PhysRevLett.56.930>
- *Spectroelectrochemistry: the best of two worlds*. Kaim W., Fiedler J., 2009. Chem. Soc. Rev. 38(12), 3373–3382. <https://doi.org/10.1039/b504286k>

- *Spectroelectrochemistry, the future of visualizing electrode processes by hyphenating electrochemistry with spectroscopic techniques.* Lozeman J. J. A., Führer P., Olthuis W., Odijk M., 2020. *Analyst*. 145, 2482–2509. <https://doi.org/10.1039/c9an02105a>

*Additional, optimal literature*

- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives.* Aksimentyeva O. I., Konopelnyk O. I., Poliovyi D. O. in *Computational and experimental analysis of functional materials.* eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. 91–150. <https://doi.org/10.1201/9781315366357>

- *Structure and properties of polyaniline micro- and nano-composites with Noble metals.* Nanooptics and photonics, nanochemistry and nanobiotechnology, and their applications. Aksimentyeva O., Horbenko Yu., Demchenko P., 2020. *Springer Proceedings in Physics*. 246, 507–522. [https://doi.org/10.1007/978-3-030-51905-6\\_35](https://doi.org/10.1007/978-3-030-51905-6_35)

## 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### APPLICATIONS OF ELECTROCHROMIC MATERIALS AND DEVICES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will present the application of electrochromic materials and devices in different areas. Each electro-optical device consists of an electrochemical cell, which includes an ion-conducting electrolyte medium (liquid or solid) and one or more electrochromic materials whose response to an electric current causes a change in their electrical/optical properties, resulting in the generation of color. Electronic and color transformations can be used to create non-radiative electrochromic devices – organic displays, safety to human eyes and health. Electrochromic displays can operate in one of two modes: reflecting light mode, where light or other radiation strikes a surface and is redirected, or transmitting light mode, which is transmitted through a substrate; the majority of displays operates in a reflective mode. Even though electrochromic devices are considered to be more “passive” since they do not emit light and need external illumination to function, electrochromic coatings on devices have been proposed for flat panel displays and visual-display units (VDUs).

Smart windows have both direct and indirect impacts on building energy consumption. Mirrors with controlled reflection use a combination of optoelectronic sensors and complex electronics that monitor ambient light and the intensity of the light shining on the surface. As soon as glare makes contact with the surface, these mirrors automatically dim reflections of flashing lights from following vehicles at night so that a driver can see them without discomfort.

Electronic paper, also known as electronic ink (e-ink) or intelligent paper, is a display device that mimics the appearance of ordinary ink on paper. Unlike conventional flat panel displays that emit light, an electronic paper display reflects ambient light like paper. It makes reading more comfortable and provides a wider viewing angle than most light-emitting displays.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Applications of conducting polymers*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Emerging electrochromic materials and devices for future displays*. Gu C., Jia A., Zhang Y., 2022. Chem. Rev. 122(18), 14679–14721. <https://doi.org/10.1021/acs.chemrev.1c01055>

- *Electrochromic smart materials: Fabrication and applications*. Xu J. W., Chua M. H., Shah K. W., 2019. Royal Society of Cambridge. <https://doi.org/10.1039/9781788016667>
- *Electrochromic glass vs. fritted glass: an analysis of glare control performance*. Ahoo M. A., Sok E., Niemasz J., 2017. Energy Procedia. 122, 343–348. <https://doi.org/10.1016/j.egypro.2017.07.334>

Additional, optional literature:

- *Large-area electrochromic glazing with ion-conducting PVB interlayer and two complementary electrodeposited electrochromic layers*. Kraft A., Rottmann M., Karl-Heinz H., 2006. Sol. Energy Mater. Sol. Cells. 90(4), 469–476. <https://doi.org/10.1016/j.solmat.2005.01.019>
- *Functionalization of conducting polymers and their applications in optoelectronics*. Khokhar D., Jadoun S., Arif R., Jabin S., 2020. Polym-Plast. Tech. Mat. 60(5), 465–487. <https://doi.org/10.1080/25740881.2020.1819312>
- *How do electrochromic (smart glass) windows work?*. Woodford C. 2021. Explain that Stuff. <https://www.explainthatstuff.com/electrochromic-windows.html>

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

#### NANOTECHNOLOGIES FOR IMPROVING ELECTROCHROMIC MATERIALS AND DEVICES

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Increasing the performance of organic electronics devices is possible due to the development of hybrid nanosystems with inorganic semiconductors. Organic-inorganic hybrid systems are materials containing inorganic nanostructures (nanocrystals, nanotubes, nanopores) embedded in an organic matrix. Hybrid systems have properties different from their components.

The formation of nanoparticles is carried out by a direct method in the presence of a polymer so that the nanocomposite is the product of a one-step reaction. The direct method is fast but unsuitable for obtaining non-contacting identical nanoparticles. According to the second method, an inorganic precursor is introduced into the polymer matrix, followed by a sequence of chemical reactions. The unique electrical and optical properties and structure of conducting polymers determine their use as components of hybrid nanosystems. During the lecture, students will learn the main approaches to improve electrochromic materials and devices: nanofabrication of hybrid electrochromic layers, formation of composites of electrochromic compounds in flexible polymer matrices, copolymerization of donor and acceptor monomers, doping of electrochromic materials by metallocomplex, carbon and oxide nanoclusters.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to *Nanotechnologies for improving electrochromic materials and devices*.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Improved electrochromic performances of NiO based thin films by lithium addition: From single layers to devices*. Moulki H., Park D. H., Min B., et al., 2012. *Electrochim. Acta*. 74, 46–52. <https://doi.org/10.1016/j.electacta.2012.03.123>.

- *Electrochromic materials and devices: present and future*. Somani P., Radhakrishnan S., 2003. *Mater. Chem. Phys.* 77(1, 2), 117–133. [https://doi.org/10.1016/S0254-0584\(01\)00575-2](https://doi.org/10.1016/S0254-0584(01)00575-2)

- *An overview of recent progress in the development of flexible electrochromic devices*. Wang B., Zhang W., Zhao F., et al., 2023. *Nano Mater. Sci.* 5(4), 369–391. <https://doi.org/10.1016/j.nanoms.2022.08.002>

Additional, optional literature:

- *Recent trends and developments in conducting polymer nanocomposites for multifunctional applications*. Sharma S., Sudhakara P., Omran A. A. B., Singh J., Ilyas R. A., 2021. *Polymers*. 13(17). <https://doi.org/10.3390/polym13172898>
- *Application of intrinsically conducting polymers in flexible electronics*. Jianyong O., 2021. *SmartMat*. 2(3), 263–285. <https://doi.org/10.1002/smm2.1059>
- *Color tuning of electrochromic TiO<sub>2</sub> nanofibrous layers loaded with metal and metal oxide nanoparticles for smart colored windows*. Eyovge C., Deenen C. S., Ruiz-Zepeda F., et al., 2021. *ACS Applied Nano Materials*. 4(8), 8600–8610. <https://doi.org/10.1021/acsanm.1c02231>
- *Conducting polymer nanomaterials: electrosynthesis and applications*. Li C., Bai H., Shi G., 2009. *Chem. Soc. Rev.* 38, 2397–2409. <https://doi.org/10.1039/b816681>

## 6. Additional notes

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## Course content – laboratory classes

### Topics 1 – Lab 1

#### 1. The subject of the laboratory classes

##### ELECTROCHEMICAL SYNTHESIS OF CONJUGATED POLYMERS

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study of the electrochemical synthesis of electrochromic material based on conjugated polyaminoarenes on the surface of optically transparent electrodes in the cyclic potential sweep mode, the study of an influence of the electrosynthesis mode on the formation processes and properties of conjugated polymers in a thin layer, determining the thickness and morphology of the obtained films. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results, and draw conclusions. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

#### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Electrochemical synthesis of electrochromic layer on transparent surfaces*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemical synthesis of electrochromic layers*, including critical analysis, synthesis, and conclusions.

#### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- Transmission electron microscope,
- Computer laboratory,
- Interference microscope MII-4

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - reading,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of methods of electrochemical synthesis of polymers, mechanism of oxidative electrochemical polymerization of anilines, methods of materials characterization, especially TEM technique,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives*. Aksimentyeva O. I., Konopelnik O. I., Poliovyi D. O. in Computational and experimental analysis of functional materials. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. 91–150. <https://doi.org/10.1201/9781315366357>
- *Cyclic Voltammetry*. David K., Grosser Jk. New York: VCH Publishers, 1994.
- *Conducting polymers: a comprehensive review on recent advances in synthesis, properties, and applications*. Namsheer K. N., Rout C. S., 2021. RSC Advances. 11(10), 5659–5697. <https://doi.org/10.1039/d0ra07800j>
- *Progress in preparation, processing and applications of polyaniline*. Bhadra S., Khastgir D., K. Singhaa N., Lee J. H., Prog. Polym. Sci. 34, 783–810. <https://doi.org/10.1016/j.progpolymsci.2009.04.00>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

#### FORMATION OF ELECTROCHROMIC LAYERS BY „LAYER BY LAYER“ ASSEMBLING TECHNIQUE

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will perform the electrochromic layers fabrication from PEDOT-PSS dispersion on the transparent conductive surface by self-assembling “layer by layer”, determine the thickness and morphology of the obtained films, and measure the optical spectrum of the film in transmission and absorption modes. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Formation of electrochromic layer by layer by layer self-assembling*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Formation of electrochromic layer by layer by layer self-assembling*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- 3 Chemical glasses,
- Timer,
- Dryer,,
- Optical microscope,
- UV-viz-spectrophotometer,
- Laser zero-elipsometer LEF-3M-1,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,

- discussion (checking students' knowledge) of methods of conducting polymer synthesis,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *High-contrast electrochromism from layer-by-layer polymer films*. DeLongchamp D. M., Kastantin M., Hammond P. T., 2003. *Chem. Mater.* 15, 1575–1586. <https://doi.org/10.1021/cm021045x>
- *Spectral and optical performance of electrochromic poly(3,4-ethylenedioxythiophene) (PEDOT) deposited on transparent conducting oxide coated glass and polymer substrates*. Sindhu S., Raoa K. N., Ahujaa S., et al., 2006. *Mater. Sci. Eng.* 132(1-2), 39–42. <https://doi.org/10.1016/j.mseb.2006.02.030>
- *Conducting polymers: a comprehensive review on recent advances in synthesis, properties and applications*. Namsheer K. N., Rout C. S., 2021. *RSC Advances*. 11(10), 5659–5697. <https://doi.org/10.1039/d0ra07800j>
- *Solution-processable electrochromic materials and devices: roadblocks and strategies towards large-scale applications*. Li X., Perera K., He J., et al., 2019. *J. Mat. Chem. C* 41, 12761–12789. <https://doi.org/10.1039/C9TC02861G>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+

71 - 80 points = C  
66 - 70 points = D+  
61 - 65 points = D  
0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

#### ELECTROCHEMICAL DOPING OF ELECTROCHROMIC LAYERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will perform electrochemical doping of the electrochromic layer based on conjugated polymers and determine the charge transfer parameters in obtained thin films – effective diffusion coefficient and speed of response. Students will work in a group, sharing tasks and working together to establish a work plan, analyze the results, and draw conclusions about the possibility of using the polymer to create electrochromic films of sufficient speed, which can be used in visualization devices, indicators, sensors, etc. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Electrochemical doping of electrochromic layers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Electrochemical doping of electrochromic layers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of types of doping of conjugated polymers, possible application of conductive polymer films,

- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Chemical doping of organic semiconductors*. Bhagat S., Hase H., Salzmann I., 2021. *Organic Flexible Electronics*. 107–141. <https://doi.org/10.1016/b978-0-12-818890-3.000>
- *The effects of secondary doping on ink-jet printed PEDOT:PSS gas sensors for VOCs and NO<sub>2</sub> detection*. Vigna L., Verna A., Marasso S. L., et al., 2021. *Sens. Actuators B*. 345, 130381. <https://doi.org/10.1016/j.snb.2021.130381>
- *Hole-limited electrochemical doping in conjugated polymers*. Keene S. T., Laulainen J. E. M., Pandya R., et al., 2023. *Nat. Mater.* 22, 1121–1127. <https://doi.org/10.1038/s41563-023-01601-5>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



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## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

SPECTROELECTROCHEMICAL STUDY OF THE ELECTROCHROMIC MATERIAL

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the spectroelectrochemical study of the effect of applied voltage on the optical spectra and color of the electrochromic layer. Students will determine the contrast ratio and electrochromic efficiency of the material. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results, and draw conclusions. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Spectroelectrochemical study of electrochromic materials*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Spectroelectrochemical study of electrochromic materials*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Device for measuring the temperature dependence of resistance,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.

c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of types of charge carriers in conjugated polymer systems, model representations of the conduction mechanism in conjugated polymers, principle of thermocouple operation,
- getting acquainted with the research equipment in the laboratory,



- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Low-dimensional variable range hopping in conducting polymers*. Epstein A., Lee W., Prigodin V., 2001. Synth. Met. 117, 9–13. [https://doi.org/10.1016/S0379-6779\(00\)00531-2](https://doi.org/10.1016/S0379-6779(00)00531-2)
- *Electrical properties of polypyrrole conducting polymer at various dopant concentrations*. Othman N., Talib Z. A., Kassim A., Shaari A. H., Liew J. Y. C., 2009. J. Fundam. Sci. 5, 29–33. <http://dx.doi.org/10.11113/mjfas.v5n1.284>
- *Conducting polymers: electrical conductivity*. Kohlman R. S., Joo J., Epstein A. J., 1996. Physical properties of polymers handbook. Mark J. E. ed.; Amer. Inst. Phys. Woodbury: New-York.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



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## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### OPTICAL PROPERTIES OF ELECTROCHROMIC POLYMERS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students will perform measurements and analysis of transmission and absorption spectra of various polyaminoarenes on optically transparent surfaces and their application in optical color indicators. Students will make the calibration curves based on the changes in optical density and shifts in the position of the absorption maximum under applied voltage. Students' theoretical knowledge of the UV-Vis spectroscopy technique will be verified. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results, and draw conclusions. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Optical properties of conjugated polymers*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Optical properties of conjugated polymers*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat,
- Electrochemical cell,
- ITO-glass, Pt wire, Ag/AgCl reference electrode,
- UV-Vis spectrophotometer,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
- discussion (checking students' knowledge) of optical phenomena in conjugated polymer systems, principles of potentiometric and optical sensors operation, UV-Vis spectroscopy,
- getting acquainted with the research equipment in the laboratory,
- students in groups, students carry out a selected experiment,
- during the experiment, students make observations, record comments and the results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Spectroelectrochemistry: the best of two worlds*. Kaim W., Fiedler J., 2009. Chem. Soc. Rev. 38(12), 3373–3382. <https://doi.org/10.1039/b504286k>
- *Electrooptic phenomena in conjugated polymeric systems based on polyaniline and its derivatives*. Aksimentyeva O. I., Konopelnyk O. I., Poliovyi D. O. in Computational and experimental analysis of functional materials. eds.: Reshetnyak O. V., Zaikov G. E., Toronto: Apple Academic Press, 2017. 91–150. <https://doi.org/10.1201/9781315366357>
- *Spectroelectrochemistry, the future of visualizing electrode processes by hyphenating electrochemistry with spectroscopic techniques*. Lozeman J. J. A., Führer P., Olthuis W., Odijk M., 2020. Analyst. 145, 2482–2509. <https://doi.org/10.1039/c9an02105a>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.

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## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

#### DESIGN AND CHARACTERIZATION OF ELECTROCHROMIC CELL

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the design of electrochromic cells in two-electrode mode with conjugated polymer layer and gel electrolyte between transparent ITO plates. Students will study the effect of applied potential on color change in electrochromic cells. They will determine the potential of switching and coloration-discoloration conditions. During laboratory classes, students will work in a group, sharing tasks and working together to establish a work plan, analyze the results, and draw conclusions. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

### 3. Learning outcomes

Students can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to *Design and characterization of electrochromic cell*. Students are able to work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions. They can prepare a theoretical introduction and final results description to the laboratories on *Design and characterization of electrochromic cell*, including critical analysis, synthesis, and conclusions.

### 4. Necessary equipment, materials, etc

- Electrochromic cell,
- Potentiostat,
- ITO-glass, Pt wire as reference electrode,
- Optical microscope,
- UV-Vis spectrophotometer,
- Computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- getting acquainted with the rules of occupational health and safety and laboratory regulations,
  - discussion (checking students' knowledge) of optical phenomena in conjugated polymers,
  - getting acquainted with the research equipment in the laboratory,
  - students in groups, students carry out a selected experiment,
  - during the experiment, students make observations, record comments and the results of the experiment,
  - completion of the experiment and formulation of preliminary conclusions.
- Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- *Polymeric electrochromics*. Sonmez G., 2005. Chem. Comm. 42, 5251. <https://doi.org/10.1039/b510230h>
- *Colours from electroactive polymers: Electrochromic, electroluminescent and laser devices based on organic materials*. Carpi F., De Rossi D., 2006. Opt. Laser Technol. 38, 292–305. <https://doi.org/10.1016/j.optlastec.2005.06.019>
- *Polymer electrolytes for electrochromic devices*. X.Fu., 2010. Polymer Electrolytes. Fundamentals and Applications. 471–523. <https://doi.org/10.1533/9781845699772.2.471>

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

- 96 - 100 points = A
- 91 - 95 points = B+
- 86 - 90 points = B
- 80 - 85 points = C+
- 71 - 80 points = C
- 66 - 70 points = D+
- 61 - 65 points = D
- 0 - 60 points = F

## 8. Optional information

Exercise manuals will be available.



The document was prepared as part of the "Materials Science Ma(s)ters - developing a new master's degree" project (2021-1-PL01-KA220-HED-000035856).



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**CREATING A STARTUP**

**Code: CS**

## Course content – lectures

### Topics 1

#### 1. The subject of the lecture

**First step to startups is an idea**

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

At the beginning of the lecture, the concept of a startup will be considered. A startup is different from a regular business activity. Normal business functions by analogy and is based on known processes. A start-up company produces an innovative product and just conquers the market. The startup does not have a well-known and stable business model - it creates and tests it, constantly improving it. To start a successful search for an idea for a startup, you need to combine two components: internal motivation and research of market needs and market environment. Although the idea is at the beginning of the creation of a startup, in addition to the realism of the idea, 5 other factors must be taken into account: time limits, team, business model and financing.

#### 3. Learning outcomes

students will be able to generate an idea for their own startup and test it for viability using various methods

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Ihor Katernyak "Innovation Spring in Tech Startup: momentum to take off". Lviv: Publ. house of the Lviv University, 2021. – 172 p.

Bill Gross. The single biggest reason why start-ups succeed. [www.youtube.com/watch?v=bNpx7gpSqBY&t=66s](https://www.youtube.com/watch?v=bNpx7gpSqBY&t=66s)

The top 20 reasons startups fail. [www.cbinsights.com/research/startup-failure-reasons-top/](https://www.cbinsights.com/research/startup-failure-reasons-top/)

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 2

### 1. The subject of the lecture

Target audience of startup

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The important concept "Target audience" (or target group) will be defined - this is a group of people who are most likely to be interested in the offer and order a specific product or service. The main value of the target audience is that representatives of the selected group are likely to want to buy a certain product. It will also be considered how a marketer creates an advertisement taking into account the taste preferences or characteristics of this particular group, which significantly increases the effectiveness of the advertising campaign.

### 3. Learning outcomes

students will be able to determine the target audience for a startup, create its portrait, and segment it using various methods

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Alexander Santo 6 real-life target audience examples to help you define your own (b2b and b2c) [www.brafton.com/blog/strategy/6-real-life-target-audience-examples-to-help-you-define-your-own-b2b-and-b2c/](http://www.brafton.com/blog/strategy/6-real-life-target-audience-examples-to-help-you-define-your-own-b2b-and-b2c/)

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 3

### 1. The subject of the lecture

#### Startup marketing

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The concept of "Marketing" will be defined as the ability to create a situation in which the client will gladly give his money for the goods or services offered by the startup. According to this concept, the main objectives of startup marketing are to research the opinion of the potential customer, create a better value proposition and bring the product to market, after which startup marketing is focused on scaling through increasing the startup's brand awareness, gaining customer loyalty and a positive business reputation. Attention will also be paid to protecting intellectual property and avoiding common mistakes in startup marketing.

### 3. Learning outcomes

students learn the basic rules of startup marketing, in particular, they will be able to research the target market, analyze the risks of competition, protect intellectual property, determine the value proposition of a startup, and avoid typical mistakes in startup marketing

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

The Role of Marketing Capabilities in Firm's Success <https://researchleap.com/the-role-of-marketing-capabilities-in-firms-success/>

The Ultimate Guide to Startup Marketing <https://neilpatel.com/blog/ultimate-guide-startup-marketing>

The Ultimate Startup Marketing Strategy For Incredible Growth <https://www.ventureharbour.com/ultimate-startup-marketing-strategy/>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 4

### 1. The subject of the lecture

#### Startup and social networks

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will first cover the general concept of digital marketing (using all possible forms of digital channels to promote a brand), with a major focus on social media. Students will get acquainted with the main advantages of using digital marketing. The main emphasis will be on digital marketing methods (online video, native (natural) advertising, personalized content, smart advertising with big data, and community development). Advertising of a startup in social networks will be considered using the examples of creating an official page, publishing posts and advertising to attract followers (targeted advertising); purchase of advertising publications on other thematic pages; promotion of advertisements to obtain conversions to the site; working with Facebook groups (free posting and paid placement).

### 3. Learning outcomes

students will be able to apply the main methods of digital marketing, including online video, native advertising, personalized content, smart advertising with big data, and development of the Internet community; students will also be able to use various methods of advertising a startup in social networks

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Megha Parikh. How to Build a Social Media Strategy for Your Startup. <https://www.startupgrind.com/blog/how-to-build-a-social-media-strategy-for-your-startup/>  
Maksym Babych. Social Media Marketing For Startups: A Beginner's Guide. <https://www.socialpilot.co/blog/social-media-marketing-for-startups>  
10 Essential Social Media Tips for Startups. <https://www.unboxsocial.com/blog/social-media-tips-for-startups/>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 5

### 1. The subject of the lecture

#### Startup funding

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

There will be various different sources of funding: investment specifics (investing personal savings), F&F (supporting family and friends in the early stages of financing), venture capital (funds that are invested or made available for investment in a new venture by a venture firm in exchange for its own a share in the company), business angels (secured individuals or former managers of companies who directly invest in small firms, owned by others, money is invested in startups or early-stage companies in exchange for an ownership stake), business incubators (focus on the high-tech sector, supporting innovative startups at various stages of development through mentoring programs in co-working spaces, university courses, hackathons with awards, pitches, prototyping labs and hardware), grant funding (provided by government, international organizations, specialized foundations and other non-profit institutions), bank loans (secured and unsecured), crowdfunding (using an online platform to raise a significant number of small investments from the public to obtain the required amount). Special attention will be paid to the activities of university Science Parks in support of startups.

### 3. Learning outcomes

students will be able to choose a source of financing for their startup, considering its features: personal investments, F&F, venture capital, business angels, business incubators, grant financing, bank loans, crowdfunding, including the analysis of the work of Ihub Science Park, Lviv University

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Jacqueline DeMarco, Lisa Anthony. Startup Funding: What It Is and How to Get Capital for a Business. <https://www.nerdwallet.com/article/small-business/startup-funding>

The 5 Types of Startup Funding. <https://www.startups.com/library/expert-advice/5-types-startup-funding>

Katrina Kirsch. Startup Funding: What It Is, How It Works, & 5 Tips for Landing It. <https://blog.hubspot.com/sales/how-startup-funding-works>

Co-Investment & Angel Investment <http://www.angelcofund.co.uk/>

Crowdcube <https://www.crowdcube.com/>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours



## Topics 6

### 1. The subject of the lecture

#### Startup business model

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will show that a business model is a conceptual framework that supports the viability of a product or company and explains how the company operates, makes money and how it is going to achieve its goals. A business model consists of three parts: everything related to the design and manufacture of a product or service; everything related to the sale of a product/service: from finding the right customers to distributing the product; and everything related to monetization: costs and profits of the company, what exactly the customer will pay the company for. The sequence of steps of creating a business model will be considered in detail: determining the value of the product on the market, attracting valuable customers, ensuring sufficiently high mark-ups, ensuring that the product is the best available solution, ensuring consumer satisfaction, determining the channel and distribution strategy, maintaining market positions, formulating a strategy financing, implementation of pilot implementation. In conclusion, the creation of a business model canvas will be considered.

### 3. Learning outcomes

students will be able to create a business model for their own startup, taking into account its features and visualize it in the form of a canvas for easier promotion

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Mullins J. "The New Business Road Test". Pearson Education Ltd, 2010. – 337 p.

Katerynak, V. Loboda, "Entrepreneurial Momentum for Sustainable Growth" in "Sustainable Organizations – Models, Applications, and New Perspectives" Jose C. Sánchez-García and Brizeida Hernández-Sánchez, IntechOpen, DOI: 10.5772/intechopen.95099. Available from: <https://www.intechopen.com/books/sustainable-organizations-models-applications-and-new-perspectives/entrepreneurial-momentum-for-sustainable-growth>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 7

### 1. The subject of the lecture

**Startup leader and team**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will show that a successful startup requires a strong leader who must put in a lot of effort to achieve success, but will also show that no matter what idea you have, the fate of your startup depends on your team. It will be considered how leaders play a leading role in the development of a startup organization: determine directions and new development opportunities for the organization; make decisions for the company, search for optimal solutions to problems; hire, fire and inspire employees to work effectively; the leader is also the "frontman" of the company and the "face" of the brand. After that, attention will be paid to the formation of the startup team: definition of positions and areas of responsibility; well-thought-out hiring process; development of a strategy for training, professional development and career development of employees. In conclusion, the formation of corporate culture will be considered.

### 3. Learning outcomes

students will be able to create their own team for the future implementation of a startup, determine the motivation for each team member, as well as test and improve their leadership skills

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

John Rampton 5 Steps for Building a Great Startup Team <https://www.inc.com/john-rampton/5-stepsfor-building-a-great-startup-team.htm>

Michael Yang. Leadership in Startups <https://www.scribd.com/document/496884739/Leadership-in-Startups-Michael-Yang>

Protima Sharma. 10 steps to cultivate the right culture in your Startup. <https://venturecenter.co.in/pdfs/Culture-cultivation-10-steps.pdf>

Hayden Young. The keys to building successful startup teams <https://www.antler.co/blog/building-successful-startup-teams>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Topics 8

### 1. The subject of the lecture

#### Startup presentation

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will cover recommendations for creating a successful startup presentation, as well as the secrets of pitch preparation. The structure of the startup's presentation will be reviewed in slides: "Startup overview", "Mission/Vision", "Team", "Problem", "Solution", "Product", "Market opportunities", "Clients", "Technologies", "Competitors", "Push", "Business model", "Marketing plan", "Finance", "Questions". After that, an analysis of the most common mistakes in startup presentations will be conducted. At the end, attention will be paid to the creation of a pitch for a startup, its structure: "Powerful start" - present a problem with bright statistics or a personal story; "Solution" – a concise description of the solution and method of solving the problem, key differences from competitors; "Client" – clear identification and quantification of the person affected by the problem; "Funds" is a description of the business model.

### 3. Learning outcomes

students will be able to create a presentation of their own startup for investors without making the most common mistakes, as well as prepare a pitch according to the best standards

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Richard, H. (2017), How To Create A Great Investor Pitch Deck For Startups Seeking Financing. <https://www.forbes.com/sites/allbusiness/2017/03/04/how-to-create-a-great-investor-pitch-deck-for-startups-seekingfinancing/#6079ce4e2003>

How to create a 3-minute demo day pitch deck <https://vip.graphics/demo-day-pitch-formula/>  
What is a Startup Demo Day? Template and Example <https://slidebean.com/blog/startup-demo-day-pitch-deck>

### 6. Additional notes

The subject of the lecture covers 2 teaching hours

## Course content – practical classes

### Topics 1

#### 1. The subject of the practical classes

##### Presentation of Startup idea

#### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will propose their own ideas for startups and discuss them in small groups to choose the most perspective. Finally, the best from them will be chosen according to market needs and market environment. Students teams will present their own startup on the basis of their previous research in the field of Material Science in the format of MS PowerPoint. In this presentation on the basis of technical characteristics the advantages of the product that will be developed for future startups must be described.

#### 3. Learning outcomes

students will be able to generate an idea for their own startup and test it for viability using various methods

#### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Ihor Katernyak "Innovation Spring in Tech Startup: momentum to take off". Lviv: Publ. house of the Lviv University, 2021. – 172 p.

Bill Gross. The single biggest reason why start-ups succeed. [www.youtube.com/watch?v=bNpx7gpSqBY&t=66s](http://www.youtube.com/watch?v=bNpx7gpSqBY&t=66s)

The top 20 reasons startups fail. [www.cbinsights.com/research/startup-failure-reasons-top/](http://www.cbinsights.com/research/startup-failure-reasons-top/)

#### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

#### 7. Optional information

After this practical classes students finished Tasks 1 and each student can received max. 10 points

## Topics 2

### 1. The subject of the practical classes

Search of the target audience of a startup.

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will analyze which target audience is most appropriate for the startup which was chosen on previous practical class and which main values of this audience.

### 3. Learning outcomes

students will be able to determine the target audience for a startup, create its portrait, and segment it by various methods

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

The Ultimate Startup Marketing Strategy For Incredible Growth  
<https://www.ventureharbour.com/ultimate-startup-marketing-strategy/>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

Inviting of the director of Science Park of Lviv University "Innovations and Entrepreneurship" Prof. Nazar Demchyshak – he will presented best startups which was participated in the Lviv Startup Fests organized by Science Park

## Topics 3

### 1. The subject of the practical classes

Analyse of startup marketing

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will analyze target market for the startup which was chosen on previous practical class define competitors and discuss steps of bringing the product to the market. Students teams will create startup site in one of social media (for example Facebook, or any other) with advertising of startup to cover target audience and target established in previous task.

### 3. Learning outcomes

students learn the basic rules of startup marketing, in particular, they will be able to research the target market, analyze the risks of competition, protect intellectual property, determine the value proposition of a startup, and avoid typical mistakes in startup marketing

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

The Role of Marketing Capabilities in Firm's Success <https://researchleap.com/the-role-of-marketing-capabilities-in-firms-success/>

The Ultimate Guide to Startup Marketing <https://neilpatel.com/blog/ultimate-guide-startup-marketing>

The Ultimate Startup Marketing Strategy For Incredible Growth <https://www.ventureharbour.com/ultimate-startup-marketing-strategy/>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

After this practical classes students finished Tasks 2 and each student can receive max. 10 points

## Topics 4

### 1. The subject of the practical classes

#### Creating of startup site in social networks

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will create site of their startup in the different social media (Facebook, Instagram, Twitter, Pinterest, LinkedIn, Snapchat). Students teams will create startup site in one of social media (for example Facebook, or any other) with advertising of startup to cover target audience and target established in previous task.

### 3. Learning outcomes

students will be able to apply the main methods of digital marketing, including online video, native advertising, personalized content, smart advertising with big data, development of the Internet community; students will also be able to use various methods of advertising a startup in social networks

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Megha Parikh. How to Build a Social Media Strategy for Your Startup. <https://www.startupgrind.com/blog/how-to-build-a-social-media-strategy-for-your-startup/>  
Maksym Babych. Social Media Marketing For Startups: A Beginner's Guide. <https://www.socialpilot.co/blog/social-media-marketing-for-startups>  
10 Essential Social Media Tips for Startups. <https://www.unboxsocial.com/blog/social-media-tips-for-startups/>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

After this paractic classes students finished Tasks 3 and each student can received max. 10 points



## Topics 5

### 1. The subject of the practical classes

#### Finding of startup funding

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will analyze different sources of their startup to choose few of most appropriate for it and propose way for support by Science Park. Students teams will demonstrate by MS PowerPoint chart with explanation of possibilities of involvement of all types of funding with comments how each type of funding appropriate to startup.

### 3. Learning outcomes

students will be able to choose a source of financing for their startup, considering its features: personal investments, F&F, venture capital, business angels, business incubators, grant financing, bank loans, crowdfunding, including the analysis of the work of Ihub Science Park, Lviv University.

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Jacqueline DeMarco, Lisa Anthony. Startup Funding: What It Is and How to Get Capital for a Business. <https://www.nerdwallet.com/article/small-business/startup-funding>

The 5 Types of Startup Funding. <https://www.startups.com/library/expert-advice/5-types-startup-funding>

Katrina Kirsch. Startup Funding: What It Is, How It Works, & 5 Tips for Landing It. <https://blog.hubspot.com/sales/how-startup-funding-works>

Co-Investment & Angel Investment <http://www.angelcofund.co.uk/>

Crowdcube <https://www.crowdcube.com/>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

After this practical classes students finished Tasks 4 and each student can received max. 10 points

## Topics 6

### 1. The subject of the practical classes

Creation of a startup business model

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will create a business model of startup by filling of all fields of canvas from <https://www.strategyzer.com/>.

### 3. Learning outcomes

students will be able to create a business model for their own startup, taking into account its features and visualize it in the form of a canvas for easier promotion

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Mullins J. "The New Business Road Test". Pearson Education Ltd, 2010. – 337 p.

Katerynak, V. Loboda, "Entrepreneurial Momentum for Sustainable Growth" in "Sustainable Organizations – Models, Applications, and New Perspectives" Jose C. Sánchez-García and Brizeida Hernández-Sánchez, IntechOpen, DOI: 10.5772/intechopen.95099. Available from: <https://www.intechopen.com/books/sustainable-organizations-models-applications-and-new-perspectives/entrepreneurial-momentum-for-sustainable-growth>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

After this practical classes students finished Tasks 5 and each student can received max. 10 points

## Topics 7

### 1. The subject of the practical classes

Creating of startup team and looking for leader

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical classes students will discuss about roles of all members of startup team and own motivation for participation in it; finally, leader of startup will choose.

### 3. Learning outcomes

students will be able to create their own team for the future implementation of a startup, determine the motivation for each team member, as well as test and improve their leadership skills

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

John Rampton 5 Steps for Building a Great Startup Team <https://www.inc.com/john-rampton/5-stepsfor-building-a-great-startup-team.htm>

Michael Yang. Leadership in Startups <https://www.scribd.com/document/496884739/Leadership-in-Startups-Michael-Yang>

Protima Sharma. 10 steps to cultivate the right culture in your Startup. <https://venturecenter.co.in/pdfs/Culture-cultivation-10-steps.pdf>

Hayden Young. The keys to building successful startup teams <https://www.antler.co/blog/building-successful-startup-teams>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

Inviting of the leader of Spartup Lviv Hydrogene Dr. Nazar Pavlyuk – he will presented his startup “Lviv Hydrogen”, winner of the first edition of the Lviv Startup Fest and spread his experience from the deep-tech business summit NORDEEP (Finland)

## Topics 8

### 1. The subject of the practical classes

#### Startup presentation

### 2. Thematic scope of the practical classes (abstract, maximum 500 words)

During practical sessions, students will create a startup presentation and discuss all possible mistakes to avoid, as well as prepare a startup pitch. Students teams will present own startup in pitch format on the base of presentation in format of MS PowerPoint which must be send for assessment 3 day ahead of "pitching day".

### 3. Learning outcomes

students will be able to create a presentation of their own startup for investors without making the most common mistakes, as well as prepare a pitch according to the best standards

### 4. Didactic methods used (description of student/teacher activities in the classroom/practical, taking into account didactic/teaching methods)

practice

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Richard, H. (2017), How To Create A Great Investor Pitch Deck For Startups Seeking Financing. [https:// www.forbes.com/sites/allbusiness/2017/03/04/how-to-create-a-great-investor-pitch-deck-for-startups-seeking-financing/#6079ce4e2003](https://www.forbes.com/sites/allbusiness/2017/03/04/how-to-create-a-great-investor-pitch-deck-for-startups-seeking-financing/#6079ce4e2003)

How to create a 3-minute demo day pitch deck <https://vip.graphics/demo-day-pitch-formula/>

What is a Startup Demo Day? Template and Example <https://slidebean.com/blog/startup-demo-day-pitch-deck>

### 6. Additional notes

The subject of the practical classes covers 2 teaching hours

### 7. Optional information

After completion of Final task (**Startup presentation**) each student can received max. 50 points (40 points for startup presentation in format of MS PowerPoint and 10 points for pitching of startup)

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**ADVANCED FUNCTIONAL MATERIALS**

**Code: AFM**

## Course content – [lecture](#)

### Topics 1

#### 1. The subject of the lecture

##### FUNCTIONALITY OF MATERIALS

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

During the lecture on the classification of inorganic compounds for practical use, modern aspects of the production and use of functional materials will be presented, which indicate the need to modernize the production technologies of such materials, as well as the need for their use. Students should systematize their knowledge of physicochemical properties and types of composite materials, as well as their meaning.

During the lecture, students will learn that in connection with the wide use of functional materials at the current stage of the development of civilization, a large number of issues arise related to their improvement, as well as environmental protection.

#### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to the production, physicochemical properties and expansion of the use of different types of functional materials.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Guralskyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.



3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 2

### 1. The subject of the lecture

#### MATERIALS AND TECHNOLOGIES FOR OBTAINING FUNCTIONAL POLYMER COMPOSITE MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

At the current stage of development of human society, the areas of use of functional polymer composite materials are expanding. At the same time, materials for obtaining them are constantly updated. It is also important to constantly modernize the technologies for obtaining such materials, taking into account the economic and environmental aspects associated with this.

During the lecture, students will get acquainted with the peculiarities of obtaining functional polymer composite materials. The main approaches to the classification of composite polymer materials will be considered. They will receive information about the main properties and applications of polymer composite materials, as well as about film polymer functional materials.

During the lecture, students will also learn about modern functional polymer materials for light industry. New areas of their application as fiber optic sensors and piezoelectric devices will be considered.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to materials and technologies for obtaining functional composite materials.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.
3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 3

### 1. The subject of the lecture

#### STRUCTURAL FUNCTIONAL MATERIALS BASED ON ALLOYS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The production and use of structural functional materials based on alloys is extremely diverse and is expanding every time. These can be superalloys and intermetallics, heat-resistant and high-strength aluminum alloys, structural steels and alloys of increased reliability, as well as armored steels, structural alloys for nuclear power.

A special place in terms of properties and use is occupied by corrosion-resistant alloys, as well as special-purpose materials, that is, amorphous materials.

At the lecture, students will be introduced to the main methods of obtaining and analyzing structural materials based on alloys. During the lecture, the listeners will get acquainted with the features of the properties of such materials, which will determine the areas of their use in the future.

Students will also receive information about the ways of modernization and modification of structural functional materials based on alloys and improvement of their production technologies.

### 3. Learning outcomes

Able to use information from lectures, literature and other available sources, interpret and critically evaluate it, draw conclusions, formulate and solve problems related to the use of structural functional materials based on alloys.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.
3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 4

### 1. The subject of the lecture

#### PROPERTIES OF INORGANIC FUNCTIONAL MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Among functional materials that are widely used today, inorganic functional materials occupy a special place.

The listeners will be introduced to the electrical properties of such materials and the zonal structure of solids. Thermoelectric phenomena in inorganic functional materials will also be considered. Special attention is paid to the features of magnetic and optical properties of solid materials.

In order to be able to propose fields of application of inorganic functional materials, it is also necessary to get acquainted with the materials from which they are obtained, as well as the technologies of obtaining them and possible prospects for their improvement.

### 3. Learning outcomes

You can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the production and use of inorganic functional materials

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**

a. Lecture conducted with the use of multimedia.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Guralskyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoretz, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.
3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 5

### 1. The subject of the lecture

#### ELECTRICAL MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Electrical materials are a large group of functional materials.

During the lecture, students will get acquainted with the phenomenon of electrical conductivity in materials and the features of superconductors. Features of technologies for obtaining superconducting materials, as well as differences between classic and modern semiconductor materials, will be considered.

Thin film materials, in particular, for solar energy, make up a separate group in terms of properties and applications.

Modern technologies require the use of dielectrics, therefore it is important to characterize the insulating and dielectric properties of materials and the influence of the structure on them, as well as distinguish the main types of industrial insulators.

Application of thermoelectric materials, understanding the effect of the nature of the material on thermoelectric properties.

Superconductors are important electrotechnical materials. Therefore, the influence of chemical, phase composition and microstructure on superconductivity, as well as modern technologies for their production, will be considered.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the properties and use of electrotechnical materials of various nature and practical use.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.



## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Guralskyi I.O. Chemistry of functional materials: textbook - K.: KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.
3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 6

### 1. The subject of the lecture

#### MAGNETIC MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Magnetic materials are important structural materials that are used in a wide variety of electrical and electronic devices in various industries and even medicine.

Students will familiarize themselves with the features of the structure and basic properties of magnetically hard and magnetically soft materials, as well as modern technologies for their production. They will receive information about ferrites and directions of their use. Magnetostrictive materials occupy a special place among functional materials.

Soft magnetic amorphous alloys are used as special purpose materials, in particular, strip alloys. Listeners will be introduced to the main methods of obtaining them, installations and conditions of their formation.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the properties, production technologies and use of magnetic functional materials.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Gural'skiy I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret's, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.

3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 7

### 1. The subject of the lecture

#### ADVANCED NANOCRYSTALLINE MATERIALS

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Nanocrystalline materials and nanotechnologies are increasingly being used. Therefore, it is important to consider issues related to nanopowders, in particular, their production and main properties.

Volumetric nanostructured materials, as well as nanofibers, nanowires, and nanotubes of various nature occupy a special place. Technologies for obtaining and using fullerenes and graphene are being improved.

However, considering the issue of the use of nanomaterials, it is necessary to pay attention to the positive and negative aspects of such materials and technologies at the current stage, as well as in the future. It is important to anticipate the possibilities of accumulation and transformation of nanoparticles in environmental objects, as well as to know the level of their possible toxicity.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the properties, production technologies of modern nanocrystalline materials, as well as the entry of nanoparticles into the environment, their accumulation and transformation.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoret's, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.
3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Topics 8

### 1. The subject of the lecture

**SMART MATERIALS**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

A new kind of functional materials with special properties - smart materials. Students will be introduced to methods of optimizing the properties of structural intelligent polymer composites. Materials with shape memory are distinguished by their special properties. Therefore, it is necessary to understand the influence of nature and structure on the shape memory effect of structural materials. The classification of such materials is based on various features.

It is important to consider the main areas of application and methods of obtaining materials with shape memory.

Smart materials include functional materials using 3-D printing. The listeners will be introduced to selective laser sintering, the possibilities of modeling by the surfacing method, as well as the production of objects using lamination.

### 3. Learning outcomes

Can use information from lectures, literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the use, production and properties of smart materials for various purposes.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **informative lecture, monographic lecture, description**  
problem methods - **conversational lecture**

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, there is a discussion with the students.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Terebilenko K.V., Guralskyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.
2. Materials and components of functional electronics: study guide / L. IN. Odnodvoretz, I. M. Sinus. – Sumy: Sumy State University, 2020. – 196 p.

3. Protsenko I. Yu. Nanomaterials and nanotechnologies in electronics: a textbook / I. Yu. Protsenko, N. AND. Shumakova. – Sumy: Sumy State University, 2018. – 155 p.

Additional, optional literature:

Journals:

1. Functional materials.
2. Advanced materials.
3. Chemistry of metals and alloys.
4. Chemistry of materials.
5. Physico-chemical mechanics of materials.
6. Journal of solid state physics and chemistry

## 6. Additional notes

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## Course content – laboratory classes

### Topics 1 Lab 1

#### 1. The subject of the laboratory classes

##### COMPOSITE MATERIALS

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge will be tested regarding modern methods of researching composite materials of various nature, in particular, determining the structure, elemental composition and properties of various samples. The conducted experiment with samples of real objects will be the basis for writing a report and completing tasks.

During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions. Team projects will be implemented.

#### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of composite materials of various nature.

Students can work in groups, setting tasks and drawing up a work plan together, analyzing the results and drawing conclusions. They can also prepare a theoretical introduction and description of final results for laboratories on the elemental composition of materials for various purposes, including critical analysis, synthesis and conclusions.

#### 4. Necessary equipment, materials, etc

- X-ray diffractometer
- scanning electron microscope,
- transmission electron microscope
- a device for measuring microhardness
- potentiostat
- computer laboratory

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

methods of learning/assessment - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**



assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining the structure, microhardness and elemental analysis of composite materials,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, methods of obtaining composite materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

### - ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Topics 2 Lab 2

### 1. The subject of the laboratory classes

#### ADVANCED MATERIALS BASED ON ALLOYS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of researching physicochemical properties of functional materials based on crystalline and amorphous alloys will be tested. The conducted experiment with samples of real objects will be the basis for writing a report and performing exercises.

During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the determination of strength, electrical conductivity, electrochemical.

Students can work in groups, setting tasks and drawing up a work plan together, analyzing the results and drawing conclusions. May also prepare a theoretical introduction and description of final results for laboratories on the physicochemical properties of composites, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- X-ray diffractometer
- scanning electron microscope,
- transmission electron microscope
- a device for measuring microhardness
- potentiostat
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - reading,

a set of practical methods - a laboratory exercise/experiment; observation

- a. Laboratory classes are conducted using special research equipment and specialized software.
- b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.
- in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods for determining the properties of functional materials based on alloys,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics))

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, methods of obtaining composite materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),

- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Topics 3 Lab 3

### 1. The subject of the laboratory classes

#### SUPERHARD MATERIALS AND POWDER CERAMIC MATERIALS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of researching the mechanical properties of materials of various nature and purpose, in particular, superhard materials and powdered ceramics, will be tested.

The conducted experiment with samples of different nature will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of the properties of superhard materials of various compositions and powdered ceramic materials.

Students can work in groups, assigning tasks and together make a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories studying the mechanical properties of materials of various compositions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- samples of materials of different composition
- installation for studying mechanical properties
- breaking machine
- scanning electron microscope,
- transmission electron microscope
- a computer

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of methods of researching the properties of materials of various nature,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, methods of obtaining composite materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),

- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available



## Topics 4 Lab 4

### 1. The subject of the laboratory classes

#### CONDUCTING, SUPERCONDUCTING AND SEMICONDUCTOR MATERIALS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern electrochemical methods of materials research, as well as methods of researching the compatibility of materials for various purposes, will be tested. The conducted experiment with samples of real objects will be the basis for writing a report and performing exercises.

During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of physicochemical properties of materials with different types of conductivity.

Students can work in groups, together setting tasks and making a work plan, analyzing the results and drawing conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the electrochemical parameters of electrodes of various compositions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat-galvanostat
- pH meter
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **a laboratory exercise/experiment; observation**

a. Laboratory classes are conducted using special research equipment and specialized software.

b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.

in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of electrochemical research of materials of different composition and purpose,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, electrochemical methods of research of functional materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),

- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Topics 5 Lab 5

### 1. The subject of the laboratory classes

#### MODERN MAGNETIC MATERIALS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Students' theoretical knowledge of modern methods of obtaining and researching magnetic materials will be tested. The conducted experiment with samples of magnetosoft amorphous alloys of different composition will be the basis for writing a report and performing exercises. During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of modern magnetic materials of various nature.

Students can work in groups, assigning tasks and together make a work plan, analyze the results and draw conclusions. May also prepare a theoretical introduction and description of the final results for the study of magnetic properties, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- pH meter
- magnetometer
- potentiostat-galvanostat
- scanning electron microscope,
- transmission electron microscope
- a computer

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - **reading**,

a set of practical methods - **laboratory exercise/experiment; observation**

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing students' knowledge) of research methods of magnetic materials,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform the selected experiment,
- during the experiment, students conduct observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, magnetic functional materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT

They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),

- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

## Topics 6 Lab 6

### 1. The subject of the laboratory classes

#### APPLICATION OF NANOMATERIALS

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words))

Students' theoretical knowledge of modern physico-chemical methods of material research, in particular nanostructured amorphous metal alloys, will be tested. The conducted experiment with samples of real objects, in particular amorphous initial and nanostructured alloys, will be the basis for writing a report and performing exercises.

During laboratory sessions, students will work in groups, assigning tasks and working together. They have to make a work plan, analyze the results and draw conclusions.

### 3. Learning outcomes

Students can use information from the literature and other available sources, interpret and critically evaluate them, draw conclusions, formulate and solve problems related to the study of electrochemical properties of materials for various purposes, in particular, amorphous metal alloys.

Students can work in groups, set tasks together and make a work plan, analyze the results and draw conclusions. They can also prepare a theoretical introduction and description of the final results for laboratories on the electrochemical parameters of electrodes of various compositions in alkaline and acidic solutions, including critical analysis, synthesis and conclusions.

### 4. Necessary equipment, materials, etc

- Potentiostat-galvanostat
- pH meter
- scanning electron microscope,
- transmission electron microscope
- computer laboratory

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods) \*

assimilation methods/providing - reading,

a set of practical methods - a **laboratory exercise/experiment; observation**

- a. Laboratory classes are conducted using special research equipment and specialized software.
- b. In laboratory classes, students independently plan the course of the experiment and carry it out independently.
- in. During the laboratory classes, students work in groups, assigning tasks and, with joint efforts, draw up a work plan, analyze the results, and draw conclusions.

Classes are held in the following order:

- familiarization with labor protection rules and laboratory rules,
- discussion (testing of students' knowledge) of methods of electrochemical research of materials of different composition and purpose,
- familiarization with the research equipment of the laboratory,
- students in groups, students perform a selected experiment,
- during the experiment, students make observations, write down comments and results of the experiment,
- completion of the experiment and formulation of preliminary conclusions.

Students prepare the final report independently at home.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read the following lab-related texts:

1. Major environmental issues and new materials / Susmita Dey Sadhu, Meenakshi Garg, Amit Kumar // New Polymer Nanocomposites for Environmental Remediation. - 2018. – P. 77-97. <https://doi.org/10.1016/B978-0-12-811033-1.00004-4>
2. Terebilenko K.V., Gural'skyi I.O. Chemistry of functional materials: textbook - K. : KNU named after Shevchenko, 2022. – 110 p.

Additional, optional literature:

- any textbooks or manuals for studying the structure, properties, nanostructured functional materials.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

- ASSESSMENT



They will be assessed:

- substantive preparation (20%),
- the ability to properly plan and execute an experiment (20%),
- the ability to observe, analyze the results and draw appropriate conclusions (20%),
- activity (20%),
- ability to work in a group (20%).

Grading scale according to the table included in the Syllabus:

96 - 100 points = A

91 - 95 points = B+

86 - 90 points = B

80 - 85 points = C+

71 - 80 points = C

66 - 70 points = D+

61 - 65 points = D

0 - 60 points = F

## 8. Optional information

Exercise manuals will be available

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**CRYSTAL CHEMISTRY (RELATIONSHIP COMPOSITION–  
STRUCTURE–PROPERTIES)**

**Code: CC(RCSP)**

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## Course content – lecture

### Topic 1

#### From ideal to real crystal structure

During the lecture, students will be familiarized with the concepts of crystalline state, which is characterized by the presence of both short-range and long-range ordering of particles. Short-range order is an arrangement of atoms, which is repeated at distances commensurate with the distances between atoms, that is, a regularity in the arrangement of nearest neighbors. Long-range order is the periodicity of the arrangement of atoms in the entire crystalline body, regardless of the distances between atoms. The lecture will remind the students about symmetry operations, Bravais lattices, and space groups. Students will get an idea of ideal, real, and average structures. The crystal structure and symmetry are critical in determining many physical properties, such as cleavage, electronic band structure, and optical transparency. The real structure is responsible for the property, without explaining the crystal structure it will not be possible to explain why exactly the material functions. In real structures, there are various defects, that is, local changes in the arrangement of atoms that break the translational symmetry of the ideal structure. The causes of structural defects will be discussed. These defects critically determine many of real materials' electrical and mechanical properties. Students will also learn about the liquids and amorphous substances.

#### LEARNING OUTCOMES

Learn the main characteristics of the crystalline state.

Describe the crystal structure and determine the crystallographic parameters.

Understand the difference between ideal, real, and average structures.

Realize the superiority of a real structure over an ideal structure concerning the physical properties of materials.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of real crystal structure of the substances and the use of materials based on them in various fields and technologies.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984; T. Hahn, Ed., *International Tables for Crystallography*, Vol. A, Kluwer Academic Publishers, Dordrecht, 2002; B.K. Vainshtein, V.M. Fridkin, V.L. Indenbom, *Modern Crystallography*, Vol. 2: *Structure of Crystals*, Springer, Berlin, 2000; *Crystal Structure*, WIKIPEDIA ([https://en.wikipedia.org/wiki/Crystal\\_structure](https://en.wikipedia.org/wiki/Crystal_structure)).

## Topic 2

### Defects in crystals

During the lecture students will learn, that defects in crystals are imperfections in the regular geometrical arrangement of the atoms in a crystalline solid. They occur during crystal growth, in particular, due to the presence of impurities (deformation of the solid), under the influence of mechanical and thermal influence (rapid cooling from high temperatures), electric and magnetic fields,

and ionizing radiation (X-rays or neutrons striking the solid). Defects significantly affect the physical properties of crystals. When one atom substitutes for one of the principal atomic components within the crystal structure, alteration in the electrical and thermal properties of the material may ensue. Defects introduce disorder into the ideal structure and increase entropy. Another aspect discussed in the lecture is the classification of defects in crystals: stoichiometric and non-stoichiometric. Defects are also divided into: points defects (0D, Schottky, Frenkel, antistructural defects), linear (1D, dislocations), planar (2D, twin boundary, grain boundary), and volume (3D, errors in the arrangement of structural fragments, crystallographic shifts). Students also will learn that defects are classified into two groups: oscillations around ideal positions and violation of periodicity in the arrangement of atoms in the crystal structure. The first concerns the short-range order, and the second concerns the long-range order. Oscillations around ideal positions are related to temperature and the violation of periodicity is a more complicated process because it is necessary to replace the atom(s), to include an additional atom.

## LEARNING OUTCOMES

Understand the origin and nature of defects in crystals.

Classify the defects in crystals.

Understand the concept of clusters of defects using the example of the mineral wüstite.

Understand, that defects introduce disorder into the ideal structure and significantly affect the physical properties of crystals.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of ionic crystals with Schottky or Frenkel defects and ionic conductivity's dependence on the defects' quantity.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conducting a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; J.W. Morris Jr., *Defects in crystals*, In: *Materials Science and Engineering*, Wiley, 2013; A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984; *Crystallographic defect*, WIKIPEDIA ([https://en.wikipedia.org/wiki/Crystallographic\\_defect](https://en.wikipedia.org/wiki/Crystallographic_defect)).

## Topic 3

### Group-subgroup relationships between space groups

During the lecture, students will be familiarized with the concepts of phase transition and superstructure. In crystal chemistry phase transitions occur when a solid changes to a different structure without changing its chemical makeup. In elements, this is known as allotropy, whereas in compounds it is known as polymorphism. The change from one crystal structure to another, from a crystalline solid to an amorphous solid, or from one amorphous structure to another (polymorphs) are all examples of solid-to-solid phase transitions. Students will also learn that there are first- and second-order phase transitions. During the first-order phase transitions basic parameters such as density, internal energy, concentration of components change abruptly, which is accompanied by the absorption or release of heat. The second-order phase



transitions occur in those cases when the symmetry of the substance structure changes, these transitions are accompanied by a decrease in symmetry. These and other transformations of the structure can be described with the help of various relationships. Among them are group-subgroup relationships between space groups and with which students will be introduced to. Students will learn that the affinity between crystal structures implies the affinity between their space groups, which can be represented by the group-subgroup relationship. These relations are derived from the relations between lattices (unit cells), point and space groups of crystal structures and can be represented as a genealogical tree called Bärnighausen.

## LEARNING OUTCOMES

Learn the causes of phase transitions.

Understand the difference between the first- and the second-order phase transitions.

Analyze the crystal parameters to derive the code for the group-subgroup relationship between space groups.

Describe the affinity between crystal structures by the codes of structural relationship.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of structural derivatives: deformation, substitution, filling, vacancy, stacking variant, and intergrowth structure using the examples of crystal structures of intermetallic compounds.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; T. Hahn, Ed., *International Tables for Crystallography*, Vol. A, Kluwer Academic Publishers, Dordrecht, 2002; E. Parthé, *Elements of Inorganic Structural Chemistry*, K. Sutter Parthé Publisher, Petit-Lancy, 1996; E. Parthé, L. Gelato, B. Chabot, M. Penzo, K. Cenzual, R. Gladyshevskii, *TYPIX – Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, Springer-Verlag, Berlin, 1993, Vol. 1; J.H. Westbrook, R.L. Fleischer, Eds., *Intermetallic Compounds*, Vol. 1,2, John Wiley & Sons, Chichester, 1993; *Phase transition*, WIKIPEDIA ([https://en.wikipedia.org/wiki/Phase\\_transition](https://en.wikipedia.org/wiki/Phase_transition)).

## Topic 4

### Modern trends in the development of structural analysis

This lecture will focus on determining defects and microstructure by diffraction methods, i.e. extracting information on the real structure of materials from their diffraction patterns. The primary features of a powder diffraction pattern are determined by the "idealized" periodic nature of the crystal structure. With the advent of computer automation, the techniques for carrying out qualitative, quantitative, and structural analysis based on the primary pattern features rapidly matured. Recent developments in precision and speed during the last

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squares in crystals are helping structural scientists deal with larger structures more efficiently. During the lecture students will learn that, the deviations of a particular specimen, from the perfect crystal structure, cause diffraction peak profiles to broaden and sometimes to become asymmetric. Thus, information on the real structure or microstructure of a specimen can be obtained from a careful study of the diffraction line profiles. Another aspect discussed in the lecture is the modern methods of X-ray diffraction on mono- and polycrystals, research at extreme temperatures and pressures, and expanding the range of samples and problems that can be addressed. Temperature and pressure have a strong influence on the structure of (crystalline) materials and their related material properties. The crystal structure of materials under high pressure and high temperature can now be determined by X-ray diffraction using powder samples and, more recently, from multi-nano single crystal diffraction. Concurrently, these experimental advancements are accompanied by a rapid increase in computational capacity and capability, enabling the application of sophisticated quantum calculations to explore a variety of material properties.

## LEARNING OUTCOMES

Understand how to extract complete information from a powder pattern.

Learn the extreme conditions that can be applied during diffraction.

Learn about *ab initio* determination based on powder data in particular using WinCSD (crystal structure determination), FOX (free objects for crystallography).

Understand the principles of determining the crystal structure of phases in multiphase samples.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of *in-situ* studies, i.e. obtaining powder pattern during a chemical reaction, which contributes to the study of phase transitions, to establish at what temperature the structure changes from one to another.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, *Methods to Determine Crystal Structures*, Publishing Center of Ivan Franko National University of Lviv, 2015; R.L. Snyder, J. Fiala, H.J. Bunge, Eds., *Defect and Microstructure Analysis by Diffraction*, Oxford University Press, 1999; V.K. Pecharsky, P.Y. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*, Springer Science + Business Media, New York, 2009; D.L. Bish, J.E. Post, Eds., *Modern Powder Diffraction*, Mineralogical Society of America, Washington D.C., 1989; *The Extreme Conditions Beamline P02.2 and the Extreme Conditions Science Infrastructure at PETRA III* (<https://doi.org/10.1107/S1600577515005937>); *A chemical perspective on high pressure crystal structures and properties* (<https://doi.org/10.1093/nsr/nwz144>)

## Topic 5

### X-ray, neutron, and electron diffraction analysis

This lecture will be devoted to advances in the theory of diffraction, in the generation of X-rays, in techniques and data analysis tools that changed the ways X-ray diffraction is performed and the quality of the data analysis. The time and space resolution of X-ray diffraction now reaches to nanoseconds and tens of nanometers. During the lecture, the principles of diffraction theory will be

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summarized, under the assumption that the students are familiar with basic concepts of the crystalline state. The basics of diffraction techniques will be briefly reviewed using laboratory and synchrotron X-ray sources. Students will learn that the key features of synchrotron radiation concerning structural studies are the wavelength tunability, which facilitates the use of resonant diffraction methods, and the high brightness and excellent vertical collimation of the source, which make possible the construction of diffractometers with unparalleled angular and space resolution. During the lecture students will be familiarized with neutron diffraction studies, which play an important role in structural solid-state chemistry, making possible the precise determination of the location of light atoms, particularly hydrogen, and enabling a distinction to be made between certain neighboring elements in the periodic table that are difficult to distinguish in experiments with X-rays. Students will also learn about electron diffraction and that the key difference between electron and neutron diffraction is that electrons are scattered by atomic electrons, whereas neutrons are scattered by atomic nuclei. Electron diffraction is the wave nature of electrons. Neutron diffraction is the phenomenon of elastic neutron scattering. Typically, electron diffraction describes the wave-like nature, while neutron diffraction describes the atomic and/or magnetic structure of a material.

## LEARNING OUTCOMES

Learn the basics of synchrotron X-ray, neutron, and electron diffraction.

Understand the key difference between X-ray, neutron, and electron diffraction.

Understand how the maximal information can be extracted by a combination of X-ray, neutron, and electron diffraction methods in solid-state chemistry.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation about the sources of synchrotron radiation, of which there are now more than 50 in the world. The principle scheme of all of them is similar, but the energy scales differ by order of magnitude. Every ten years, the brightness of X-ray sources of synchrotron radiation increases a thousand times.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, *Methods to Determine Crystal Structures*, Publishing Center of Ivan Franko National University of Lviv, 2015; R.L. Snyder, J. Fiala, H.J. Bunge, Eds., *Defect and Microstructure Analysis by Diffraction*, Oxford University Press, 1999; V.K. Pecharsky, P.Y. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*, Springer Science + Business Media, New York, 2009; Synchrotron X-ray and Neutron Diffraction Studies in Solid-State Chemistry (<https://doi.org/10.1002/anie.199215571>); J. Milos, R. Kral, Eds., *Modern Electron Microscopy in Physical and Life Sciences*, InTech, 2016; R.A. Young, A.C. Larson, C.O. Paiva-Santos, *Rietveld Analysis of X-Ray and Neutron Powder Diffraction Patterns*, School of Physics, Georgia Institute of Technology, Atlanta, Georgia, 1998.

## Topic 6

### Material creation algorithm

During the lecture, students will get acquainted with the solution of an important scientific problem, that the creation of the novel materials requires the establishment of chemical composition – crystal structure – physical property

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relationship. The use of modern methods in chemistry, a complex approach to the search for compounds with unique properties, optimization of their characteristics by controlling the synthesis are decisive in conducting research. Students will learn, that correctly selected alloy compositions will allow determining the main physico-chemical factors, which affect the formation and properties of phases. Thus, a complex of experimental studies of state diagrams, precise determination of the crystal structure, calculation of the electronic structure and chemical bond characteristics, measurement of properties and controlled change in the concentration of valence electrons is a prerequisite for the synthesis of new phases, which can become the basis of materials for practical use. The lecture will focus on the unique properties of intermetallics, which are widely used in many industries. Modified  $\text{LaNi}_{5-x}(\text{Al/Sn})_x$ ,  $\text{Mg}_2\text{Ni}$ ,  $\text{TiFe}$  phases are used in hydrogen storage and metal hydride batteries;  $\text{LiC}_6$ ,  $\text{Li}_{22}\text{Si}_5$ ,  $\text{LiAl}$ ,  $\text{Na}_{15}\text{Sn}_4$  are electrode materials in Li- and Na-ion batteries; doped Mg-Al alloys are the basis of structural materials; heat-resistant materials ( $\text{HfC}$ ,  $\text{TiNi}_3\text{C}_x$ ,  $\text{ZrNi}_4$ ), semiconductors ( $\text{GaAs}$ ,  $\text{GaP}$ ,  $\text{GaN}$ ,  $\text{PtSi}$ ), thermoelectrics ( $\text{FeSi}_2$ ,  $\text{BaGe}_5$ ), magnets, among which  $\text{SmCo}_5$ ,  $\text{Nd}_2\text{Fe}_{14}\text{B}$ , have the best properties. Another aspect discussed in the lecture is the relationship between the symmetry of crystals, the symmetry of their physical properties, and the dependence of properties on the symmetry of external influences, which is determined by the principles of Neumann and Curie.

## LEARNING OUTCOMES

Understand the relationship between chemical composition, crystal structure, and physical properties.

Learn in which industries materials based on intermetallic compounds are used.

Realize that the presence or absence of certain properties of the crystal can be predicted based on the elements of symmetry.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of magnetically ordered materials, which are characterized not only by the symmetry of the crystal lattice but also by a certain ordering of magnetic moments, which are vector quantities. In the case of magnetic symmetry, one more parameter must be taken into account – the inversion operator ( $i$ ) associated with the magnetic moment of an atom (ion).

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984; J.H. Westbrook, R.L. Fleischer, Eds., *Intermetallic Compounds*, Vol. 1,2, John Wiley & Sons, Chichester, 1993; R.E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure*, Oxford University Press, 2005; *Solid-state chemistry*, WIKIPEDIA [https://en.wikipedia.org/wiki/Solid-state\\_chemistry](https://en.wikipedia.org/wiki/Solid-state_chemistry)).

## Topic 7

### Semiconductors and superconductors

During the first part of the lecture, students will learn about semiconductors, which are crystalline or amorphous solids with different electrical characteristics. Semiconductors are materials whose electrical conductivity has an intermediate value between the conductivity of a conductor and a dielectric (insulator). Semiconductors differ from conductors by the strong dependence of



specific conductivity on the concentration of impurities, temperature, various types of radiation, and external electric and magnetic fields. The main property of these materials is an increase in electrical conductivity with increasing temperature. At low temperatures, the electrical conductivity of semiconductors is low. At a temperature close to absolute zero, semiconductors have the properties of insulators. Students will learn, that semiconductors have a completely filled valence band, separated from the conduction band by a narrow band gap. The band gap of semiconductors is usually several eV. For example, diamond can be attributed to wide-bandgap semiconductors (6 eV), and indium arsenide to narrow-bandgap semiconductors (0.35 eV). One of the main characteristics of semiconductors is the valence electron concentration. It is defined as the number of valence electrons per formula unit. This parameter has been reported to be a significant indicator of the structural, thermodynamic and mechanical properties of compounds in various materials systems.

The second part of the lecture will be devoted to superconductivity, which is one of the unique properties inherent in various compounds. The concept of superconductivity is closely related to the Meissner effect, which is the expulsion of a magnetic field from a superconductor during its transition to the superconducting state when it is cooled below the critical temperature. The discovery of the Meissner effect led to the phenomenological theory of superconductivity. This theory explained resistanceless transport and the Meissner effect and allowed the first theoretical predictions for superconductivity to be made. Students will learn that superconductors are characterized by several critical parameters: critical temperature  $T_c$ , critical magnetic field  $B_c$ , critical current  $I_c$ , and critical current density  $J_c$ . There are low-temperature (classical) and high-temperature superconductors. High-temperature superconductors are layered cuprates, while the chemical and structural classes of low-temperature superconductors are diverse.

## LEARNING OUTCOMES

Learn semiconductors as a class of materials, their main characteristics, and applications.

Understand what the valence electrons concentration in semiconductors is responsible for.

Acquaint with the background and history of the discovery of superconductivity.

Learn superconductivity as a phenomenon, and superconductors as a class of materials.

Realize the great benefits of using superconductivity, which will reduce losses during the generation, transmission, transformation, and use of electricity.

#### DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Case study** – presentation of structural features of high-temperature superconductors and derivation of hypothetical structures.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

#### RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): R.E. Gladyshevskii, *Methods to Determine Crystal Structures*, Publishing Center of Ivan Franko National University of Lviv, 2015; E. Parthé, *Elements of Inorganic Structural Chemistry*, K. Sutter Parthé Publisher, Petit-Lancy, 1996; R. Gladyshevskii, K. Cenzual, *Crystal Structures of Classical Superconductors*, In: *Handbook of Superconductivity*, Ch. P. Poole, Jr., Ed., Academic Press, San Diego, California, 2000, Ch. 6; R. Gladyshevskii, Ph.

Galez, *Crystal Structures of High- $T_c$  Superconducting Cuprates*, In: *Handbook of Superconductivity*, Ch. P. Poole, Jr., Ed., Academic Press, San Diego, California, 2000, Ch. 8.

## Topic 8

# Analysis of relationships between the crystal structure and physical properties of individual groups of compounds

During the lecture, students will be introduced to selected physical properties of substances. Crystalline substances mainly are anisotropic and their physical properties depend on crystallographic directions. The symmetry of the property is higher than or equal to the point group of the crystal (Neumann, Curie principles). Properties of crystals are described by corresponding tensors. Based on the elements of symmetry, it is possible to predict the presence or absence of certain properties of the crystal. Many properties of crystals (color, luminescent properties, strength, plasticity) depend significantly on the types and quantity of defects. Pyroelectric and piezoelectric effects, optical activity, and enantiomorphism are manifested only in crystals that belong to non-centrosymmetric point groups. Students will also learn explanations of selected physical properties. The pyroelectric effect is the property of some dielectric crystals to change the amount of electric polarization when the temperature changes. The piezoelectric effect consists in the fact that electrical polarization occurs in the crystal under the action of mechanical stress or deformation. Optical activity is the ability of crystals to rotate the plane of light polarization. Enantiomorphism is the property of some crystals to exist in modifications that are mirror images of each other.

## LEARNING OUTCOMES

Acquaint with the concept of anisotropy of properties.

Understand the essence of such properties of substances as thermal expansion, elasticity, cleavage, pyroelectric effect, piezoelectric effect, refractive indices, enantiomorphism, and optical activity.

Realize that physical properties depend on the peculiarities of the crystal structure of the substance.

## DIDACTIC METHODS USED

**Multimedia presentation** – the use of PowerPoint presentation for the visual presentation of the discussed issues.

**Discussion** – encouraging students to actively participate in the discussion on the discussed issues.

**Quiz** – conduct a short quiz after the lecture to check how well the students have absorbed the knowledge discussed.

## RECOMMENDED READING

Students are expected to read the following texts (selected parts of monographs or textbooks related to the lecture): A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984; R.E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure*, Oxford University Press, 2005; A. Authier, Ed., *International Tables for Crystallography, Vol. D*, Kluwer Academic Publishers, Dordrecht, 2003.

## Course content – laboratory classes

### Topic 1

## Real crystal structure

The laboratory aims to search for voids in the structures of intermetallic compounds, draw the projection of the crystal structures of hydrides, and determine the coordination polyhedra of hydrogen or deuterium atoms.

### LEARNING OUTCOMES

Acquaint with the concept of crystalline state.

Understand the essence of ideal, real, and average structures.

Realize that crystal structures are characterized by the presence of voids that can be filled with atoms. In particular, in the case of hydrogenation of intermetallic compounds, these voids are occupied by hydrogen or deuterium atoms.

### NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

### DIDACTIC METHODS USED

Laboratory course outline:

1. Knowledge check from lecture:

A brief test on symmetry operations, Bravais lattices, space groups, and the difference between ideal, real, and average structures from the lecture to ensure students are well prepared for the laboratory.

2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

### 3. Research:

Each student will receive an individual task with the crystallographic parameters of the intermetallic compound and its hydride.

Each student will draw the projection of the crystal structure of the intermetallic compound and its hydride and determine the coordination polyhedra of hydrogen or deuterium atoms.

### 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

### 5. Summary and conclusions:

From the summary of all the results, students will draw conclusions regarding the voids in crystal structures, that are occupied by of hydrogen or deuterium atoms.

Summarizing the experience and identifying the voids in the crystal structures for materials characterization.

All students will prepare individual reports.

## RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984.

## OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 2

### Defects in crystals

The laboratory aims to determine the defects in crystals, calculate the enthalpy and temperature of defect formation, and establish the influence of impurity phases on the ionic conductivity of crystals.

#### LEARNING OUTCOMES

Learn by which criteria to classify the defects in crystals.

Determine quantitative characteristics related to defects.

Analyze the impact of defects on the crystal structure and physical properties of crystals.

#### NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

#### DIDACTIC METHODS USED

Laboratory course outline:

1. Knowledge check from lecture:

A brief test on different kinds of defects: point defects, clusters of defects, antistructural defects, linear and planar defects from the lecture to ensure students are well prepared for the laboratory.



## 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

## 3. Research:

Each student will receive an individual task with the crystallographic parameters of different modifications of some substances. Each student will do the appropriate calculations to say which of these modifications is stable: (i) at normal temperature and pressure, (ii) at high temperature, (iii) at increased pressure.

Each student will receive the data with the concentration of defects in the crystals of some substances depending on the temperature. The task is to determine the enthalpy of the formation of Schottky or Frenkel defects using the appropriate calculations.

Students in groups will analyze what type of defects dominate in crystals of different substances and what effect small additives have on the conductivity of the crystals.

## 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

## 5. Summary and conclusions:

From the summary of all the results, students will conclude the influence of local changes on the formation of related ordered structures and the appearance of some defects in real crystals.



Summarizing the experience of classification of different kinds of defects in crystals.

All students will prepare individual reports.

#### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; J.W. Morris Jr., *Defects in crystals*, In: *Materials Science and Engineering*, Wiley, 2013.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

### Topic 3

## Crystal chemical analysis of structures

The laboratory aims to establish the relationship between the structures (deformation, substitution, interstitial, and vacancy derivatives) and build a genealogical tree of the  $AlB_2$  family structures based on the group-subgroup relationship between space groups.

#### LEARNING OUTCOMES

Distinguish the first- and the second-order phase transitions.

Learn the types of the relationship between the structures.

Analyze the relations between lattices (unit cells), point and space groups of crystal structures, and as a result establish the relationship between the structures.

## NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

## DIDACTIC METHODS USED

Laboratory course outline:

### 1. Knowledge check from lecture:

A brief test on phase transitions and the parameters that change during them, group-subgroup relationships from the lecture to ensure students are well prepared for the laboratory.

### 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

### 3. Research:

Each student will receive an individual task with the crystallographic data of three intermetallic compounds.

Each student will draw the projection of the crystal structure of the intermetallic compounds and look for similar fragments, as well as analyze the unit cell, point and space groups and get the structural relationship code.

All student will combine their results and build a genealogical tree of the  $AlB_2$  family structures based on the group-subgroup relationship between space groups.

### 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 5. Summary and conclusions:

From the summary of all the results, students will conclude the relationship between different crystal structures.

Summarizing the experience in building a genealogical tree of some family structures and realizing that the affinity between crystal structures implies the affinity between their space groups, which can be represented by the group-subgroup relationship.

All students will prepare individual reports.

#### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; E. Parthé, L. Gelato, B. Chabot, M. Penzo, K. Cenzual, R. Gladyshevskii, TYPIX – Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Gmelin Handbook of Inorganic and Organometallic Chemistry, Springer-Verlag, Berlin, 1993, Vol. 1.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 4

### Modulated structures

The laboratory aims to derive the crystal structure of the compound  $\text{Er}_3\text{Si}_{5-x}$  using crystallographic transformations, calculate interatomic distances in it, plot the dependence of interatomic distances on superspace coordinate  $x_4$ , and determine in which regions of  $x_4$  Si atoms occupy the crystallographic sites.

## LEARNING OUTCOMES

Carry out a description (crystal structure, interatomic distances) of the ideal and real structures.

Construct a matrix transformation from ideal to real structure.

Find out the dependence of interatomic distances on modulation parameters.

## NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

## DIDACTIC METHODS USED

Laboratory course outline:

### 1. Knowledge check from lecture:

A brief test on peculiarities of ideal and real crystal structures and how they are displayed at powder patterns, research at extreme temperatures and pressures from the lecture to ensure students are well prepared for the laboratory.

### 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

### 3. Research:

Each student will receive an individual task with the crystallographic data of the ideal crystal structure and the matrix transformation (through 3 intermediate structures) to the real structure, as well as the crystallographic data for the real structure in terms of the modulated structure.

Each student using matrix transformation will find cell parameters, Wyckoff position and atom coordinates of three intermediate and real structures. The next task is to calculate interatomic distances for modulated structure, plot the dependence of interatomic distances on superspace coordinate  $x_4$ , and determine in which regions of  $x_4$  Si atoms occupy the crystallographic sites.

#### 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 5. Summary and conclusions:

From the summary of all the results, students will conclude that the real crystal structure can be represented with a large unit cell in 3D space, while the unit cell can be rather smaller in 4D space for example in the case of modulated structures.

Summarizing the experience in building crystal structures using matrix transformations.

All students will prepare individual reports.

### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; V.K. Pecharsky, P.Y. Zavalij,

*Fundamentals of Powder Diffraction and Structural Characterization of Materials*, Springer Science + Business Media, New York, 2009.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 5

### Structure refinement

The laboratory aims to refine the crystal structure parameters of the intermetallic compounds: atomic coordinates, displacement parameters, and occupancies.

#### LEARNING OUTCOMES

Refine the crystal structures of the compounds according to the algorithm.

Understand the peculiarities of the crystal structure refinement in multiphase samples.

Correctly interpret and present the obtained results of refinement.

#### NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

#### DIDACTIC METHODS USED

Laboratory course outline:

1. Knowledge check from lecture:

A brief test on the principles of diffraction theory and basics of diffraction techniques from the lecture to ensure students are well prepared for the laboratory.

## 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

## 3. Research:

Each student will receive an individual task with the X-ray powder diffraction pattern of some sample. The task is to perform the phase and structural analysis of the sample. Using crystallographic databases and specialized software each student will carry out these analyses.

The structure parameters are refined gradually in the following sequence: scale factor, unit cell parameters, zero shift parameter, peak width parameters, profile function mixing parameter, texture parameter (preferred orientation of crystal grains), peak asymmetry parameter, atomic coordinates, occupancies (if necessary), isotropic displacement parameters of the atoms in the structure of the compound.

## 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

## 5. Summary and conclusions:

From the summary of all the results, students will conclude that it is important to follow the structure refinement algorithm. They will realize that advances in diffraction theory and modern equipment facilitate qualitative phase and structural analyses.

Summarizing the experience in the refinement of crystal structures in multiphase samples.

All students will prepare individual reports.

#### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; R.A. Young, A.C. Larson, C.O. Paiva-Santos, *Rietveld Analysis of X-Ray and Neutron Powder Diffraction Patterns*, School of Physics, Georgia Institute of Technology, Atlanta, Georgia, 1998.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 6

### Magnetic structure

The laboratory aims to derive magnetic symmetry groups, determine the change in the direction of the atom's spin (magnetic moment) when applying symmetry elements and the inversion operator, and, as a result, make a conclusion about the magnetic properties of the compound.

#### LEARNING OUTCOMES

Understand the magnetic structures and action of the inversion operator.

Know the way of changing the direction of the atom's spin, when applying symmetry elements and the inversion operator.



Learn about the methods by which magnetic structure can be studied.

## NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

## DIDACTIC METHODS USED

Laboratory course outline:

### 1. Knowledge check from lecture:

A brief test on the peculiarities of magnetic structures and the concept of inversion operator from the lecture to ensure students are well prepared for the laboratory.

### 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

### 3. Research:

Each student will receive an individual task with the crystallographic data (including the magnetic symmetry group) of three compounds. Each compound contains at least one magnetic element.

Each student will draw a projection of the structure using symmetry elements, establish the direction of the atom's spin, depict the location of the magnetic moments, and make a conclusion about the magnetic properties of the compound.

### 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 5. Summary and conclusions:

From the summary of all the results, students will conclude that magnetically ordered materials are characterized not only by the symmetry of the crystal lattice but also by a certain ordering of magnetic moments.

Summarizing the experience in the analyzing of magnetic structures.

All students will prepare individual reports.

#### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; R.E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure*, Oxford University Press, 2005.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 7

### Valence electron concentration

The laboratory aims to calculate the valence electron concentration of the chemical compounds, draw projections of crystal structures of the compounds, and indicate homoatomic structural details.

## LEARNING OUTCOMES

Understand the way of formation of valence compounds, the type of chemical bond, that is realized in these compounds, and their classification.

Learn the concept of valence electron concentration and its calculation.

Find out the most common homoatomic structural details, that are observed in the structures of valent compounds.

## NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

## DIDACTIC METHODS USED

Laboratory course outline:

### 1. Knowledge check from lecture:

A brief test on the types of chemical bonds in the compounds, the number of valence electrons in atoms, and the concept of valence electron concentration from the lecture to ensure students are well prepared for the laboratory.

### 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

### 3. Research:

Each student will receive an individual task with the crystallographic data of five chemical compounds.

Each student for each compound will draw a projection of the crystal structure along the shortest translation period, calculate the valence electron

concentration of the chemical compound, determine the number of homoatomic bonds (polyanionic or polycationic), and indicate them as fragments at the projection.

#### 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 5. Summary and conclusions:

From the summary of all the results, students will conclude that in valent compounds, either the cations do not transfer all their valence electrons, but use them to bond with each other (cation-cation), or the anions do not receive enough electrons to complete octets, and therefore form bonds with each other (anion-anion).

Summarizing the experience in the calculation of valence electron concentration and realizing that this value is responsible for the way of atom arrangement in the structures.

All students will prepare individual reports.

### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; A.R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, Chichester, 1984; E. Parthé, *Elements of Inorganic Structural Chemistry*, K. Sutter Parthé Publisher, Petit-Lancy, 1996.

### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

## Topic 8

### High-temperature superconductors

The laboratory aims to derive hypothetical structures of the family of high-temperature superconductors, i.e., determine the stacking of layers in the structure of a high-temperature superconductor and derive the Wyckoff positions, based on the established coordinates of atoms.

#### LEARNING OUTCOMES

Know the essence of the Meissner effect and the classification of superconductors.

Get to know critical parameters, that are characterized superconductors.

Understand the role of atomic layers and the rules of their stacking in high-temperature superconductors.

Derive hypothetical structures of high-temperature superconductors, based on a four-digit code.

#### NECESSARY EQUIPMENT

Computer laboratory equipped with crystallographic databases and specialized software.

#### DIDACTIC METHODS USED

Laboratory course outline:

1. Knowledge check from lecture:

A brief test on superconductivity, the Meissner effect, and classical and high-temperature superconductors from the lecture to ensure students are well prepared for the laboratory.

## 2. Introduction:

Introduction to the topic of the laboratory.

Presentation of goals, procedures, and expected results of the exercise.

## 3. Research:

Each student will receive an individual task with three four-digit codes. The task is to derive hypothetical structures of high-temperature superconductors.

Each student for each four-digit code will establish the general formula and the space group, find out the types and numbers of atomic layers, calculate unit cell parameters, arrange the atomic layers along the crystallographic direction [001] according to the rules of their stacking in high-temperature superconductors, and finally determine atomic coordinates and derive the Wyckoff positions.

## 4. Results analysis:

Each student will discuss the result obtained in the group forum, its correctness and sense.

The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

## 5. Summary and conclusions:

From the summary of all the results, students will conclude that the main class of high-temperature superconductors is copper oxides combined with other metals, especially the rare-earth barium copper oxides (REBCOs) such as yttrium barium copper oxide (YBCO). Cuprates are layered materials, consisting of superconducting layers of copper oxide, separated by spacer layers. Their superconducting properties are determined by electrons moving within weakly coupled copper-oxide ( $\text{CuO}_2$ ) layers.

Summarizing the experience in the deriving of hypothetical structures of high-temperature superconductors.

All students will prepare individual reports.

#### RECOMMENDED READING

R.E. Gladyshevskii, S.Ya. Pukas, *Applied Crystal Chemistry*, Publishing Center of Ivan Franko National University of Lviv, 2022; R. Gladyshevskii, Ph. Galez, *Crystal Structures of High- $T_c$  Superconducting Cuprates*, In: *Handbook of Superconductivity*, Ch. P. Poole, Jr., Ed., Academic Press, San Diego, California, 2000, Ch. 8.

#### OPTIONAL INFORMATION

Exercise manuals will be available.

Students should prepare a theoretical introduction to the laboratories.

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv



**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

The Teachers' Guide is a supplement to the information  
contained in the course syllabus

**PHASE DIAGRAMS OF MULTICOMPONENT SYSTEMS**

**Code: PDMS**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

Introduction to the phase diagrams

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture introduces students to the fundamental theory applicable to all phase diagrams, including the basis of thermodynamics, Gibbs phase rule and condensed phase rule, and other principles and rules. Students will learn the main definitions such as thermodynamic system, system parameter, system component, variance, phase, phase transition, etc. They will get acquainted with the theoretical basis of the construction and interpretation of the phase diagrams of equilibrium systems. Students will realize that by reading the diagram of a substance properly, they will be able to determine the stability of phases under specific conditions and anticipate how these phases will respond to their changes. Since the phase diagram is a graphical representation of substance behaviour under varying conditions of temperature and pressure it allows scientists to comprehend the transitions between different phases of matter, such as solid, liquid, and gas.

#### 3. Learning outcomes

- Students will know the basis of thermodynamics, main concepts and definitions concerning phase diagrams;
- students will understand and know the basic terminology related to phase diagrams;
- students will comprehend the classification of phase diagrams by the number of components;
- students will realize the importance of reading and interpreting the phase diagrams properly in material science and engineering;
- students will be able to use theoretical approaches to the construction and interpretation of the phase diagrams of equilibrium systems.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.

3. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.
4. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

## Topics 2

### 1. The subject of the lecture

Unary phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture aims to acquaint students with single-component systems and their graphical representation in the form of  $p$ - $T$  diagrams. The Gibbs phase rule for these systems will be presented. During the lecture, students should be introduced to the main types of unary phase diagrams such as water and sulphur. They will gain insight into the effects of temperature, pressure, and composition on phase transitions and learn how to predict and interpret them. Invariant, univariate and divariant equilibria, as well as metastable equilibria in these systems, will be described in detail. Allotropy and allotropic modifications will be outlined. After all, the presence of polymorphism in substances complicates the state diagram, since each modification on the state diagram will have its own lines of monovariant equilibrium and areas of existence of phases.

### 3. Learning outcomes

- Students will know the definition of single-component systems and the ways of its graphical representation;
- students will be able to determine the type of the unary phase diagram (water or sulfur) and know the algorithm of its description;
- students will understand the effects of temperature, pressure, and composition on the phase transitions and the ways to predict and describe them;
- students will be able to distinguish invariant, univariate and divariant equilibria and characterize them;
- students will realize the essence of allotropy and allotropic modification, will be able to distinguish stable and metastable equilibria and understand their influence of the properties of the substance;
- will collaborate effectively to explore and discuss the practical applications of unary phase diagrams in materials science and engineering.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.

3. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.
4. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

## Topics 3

### 1. The subject of the lecture

Binary phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture acquaints students with two-component condensed systems and their geometric representation in the coordinates temperature-composition. Gibbs phase rule for this type of systems will be presented. Three main types of phase states in the interaction of heterogeneous components (compounds, solid solutions and mechanical mixtures) and the conditions of their formation will be considered. General regularities of the construction of binary phase diagrams will be covered. Application of the continuity and conformity principles to the phase diagrams will be demonstrated. Students will learn how to present phase equilibria in binary systems, describe and interpret phase transformations that occur in these systems during heating and cooling. A clear algorithm of the description of binary phase diagrams will be presented to the students.

### 3. Learning outcomes

- Students will know the definition of a two-component system and the ways of its graphical representation in the form of the phase diagrams;
- students will know the Gibbs phase rule, the principles of continuity and conformity for this type of system and understand how to apply them;
- students will comprehend the general regularities of the construction of the  $p$ - $T$  binary phase diagrams;
- students will remember the algorithm of the description of binary phase diagrams and will be ready to use it;
- students will realize the importance of reading and interpreting the binary phase diagrams properly in material science and engineering.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

4. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

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## Topics 4

### 1. The subject of the lecture

Topology of binary phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture introduces students to the classification of binary phase diagrams and the relationships between them. The systems with complete mutual solubility of components in liquid and solid state (isomorphous systems); with unlimited solubility of components in a liquid state and a lack of mutual solubility in a solid state; with limited solid solutions and with intermediate phases; with polymorphic transformations of the initial components and intermediate phases; with complete insolubility or limited solubility of components in the liquid state will be considered in detail. The crystallization of samples and the development of their microstructure are highlighted. General patterns of the construction of different types of binary systems will be highlighted. The correlation between the type of phase diagram and the properties of alloys will be demonstrated and illustrated on real examples.

### 3. Learning outcomes

- Students will know the main types of binary phase diagrams and nonvariant equilibrium transitions occurring in them;
- students will comprehend the main differences and the relationships between these phase diagrams;
- students will understand the processes that take place during the crystallization of the samples and the changes in their microstructure caused by this;
- students will remember the general patterns of the construction of different types of binary systems and be ready to use them;
- students will be able to search and review literature data on binary phase diagrams from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.);
- students will realise the correlation between the type of the phase diagram and the properties of alloys.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.



3. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.
4. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

## Topics 5

### 1. The subject of the lecture

Ternary phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture is devoted to the phase diagrams of three-component systems, the main regularities and the geometric bases of their construction. Students will get acquainted with the methods of presenting and determining the quantitative composition of three-component samples, in particular, the method of Roozeboom and Gibbs. They will consider the properties of the concentration Gibbs-Roozeboom triangle and learn to determine the relative amounts of equilibrium phases in three-component alloys using the lever rule and the triangle centre of gravity rule. General approaches to the interpretation of ternary phase diagrams will be discussed. A clear algorithm of their description will be presented to the students.

### 3. Learning outcomes

- Students will know the definition of a three-component system and the ways of its graphical representation in the form of the phase diagram;
- students will understand the main regularities and geometric bases of the ternary phase diagrams construction;
- students will know the Gibbs phase rule for this type of system, and understand how to apply it;
- students will know the methods of presenting and determining the quantitative composition of three-component samples;
- students will remember the algorithm of the description of ternary phase diagrams and be ready to use on real examples;
- students will realize the importance of reading and interpreting the ternary phase diagrams properly in material science and engineering.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.
3. Mats Hillert, Phase Equilibria, Phase Diagrams Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

4. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

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## Topics 6

### 1. The subject of the lecture

Topology of ternary phase diagrams. Isothermal and polythermal sections

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture aims to present the main types of the phase diagrams of three-component system (with unlimited solubility of components in liquid and solid states (isomorphic); with unlimited solubility of components in liquid state and lack of solubility in solid state; with intermediate phases; with limited mutual solubility of components in solid state) and their peculiarities. Students will get acquainted with surfaces, curves and regions of the phase diagrams, their projections on a concentration triangle. They will learn the algorithm of the construction of isothermal and polythermal sections of ternary phase diagrams. The process of crystallization of three-component samples and methods of construction of their cooling curves will be considered. Students will also learn The main approaches to the description of the microstructural components of three component alloys will be pointed out and illustrated.

### 3. Learning outcomes

- Students will know the main types of ternary phase diagrams, the ways of their representation, and comprehend the main differences and the relationships between them;
- students will know general approaches to the description of surfaces, curves, regions and nonvariant equilibrium transitions occurring in these phase diagrams,
- students will understand the processes that take place during the crystallization of three-component samples and the changes in their microstructure caused by this;
- students will remember the general patterns of the construction of isothermal and polythermal sections of ternary phase diagrams and be ready to use them;
- students will be able to search and review literature data on binary phase diagrams from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.);
- students will realise the correlation between the type of the phase diagram and the properties of alloys.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

### 6. Additional notes





Co-funded by  
the European Union

The subject of the lecture covers 2 teaching hours.

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## Topics 7

### 1. The subject of the lecture

Quaternary phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture introduces students to the basics of interpretation and construction of phase diagrams of  $n$ -component systems using the example of quaternary systems. Students will be introduced to the classification of quaternary phase diagrams and ways of their representation. The main methods of presenting and determining the composition of four-component samples will be considered. Peculiarities of the construction of primary and secondary cross-sections, as well as their practical significance for the formation of an idea of the transformations that occur in four-component systems, will be revealed. This knowledge, in particular, can help to correctly choose the temperature regimes of melting and casting of four-component alloys, as well as their heat treatment in metallurgy. Polyhedration as a method of dividing the quaternary phase diagrams with intermediate phases into simpler parts and the regularities of its implementation to facilitate the study of phase equilibria and the interpretation of phase diagrams will be explained. The main types of tetrahedration of the quaternary phase diagram A-B-C-D, depending on the number and composition of compounds, will be considered in detail and illustrated with examples.

### 3. Learning outcomes

- Students will know the definition of multicomponent systems and the ways of their graphical representation in the form of phase diagrams;
- students will understand the main regularities and geometric bases of their construction on the example of quaternary systems;
- students will know the classification of quaternary phase diagrams and the algorithm of their description, the main methods of presenting and determining the composition of four-component samples,
- students will comprehend general approaches to the construction of primary and secondary cross-sections of the quaternary phase diagrams, the main types of their tetrahedration and the practical significance of these procedures.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.

2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

#### 6. Additional notes

The subject of the lecture covers 2 teaching hours.

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## Topics 8

### 1. The subject of the lecture

Methods of the investigation of phase equilibria in multicomponent systems

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture describes the main methods of the investigation of the phase equilibria in multicomponent systems, identification of intermediate phases and solid solutions and studying their homogeneity ranges, construction of binary phase diagrams, isothermal and polythermal sections of ternary and quaternary systems. Thermal analysis (TA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), X-ray powder diffraction (XRD), microstructural analysis, measurement of hardness (microhardness) etc. and opportunities which they provide in the study of phase diagrams will be discussed. Gibbs phase rule and its application in the construction of the phase diagrams of multicomponent systems will be covered. Students will also get acquainted with possible experimental difficulties appearing during the study of the phase equilibria. Typical mistakes during the construction of isothermal and polythermal sections of the phase diagrams will be pointed out.

### 3. Learning outcomes

- students will know the main methods of physicochemical analysis of the phase equilibria in multicomponent systems (thermal, differential thermal, X-ray phase, X-ray structural, microstructural, measurement of hardness (microhardness), etc.)
- students will understand what data each method can provide for the researchers studying the phase diagrams;
- students will comprehend the application of the Gibbs phase rule in the construction of the phase diagrams of multicomponent systems;
- students realize the importance of reading and interpreting multicomponent phase diagrams properly in material science and engineering.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

The lecture will be conducted using multimedia (PowerPoint presentation) and a traditional board to cover key concepts and provide examples illustrating the discussed topics. Conversations with students and active discussion of the main issues will take place. A case study of the real examples of the phase diagrams will be performed.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.
3. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.

### 6. Additional notes

The subject of the lecture covers 2 teaching hours.



## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

Phase diagrams of unary systems: analysis and description

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The thematic scope of the laboratory session is focused on providing students with a deep understanding of the application of fundamental concepts and principles for reading and interpreting phase diagrams of single-component systems. During laboratory classes, students will analyse  $p$ - $T$  diagrams of metallic and non-metallic unary systems interesting from the point of view of their application in particular helium, carbon, iron, silicon dioxide, titanium dioxide, etc. Students will learn to describe phase regions, lines of monovariant equilibria and triple (invariant) points, determine the number of phases which coexist in equilibria in each part of the phase diagram. By characterizing the melting, evaporation and sublimation curves, students will be able to assess the effect of pressure on the melting point and the effect of temperature on the pressure of saturated vapours, understand the meaning of the critical point above which the difference between liquid and gas disappears. During the second part of the laboratory class students will also perform a reverse task - construct an unary phase diagram according to the description. This laboratory class aims to develop students' expertise in searching and analysis of literature data on unary phase diagrams from various scientometric bases (Scopus, Web of Science, Google Scholar, etc.). They will be prompted to carry out a critical analysis of scientific publications and data, extract valuable insights from them, and interpret phase diagrams found there.

#### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation and construction of unary phase diagrams of equilibrium systems;
- to describe phase regions, lines of monovariant equilibria and triple (invariant) points, determine the number of phases which coexist in equilibria in each part of the phase diagrams;
- to assess the effect of pressure on the melting point and the effect of temperature on the pressure of saturated vapours by characterizing the melting, evaporation and sublimation curves;
- to search and critically analyze literature data on unary phase diagrams from different scientometric databases (Web of Science, Google Scholar, etc.) and scientific publications, extract valuable insights from them, and data found there;
- to construct an unary phase diagram according to the description;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

#### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.

## Topics 2

### 1. The subject of the laboratory classes

Binary isomorphous systems: interpretation of the phase diagrams, construction of sample cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will learn to read and interpret phase diagrams of the binary systems with unlimited solubility of components in liquid and solid states, which are called isomorphous. Students will consider the conditions for the formation of continuous series of solid solutions. They will learn Vegard's rule, which states that lattice periods change linearly within the region of their homogeneity, and will see examples of such systems. During the laboratory class, students will learn to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule, as well as build cooling curves for different samples. They will calculate the mass of the starting components for the synthesis of the samples by hand and with special software. A case study of the miscibility gap in the solid state and the formation of ordered solid solutions on the example of the system Au-Cu will be carried out. The laboratory will help students to understand the universality of the phenomenon of solutions for organic and inorganic substances and natural materials and realize their practical significance in materials science and engineering.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of binary isomorphous phase diagrams;
- to search and critically analyze literature data on binary systems from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to calculate the mass of the starting components for the synthesis of the samples by hand and with special software and to choose the conditions necessary for the synthesis of samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

## 8. Optional information

Required software and exercise instructions will be available.

## Topics 3

### 1. The subject of the laboratory classes

Phase diagrams of the binary systems with eutectic and peritectic nonvariant equilibria: analysis, description and construction of samples cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will analyse and interpret binary phase diagrams with unlimited solubility of components in liquid state and without solubility or with limited solubility in solid state. They will describe eutectic and peritectic reactions and write their equations, characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the eutectic and peritectic horizontals. Students will determine the phase composition of samples and build cooling curves. Detailed analysis of the microstructural constituents of eutectic alloys will be conducted during laboratory sessions. A case study of the phase diagrams interesting from the point of view of their practical use will be carried out.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on binary systems from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- describe eutectic and peritectic reactions and write their equations;
- to characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the eutectic and peritectic horizontals;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to analyze the microstructural constituents of eutectic alloys;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks

and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

## 8. Optional information

Exercise instructions will be available.



## Topics 4

### 1. The subject of the laboratory classes

Phase diagrams of binary systems with intermediate phases melting congruently and incongruently: analysis, interpretation and construction of samples cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will consolidate the concept of a chemical compound and a phase, a daltonide and a berthollide. They will consider the nature of the open maximum on the liquidus and solidus curves of the intermediate phase depending on its stability. Using real examples students will learn to interpret the phase diagrams of binary systems with intermediate phases melting congruently and incongruently, having fixed compositions or broad homogeneity range. They will analyse and describe the phase diagrams with intermediate phases forming exclusively from the solid. Such compounds include ordered solid solutions of stoichiometric composition or compounds that are formed from two limiting solid solutions based on the initial components. After considering the last example, students will understand the essence of peritectoid transformation and write its equation. Determining the phase composition of the samples and constructing their cooling curves will also be the task of the laboratory session.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation and construction of binary phase diagrams with intermediate phases melting congruently and incongruently and the phase diagrams with intermediate phases forming exclusively from the solid;
- to search and critically analyze literature data on binary systems from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- to describe congruent and incongruent melting of binary compounds, peritectoid reaction of their formation and write their equations;
- to characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the nonvariant horizontals;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Wiley, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.



## Topics 5

### 1. The subject of the laboratory classes

Phase diagrams of binary systems with polymorphic transformation of intermediate phase: analysis, interpretation and construction of samples cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will consolidate their knowledge of polymorphic transition as the ability of substances to have a different crystal structure depending on external conditions. During polymorphic transformation, not only the type of crystal lattice can change, but also the density of its arrangement, which leads to changes in its physical and chemical properties. Taking this into account students consider the real phase diagrams containing polymorphic modifications of intermediate phases. They learn to interpret these phase diagrams, determine the phase composition of the samples from different parts of the phase diagrams and build their cooling curves.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of polymorphic transitions and polymorphic modifications;
- to search and critically analyze literature data on binary systems from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- to describe phase diagrams of binary systems with polymorphic transformation of intermediate phase;
- to characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the nonvariant horizontals;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan,

analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

## 8. Optional information

Exercise instructions will be available.

## Topics 6

### 1. The subject of the laboratory classes

Phase diagrams of binary systems with allotropic modifications of the initial components: analysis, interpretation and construction of samples cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will continue to consolidate their knowledge of polymorphic transitions by interpreting phase diagrams with allotropic modifications of the initial elements. They will carry out a case study of the phase diagrams with solid solutions, in particular with a continuous series of solid solutions formed on the basis of allotropic modifications of both components, with the solid solution of closed homogeneity region on the basis of one of the components. They will also describe the phase diagrams with eutectoid, monotectoid and metatectic nonvariant equilibria. Students will write the equations of corresponding reactions and characterize phase regions of the phase diagrams. They will determine the phase composition of different samples and build their cooling curves.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of allotropic modifications substances;
- to search and critically analyze literature data on binary systems from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- to analyse phase diagrams of binary systems with allotropic modifications of the initial components,
- to describe eutectoid, monotectoid and metatectic reactions and write their equations;
- to characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the nonvariant horizontals;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes,

students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

## 8. Optional information

Exercise instructions will be available.

## Topics 7

### 1. The subject of the laboratory classes

Phase diagrams of binary systems with limited solubility of components in liquid state: analysis, interpretation and construction of sample cooling curves

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will expand their knowledge of the mutual solubility of components in two-component systems by carrying out a case study of the binary phase diagrams with limited solubility of components in a liquid state. Students will understand how the delamination of components occurs in the solid state and what can cause it. They will learn to recognize and distinguish monotectic and syntectic nonvariant transitions, describe and write their equations. They will determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule, as well as build cooling curves for different samples.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on binary phase diagrams from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications, and describe phase diagrams found there;
- to analyse and interpret phase diagrams of binary systems with limited solubility of components in liquid state,
- to describe monotectic and syntectic reactions and write their equations;
- to characterize phase regions, liquidus, solidus curves and solubility limiting curves (solvus), describe by figurative points the nonvariant horizontals;
- to determine the phase composition of the sample and the quantitative ratio of phases in it using the lever rule;
- to build cooling curves of two-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks

and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases are expected to use in the laboratory class:

1. Binary Alloy Phase Diagrams. 2nd ed. Eds. T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak. ASM International, Materials Park, Ohio-USA, 1990. ISBN 9780871704030.
2. Hiroaki Okamoto, Desk Handbook: Phase Diagrams for Binary Alloys. Second Edition, ASM International, Materials Park, Ohio-USA, 2000. ISBN 9781615030460.
3. Pauling File. Inorganic Materials Database and Design System. Binaries Edition. Eds. P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince, S. Iwata. ASM International, Materials Park, Ohio-USA, 2002.

Students should prepare a theoretical introduction to the laboratories.

## 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

## 8. Optional information

Exercise instructions will be available.



## Topics 8

### 1. The subject of the laboratory classes

Construction of the binary phase diagrams based on their description

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

This laboratory class is devoted to the construction of the phase diagrams of two-component systems. Students will get acquainted with the construction of phase diagrams using the thermodynamic potential method. Applying the Gibbs phase rule and other thermodynamic principles, students will develop skills to construct binary phase diagrams based on the results of their physicochemical analysis, for example, thermal analysis. Having the composition of alloys and the values of their melting points and nonvariant equilibrium transitions, students will be able to draw a figure of a  $p$ - $T$  phase diagram of isomorphous systems or systems with eutectic or peritectic equilibria. Students will also practice constructing the phase diagrams by the amount of data sufficient for constructing a phase diagram regarding pure components, their melting points and mutual solubility, temperature and concentration limits of the existence of binary compounds and the temperatures of other nonvariant transformations. During laboratory sessions, students will see possible difficulties and typical mistakes appearing during the construction of the phase equilibria and will discuss how to avoid them.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on binary phase diagrams from different databases (Pauling File, Scopus, Web of Science, Google Scholar, etc.) and scientific publications;
- to construct binary phase diagrams using the thermodynamic potential method,
- to construct binary  $p$ - $T$  phase diagrams based on the results of their physicochemical analysis, e.g. thermal analysis;
- to construct binary phase diagrams from their description;
- to avoid typical mistakes appearing during the construction of the phase equilibria;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan,

analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions and issues for the test will be available.



## Topics 9

### 1. The subject of the laboratory classes

Ternary systems. Exercises with Gibbs-Rooseboom triangle

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will consolidate their knowledge of three-component systems, the main regularities and the geometric bases of construction of their phase diagrams. They will use the Rooseboom and Gibbs methods to determine the quantitative composition of three-component samples marked by the instructor. They will practice with concentration Gibbs-Rooseboom triangle calculating the relative amounts of equilibrium phases in three-component alloys using the lever rule and the triangle centre of gravity rule. Students will receive individual assignments from the teacher regarding the initial components of the system (chemical elements) and sample masses. Based on these data they will calculate the mass of the starting components for the synthesis of three-component samples manually and with special software, e.g. Weight.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of ternary phase diagrams;
- to use Rooseboom and Gibbs methods to determine the quantitative composition of three-component samples;
- to determine relative amounts of equilibrium phases in three-component alloys by the lever rule and the triangle centre of gravity rule;
- to calculate the mass of the starting components for the synthesis of three-component samples manually and with special software;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Required software and exercise instructions will be available.

## Topics 10

### 1. The subject of the laboratory classes

Ternary systems with unlimited solubility of components in liquid and solid state or without solubility in solid state

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During the first half of the laboratory session, students will analyse a ternary system with unlimited solubility of components in liquid and solid state. This is the simplest type of interaction of three components, when they form a continuous series of solid solutions. A system corresponding to this type of interaction is called isomorphic and is formed by three also isomorphic binary systems. During the second half of the laboratory session, students will analyse a ternary system with unlimited solubility of components in liquid state and without solubility in solid state, which is formed by three binary systems of the eutectic type also without solubility of components in solid state. Students will practice with 3D models of the corresponding phase diagrams, describe all surfaces, curves and phase regions and project them on the concentration triangles. They will construct isothermal sections of the diagrams dividing the spatial diagram in the mind by horizontal planes parallel to the plane of the concentric triangle. They will also construct polythermal sections of the phase diagrams parallel to one of the sides of the spatial diagram (the content of one of the three components in the samples is constant) or from one of the corners of the spatial diagram (the ratio between the contents of the two components in the sample is constant). Students will schematically draw cooling curves of the samples selected by the instructor.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of ternary isomorphic phase diagrams;
- to search and critically analyze literature data on ternary systems from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications, describe phase diagrams found there;
- to be familiar with 3D model of the corresponding phase diagrams, describe all surfaces, curves and phase regions and project them on the concentration triangles;
- to construct different isothermal and polythermal sections of the phase diagrams;
- to build cooling curves of three-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychyporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.

## Topics 11

### 1. The subject of the laboratory classes

Ternary systems with limited solid solutions

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will analyse ternary systems with unlimited solubility of components in liquid state and with limited mutual solubility of components in the solid state. They will distinguish systems with four-phase equilibria of the first, second and third classes. Practising with 3D models of the corresponding phase diagrams, students will describe all surfaces, curves and phase regions and project them on the concentration triangle. They will construct isothermal sections of the phase diagram dividing it in the mind by horizontal planes parallel to the plane of the concentric triangle. They will also construct polythermal sections of the phase diagram parallel to one of the sides of the spatial diagram or from one of the corners of the spatial diagram, which make it possible to trace the changes that occur in the samples at different temperatures - from the liquid state to the solid state. Students will also draw cooling curves of the samples selected by the instructor.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of mutual solubility of the components in ternary systems;
- to search and critically analyze literature data on ternary systems from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications, describe phase diagrams found there;
- to be familiar with 3D model of the phase diagrams with limited solid solutions, describe all surfaces, curves and phase regions and project them on the concentration triangles;
- to describe four-phase equilibria of the first, second and third classes and distinguish the corresponding phase diagrams;
- to construct different isothermal and polythermal sections of the phase diagrams;
- to build cooling curves of three-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic

will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.

## Topics 12

### 1. The subject of the laboratory classes

Ternary systems with intermediate phases

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will interpret the phase diagrams of three-component systems with phase transitions different from those considered before and the phase diagrams with the formation of intermediate binary and ternary phases. Students will receive individual tasks from the instructor and, based on the knowledge and skills obtained before, will describe certain types of the ternary system and draw a projection of its phase diagram on the concentration triangle. They will be asked to describe all surfaces, curves and phase regions of the phase diagram and build certain isothermal and polythermal sections of the phase diagrams. For the specified compositions, students should also depict the cooling curves of the samples.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to use theoretical approaches for the interpretation of ternary systems with phase transitions different from those considered before and with the formation of intermediate binary and ternary phases;
- to search and critically analyze literature data on ternary systems from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications, describe phase diagrams found there;
- to be familiar with 3D model of the phase diagrams of corresponding systems, describe all surfaces, curves and phase regions and project them on the concentration triangles;
- to construct different isothermal and polythermal sections of the phase diagrams;
- to build cooling curves of three-component samples;
- to apply knowledge gained from the lab to predict material behaviour;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks



and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.



## Topics 13

### 1. The subject of the laboratory classes

Interpretation of the isothermal sections of ternary systems

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The isothermal section makes it possible to detect a change in phase equilibria from a change in the concentration of components at a constant temperature. Such a section helps to determine the compositions of the equilibrium phases in each three-component sample and estimate their relative amounts, characterize the phase equilibria in qualitative and quantitative terms, and determine the extent of the homogeneity ranges of the formed compounds and solid solutions. During laboratory classes, students will analyse and describe the isothermal sections of ternary phase diagrams found in databases. They will receive individual tasks from the instructor and work on them in groups. The description of the isothermal section of the phase diagram students will carry out following the sequence: 1) describe the mutual solubility of the components; 2) characterize the phase equilibria in binary systems limiting the ternary system (the number and composition of binary compounds, their regions of homogeneity, the solubility of the third component in them, etc.); 3) characterize the phase equilibria in the ternary system (the number and compositions of ternary compounds, their regions of homogeneity, two-phase and three-phase equilibria, etc.).

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on ternary phase diagrams from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications;
- to analyse and describe the isothermal sections of ternary phase diagrams;
- to characterize the phase equilibria (the number and compositions of ternary compounds and solid solutions, their regions of homogeneity, two-phase and three-phase equilibria, etc.);
- to determine the compositions of the equilibrium phases in three-component samples and estimate their relative amounts;
- to collaborate effectively to explore and discuss the practical applications of phase diagrams in materials science and engineering;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- figures of the isothermal sections of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic

will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.

## Topics 14

### 1. The subject of the laboratory classes

Determination of the composition of samples in quaternary systems, calculation of the weight of components for sample production

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Four-component metallic systems with intermediate phases are of great practical importance, as metallurgical and chemical processes, in particular, are based on them. The study of their phase diagrams is an important scientific task. During laboratory classes students will apply acquired knowledge in the representation of quaternary systems, practice in determining the composition of four-component samples by different methods. To depict the compositions of four-component systems, students will use the correct concentration tetrahedron. The vertices of this tetrahedron denote pure components, the compositions of samples of binary systems are depicted on six edges, and samples of ternary systems are depicted on four faces. Compositions of four-component samples are indicated by figurative points inside the tetrahedron. To determine the composition of four-component samples, students will use two methods: 1) by the values of the perpendiculars dropped from the figurative point of the sample on the face of the tetrahedron; 2) by the values of segments that cut off four planes on the edges of the tetrahedron that pass through the figurative point of the alloy parallel to the faces of the tetrahedron. Using the algorithm learned in the lecture, students will calculate the weight of components for the synthesis of four-component samples.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on quaternary systems from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications, describe phase diagrams found there;
- to be familiar with 3D model of the phase diagrams of corresponding systems;
- to determine the composition of four-component samples by different methods;
- to calculate the weight of components for the synthesis of four-component samples;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes,

students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.

2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### **7. Additional notes**

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### **8. Optional information**

Required software and exercise instructions will be available.

## Topics 15

### 1. The subject of the laboratory classes

Polyhedration of quaternary systems

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During laboratory classes, students will learn to describe quaternary systems and characterise phase regions and transitions. They will also acquire skills in performing polyhedration of a four-component system by means of breaking its phase diagram into simpler component parts (secondary systems). After all, knowing the regularities of polyhedration facilitates the study of phase equilibria in four-component systems with intermediate phases, as well as the construction and interpretation of their phase diagrams. For the quaternary system provided by the lecturer students will perform singular tetrahedration of its phase diagram and determine its type (vertex type, free vertex type, ternary compound type or quaternary compound type). They will describe quasi-binary and quasi-ternary systems, and secondary four-component systems that appear during tetrahedration according to the individual tasks obtained from the instructor.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to search and critically analyze literature data on quaternary systems from different databases (Scopus, Web of Science, Google Scholar, etc.) and scientific publications;
- to be familiar with 3D model of the phase diagrams of corresponding systems, describe them and characterise phase regions and transitions;
- to perform singular tetrahedration of quaternary phase diagram and determine its type;
- to describe quasi-binary and quasi-ternary systems, and secondary four-component systems that appear during tetrahedration;
- to collaborate effectively exploring and discussing the practical applications of phase diagrams in materials science and engineering
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop with internet connection;
- 3D models of the phase diagrams;
- figures of the phase diagrams;
- databases;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of databases, specialized software and 3D models of the phase diagrams. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, analyze and discuss the results and draw conclusions. They will also receive individual tasks

and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted

The topic will be covered in 2 teaching hours.

#### 8. Optional information

Exercise instructions will be available.

## Topics 16

### 1. The subject of the laboratory classes

Construction of the phase diagrams based on experimental data

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Laboratory session aims to gain students' understanding of how experimental methods help researchers investigate phase equilibria in multicomponent systems and identify and characterise intermediate phases. During laboratory classes students will perform differential thermal analysis (DTA)/differential scanning calorimetry (DSC)/thermogravimetry (TG), X-ray diffraction (XRD), energy dispersive X-ray analysis (EDX) of the samples, collect experimental data, treat and analyse them. Using the obtained information, students will try to construct a phase diagram of the binary system or the isothermal section of the ternary system according to the task obtained from the instructor. During the lab session students will also get acquainted with the methods of calculating and modelling phase equilibria in the binary system as an example.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to identify key characteristics and ways to obtain necessary information for completing the task;
- to collect, treat and analyse experimental data effectively and use them to construct the phase diagram of the binary system or the isothermal section of the ternary system;
- to implement theoretical knowledge and skills gained during the course to complete the task;
- to discuss own choices and propositions;
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- differential scanning calorimeter;
- X-ray diffractometer;
- scanning electron microscope with EDX-detector;
- personal computer or laptop with internet connection;
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Laboratory classes will be carried out with the use of special equipment and specialized software. At the beginning of the lab session a short quiz on the lab topic will be carried out to ensure that students are ready for the lab. During laboratory classes, students will work in groups, sharing tasks and working together to establish a work plan, carry out an experiment, analyze and discuss the results and draw conclusions. They will also receive individual tasks and perform them independently. Students perform the calculations and prepare the laboratory report on their own. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.



Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, and practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. I.Ye. Barchiy, Ye.Yu. Peresh, V.M. Rizak, V.O. Khudoliy, Heterogeneous equilibria. Uzhhorod, Zakarpattia, 2003. ISBN 966-7400-25-6.
2. B.Ya. Kotur, Z.M. Shpyrka, G.P. Nychyporuk, O.Ya. Zelinska, Physico-chemical analysis of multicomponent systems: laboratory practicum. Lviv: Publishing center of IFNUL, 2013.
3. Anthony R. West, Solid State Chemistry and its Application (Ch.7). Willey, 2014, ISBN 9781119942948.
3. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
4. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Students should prepare a theoretical introduction to the laboratories.

#### 7. Additional notes

ASSESSMENT: laboratory report should be submitted  
The topic will be covered in 2 teaching hours.

#### 8. Optional information

Required software, exercise instructions and issues for the test will be available.



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**ASSEMBLING ELECTRICAL BATTERIES**

**Code: AEB**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

**Fundamental aspects of electrochemical energy sources. Mechanism of generation of electrical energy in batteries**

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture will explain the basic concepts of electrode materials science, as well as the main principles and mechanisms of electrical energy generation during chemical processes. The historical aspect of the development of battery production technologies will also be considered. Considerable attention is paid to the synthesis of new electrode and electrolyte materials. The main criteria for the selection of electrode materials and their influence on the operational characteristics of the battery are discussed. The lecture is focused on the tasks of energy supply, including methods of synthesis of electrode materials, research of their chemical composition and structure, technology of battery manufacturing and their testing. Problems faced by battery technologies and ways to overcome them are presented. The lecture will also outline the prospects of the battery industry.

#### 3. Learning outcomes

- historical aspect of the development of battery materials;
- basic parameters of electrode materials;
- basic structural characteristics of electrode materials;
- able to compare the effectiveness of electrode materials;
- discuss the potential benefits of using battery technologies.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley & Sons, 2012.
3. Beard, Kirby W. Linden's handbook of batteries. McGraw-Hill Education, 2019.
4. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.

## Topics 2

### 1. The subject of the lecture

#### Components of cells and batteries

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture focuses on important characteristics of components of cells and batteries. Cathode materials for Li-, Na- and Mg-ion batteries: synthesis, structure and characterization. Cathode materials for metal hydride batteries. Anode materials for Li-, Na- and Mg-ion batteries: synthesis, structure and characterization. Anode materials for metal hydride batteries (Ni-MH). Intermetallic electrodes for batteries. The lecture highlights the importance of crystal structures of electrode materials and influence on energy capacity and cyclic stability. The lecture explains how to solve the problems of cycle stability of electrode materials. Different ways to improve activity of electrodes. Composite electrodes. Electrolytes for batteries: non-aqueous electrolytes, aqueous solutions, ionic liquids, polymer electrolytes, and hybrid electrolytes will also be discussed.

### 3. Learning outcomes

- basic parameters of cathode materials for Li-, Na- and Mg-ion batteries materials;
- basic parameters of anode materials for Li-, Na- and Mg-ion batteries;
- basic parameters of electrolytes for batteries;

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

1. Besenhard, Jürgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley & Sons, 2012.
3. Beard, Kirby W. Linden's handbook of batteries. McGraw-Hill Education, 2019.
4. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.

## Topics 3

### 1. The subject of the lecture

**The most important characteristics of batteries**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture enables knowledge of important characteristics of batteries: theoretical cell voltage, capacity, and energy, specific energy and energy density. Coulometric efficiency and energy efficiency. Among the important operational characteristics, one should highlight the validity period, cycle life, charge retention, temperature range of performance, and toxicity. Considerable attention in this lecture will be paid to methods of studying these characteristics, namely chronopotentiometry, cyclic voltammetry, electrochemical impedance spectroscopy and others. Charge and discharge process. Thermodynamics and electrode processes at equilibrium. Concentration dependence of the equilibrium cell voltage. Temperature dependence of equilibrium cell voltage. Overpotential of half-cells and internal resistance.

### 3. Learning outcomes

- knowledge of important characteristics of batteries: theoretical cell voltage, capacity, and energy, specific energy and energy density;
- important operational characteristics;
- basic knowledge in thermodynamics of batteries;
- basic knowledge in electrochemical impedance spectroscopy.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley & Sons, 2012.
2. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
3. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
4. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 4

### 1. The subject of the lecture

#### Primary Batteries

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture explains fundamentals and principles of main types of primary batteries: Alkaline batteries (Zinc/alkaline/Manganese Dioxide), Zinc-carbon batteries, Zinc-chloride batteries, Silver-oxide battery, Zinc-air battery. Also will be discussed Lithium-based primary cells, which is batteries that have metallic lithium as an anode. These types of batteries are also referred to as lithium-metal batteries. Materials for anodes and cathodes for primary cells, construction of batteries. The lecture also presents the main characteristics of primary batteries: theoretical cell voltage, capacity, and energy. Recycling and disposal of primary batteries. Reserve cells: Water activated batteries, Electrolyte activated batteries, Gas activated batteries and Heat activated batteries.

### 3. Learning outcomes

- knowledge of specific characteristics of main types of primary batteries;
- future trends development of primary batteries;
- basic knowledge in science and engineering of the primary battery technologies.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
2. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
3. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 5

### 1. The subject of the lecture

**Secondary Batteries. Li-ion batteries**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture presents the most important data for Li-ion secondary batteries that have been developed for mobile applications like cellular phones, power tools, and cars. Li-ion battery performance, charge characteristics of Li-ion batteries. Specific characteristics and safety testing of  $\text{LiC}_6/\text{LiCoO}_2$  Batteries, Polymer Li-Ion Batteries, Thin-Film, and Solid-State Li-Ion Batteries. The future trends development of Li-ion batteries. Intermetallic electrodes for Li-ion batteries. The newest development for secondary flow-cell battery, which allows for cheap large-scale (GWh) energy storage using large basins also discussed. This lecture also presents the Li-ion battery science and engineering, the chemistry of the most relevant secondary battery technologies, kinetics, energy efficiency reduction contributions, and potential in development.

### 3. Learning outcomes

- knowledge of specific characteristics of Li-ion batteries;
- future trends development of Li-ion batteries;
- basic knowledge in science and engineering of the secondary Li- battery technologies.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
2. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
3. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 6

### 1. The subject of the lecture

**Secondary Batteries. Na-ion batteries**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture presents the current state in development of Na-ion batteries. Operating principle and electrode materials. Hard carbon's anodes and their ability to absorb sodium. Carbon arsenide( $\text{AsC}_5$ ) mono/bilayer as an anode material. Metals and semi-metals (Pb, P, Sn, Ge, etc.) electrodes for Na-ion batteries. The layered structure  $\text{MoS}_2$  as a new type of anode for sodium-ion batteries. Cathode materials based on layered transition metal oxides which can reversibly intercalate sodium. The lecture discusses the technological requirements, preparation and properties of new electrode materials for the Na-ion batteries.

### 3. Learning outcomes

- knowledge of specific characteristics of Na-ion batteries;
- future trends development of Na-ion batteries;
- basic knowledge in science and engineering of the secondary Na- battery technologies.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
2. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
3. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.



## Topics 7

### 1. The subject of the lecture

**Metal hydride batteries and fuel cells**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture presents a description of energy sources that are related to hydrogen. Metal hydride and fuel cells are a subclass of alkaline fuel cells that are under research and development. The main types of metallic and intermetallic electrodes capable of absorbing electrochemically released hydrogen will be considered. Metal Hydride-Nickel Batteries.  $AB_5$ ,  $AB_2$  and  $AB$  hydride electrodes. Effect of temperature. Electrode corrosion and storage capacity. Effect of metal substitution. Magnesium based electrodes for Ni-MH. This lecture describes the materials used in fuel cell technology connected with the commercialization of fuel cells for large scale (stationary power units, hydrogen transport, drones, and other applications

### 3. Learning outcomes

- knowledge of specific characteristics of metal hydride batteries;
- knowledge of specific characteristics of fuel cells;
- future trends development of metal hydride batteries;
- basic knowledge in science and engineering of the secondary metal hydride battery technologies.
- 

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 8

### 1. The subject of the lecture

#### Battery manufacturing

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture described in detail the 3 main technological phases: (i) electrode manufacturing, (ii) cell assembly, and (iii) training, aging, and testing that validate the right performance of the assembled battery cells. Electrode manufacturing - from lab to mass production. Coating of electrode foils as per individual desired formulation and material, tailoring to the particular application. Manufacture a battery from a cell is discussed, especially: Electrode Shaping, Electrode Stacking, Tab Welding, Packaging (Pouch Cells), Packaging (Prismatic and Cylindrical Cells), Electrolyte Filling, and Cell Finishing – Formation.

### 3. Learning outcomes

- knowledge of electrode manufacturing;
- knowledge of cell assembly;
- basic knowledge in training, aging, and testing that validate the right performance of the assembled battery cells.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Lecture conducted with the use of multimedia.
- b. During the lecture, presentations of experiments illustrating the discussed topics are made.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

**Synthesis of electrode materials**

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory is the synthesis of samples will by induction or arc melting as conventional methods or by high energy ball milling and reactive mechanical alloying. Preparation and homogenizing annealing of sample in Ta-crucibles. The overall composition of the alloys will be chosen with respect to the nominal composition of the known or expected compounds. Deviations from these nominal compositions will be selected to probe the homogeneity ranges of solid solutions of the included phases. For all systems temperature of annealing will be adjusted individually, depending on the composition of samples.

#### 3. Learning outcomes

The student should be able to:

- synthesize material (alloys, intermetallic compounds);
- carry out heat treatment of the material;
- prepare material for phase and structural analysis;
- prepare material for electrochemical studies;
- will interpret and analyze of the research results.

#### 4. Necessary equipment, materials, etc

- arc melting furnaces;
- induction melting furnaces;
- x-ray diffractometer
- electron microscope

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- d. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015..

## Topics 2

### 1. The subject of the laboratory classes

**Phase analysis of the samples**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory is to determine the phase content of prepared samples. X-ray powder diffraction will be applied as the method of choice for phase analysis. The phase analysis will be performed by Rietveld refinements with FULLPROF. In order to determine the quantitative and qualitative composition of phases, the analysis will be performed using a scanning electron microscope with EDS/WDS analyzer. Microstructures will be observed and phase content will be measured by SEM.

### 3. Learning outcomes

The student should be able to:

- determine the phase content of prepared samples;
- carry out of the Rietveld refinements with FULLPROF;
- prepare material for phase and microstructural analysis;
- prepare material for EDS/WDS analyzing;
- will interpret and analyze of the research results.

### 4. Necessary equipment, materials, etc

- X-ray diffractometer;
- Electron microscope;
- - Polishing machine.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- d. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley

3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 3

### 1. The subject of the laboratory classes

**Investigation of the crystal structures of compounds**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory is to investigate the crystal structures of phases by powder methods. High-temperature powder diffraction and thermal analysis will be carried out. Determination, calculation and interpretation of the electronic and band structures. Bader's topological analysis.

### 3. Learning outcomes

The student should be able to:

- prepare sample for structural investigations;
- powder diffraction measurements;
- carry out of the Rietveld refinements with FULLPROF;
- analyzing of the research results.

### 4. Necessary equipment, materials, etc

- X-ray diffractometer;
- Powdering equipment;
- Computing software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- d. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.



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## Topics 4

### 1. The subject of the laboratory classes

Electrochemical properties of electrode materials.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory is determination of electrochemical properties of electrode materials by electrochemical methods: Cyclic voltammetry (CVA), Chronopotentiometry (CP), Chronocoulometry (CC), and Electrochemical Impedance Spectroscopy (EIS).

### 3. Learning outcomes

The student should be able to:

- prepare sample for electrochemical investigations;
- Cyclic voltammetry (CVA) measurements;
- Chronopotentiometry (CP), Chronocoulometry (CC) measurements;
- Electrochemical Impedance Spectroscopy (EIS) measurements;
- analyzing of the results.

### 4. Necessary equipment, materials, etc

- electrochemical work station;
- computing software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
  - b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
  - c. During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
  - d. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- etc.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

## Topics 5

### 1. The subject of the laboratory classes

Battery prototype manufacturing

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory is to creation of battery prototype. Battery simulations will also be performed, allowing the prediction and optimization of some key battery parameters, such as state of charge, battery life, and charge/discharge characteristics. The temperature range of battery operation will also be investigated

### 3. Learning outcomes

The student should be able to:

- prepare of electrodes for battery prototype;
- prepare of electrolytes for battery prototype;
- electrochemical measurements;
- analyzing of the results.

### 4. Necessary equipment, materials, etc

- press and welding equipment's
- electrochemical work station;
- computing software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. During laboratory classes, students independently plan the course of the experiment and perform it on their own.
- c. During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- d. During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

1. Besenhard, Jurgen O., ed. Handbook of battery materials. John Wiley & Sons, 2008..
2. Daniel, Claus, and Jürgen O. Besenhard, eds. Handbook of battery materials. John Wiley
3. Ma, Jianmin, ed. Battery technologies: Materials and components. John Wiley & Sons, 2021.
4. Korthauer, Reiner, ed. Lithium-ion batteries: basics and applications. Springer, 2018.
5. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of solid state batteries. Vol. 6. World Scientific, 2015.

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**MAGNETISM AND MAGNETIC MATERIALS**

**Code: MAG**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

Classification of magnetic materials. Evolution of magnetic moments.

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to introduce the classification of materials based on their magnetic behaviour. The students will learn the main definitions and magnetic characteristic, including spin and orbital magnetic moments, magnetization, magnetic flux density, magnetic field strength, magnetic susceptibility (volume, mass, molar). The conventional systems of magnetic unit will be presented (SI and CGS), as well as the relationships between them. Diamagnetic, paramagnetic, and magnetically ordered materials will be introduced, typical chemical compositions and electronic structures will be discussed. The relationship between diamagnetism and superconductivity will be demonstrated. Atomic paramagnetism and weak Pauli paramagnetism will be introduced. The student will learn to evaluate the possibility of evolution of magnetic moments based on the electronic structure of the elements. The quantum mechanical tools, such as Aufbau principle and Hund's rules, will be applied. The meaning of the quantum numbers will be repeated, the quantum number  $J$  (total angular quantum number) will be introduced. The students will learn to use a term symbol for the representation of the electronic structure of individual atoms and ions. The dependence of magnetization of a paramagnet as a function of temperature and magnetic field will be discussed, the Brillouin function and Lande factor  $g$  will be presented. The paramagnetic effective moment and saturation moment will be introduced. The Curie law, its quantitative parameters, and its application will be discussed. The students will learn how to calculate theoretical effective moments and saturation moments for the ions of  $3d$  and  $4f$  metals, the difference between these two groups of elements in the terms of orbital moment quenching will be discussed.

#### 3. Learning outcomes

- **Knowledge:** The student will be able to distinguish which chemical elements have the potential to carry magnetic moments of their atoms or ions.
- **Comprehension:** The student will learn which criteria must be fulfilled for an atom/ion to become magnetic
- **Application:** The student will be able to calculate the theoretical values of effective and saturation moments for magnetic atoms/ions
- **Analysis:** The student will be able to interpret the difference between the magnetic atoms of  $3d$ - and  $4f$ -elements
- **Synthesis:** The student will be able to choose the chemical elements to synthesize the compound with desired paramagnetic characteristics
- **Evaluation:** The student will be able to estimate the magnetic properties of compounds with given composition

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – the comparison of the calculated values of effective moments and saturation moments with the experimental ones.

Discussion - encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

- Ch. Kittel. Introduction to Solid State Physics, 7th Ed., Wiley, 1996.

- S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

#### 6. Additional notes

- ASSESSMENT: complete the table with the values of theoretical effective and saturation moments for  $3d$ - and  $4f$ -ions

- The topics will be covered in one lecture

## Topics 2

### 1. The subject of the lecture

Magnetically ordered systems

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will cover the magnetic exchange interaction and, subsequently, the magnetically ordered systems. The students will learn how to distinguish paramagnetic and magnetically ordered state, what are the factors to accomplish a phase transition between the paramagnetic and magnetically ordered state. The basic quantum explanation of the spin correlations will be discussed within the Heisenberg theory and Ising model. The mechanisms of magnetic exchange interaction will be discussed (direct exchange interaction, indirect exchange interaction by superexchange mechanism, conducting electrons mediated indirect RKKY exchange interaction), as well as their relationship to the chemical composition and the crystal structure of the compounds. The relative strength of each type of exchange interaction and the typical representatives will be presented. The magnetic ordering will be regarded in the terms of collective phenomena. Special features of ferromagnetism, antiferromagnetism, ferrimagnetism will be discussed, as well as more complex magnetic systems (i.e. helical and spiral structures). Various type of magnetic critical temperatures (Curie temperature, Neel temperature) will be analysed. The theory of mean-field approach (Weiss field) will be applied to describe the behaviour of magnetic systems with exchange interactions. The Curie-Weiss law will be introduced, its difference from Curie law will be discussed, the meaning of paramagnetic Curie temperature with respect to the exchange interactions will be discussed. The ferromagnet-paramagnet phase transition will be explained within the framework of Landau theory of ferromagnetism (II order phase transition). The theoretical background for constructing Arrott plots will be presented. The classification of the ferromagnetic materials based on the shape of hysteresis curve will be introduced, hard and soft magnetic materials will be discussed, the areas of application for each group will be outlined. The theory of sublattices will be demonstrated for antiferromagnetic materials. The interplay between the compensation and Curie temperature will be discussed. Exchange interactions for geometrically complex systems will be considered, giving way to magnetic frustrations or the formation of *kagome* nets.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define the mechanism and the type of exchange magnetic interactions
- **Comprehension:** The student will be able explain the magnetic properties of bulk materials based on exchange interactions
- **Application:** The student will be able to choose the potential applications for materials with given types of exchange interactions
- **Analysis:** The student will be able to discuss the peculiarities of various groups of magnetically ordered systems
- **Synthesis:** The student will be able to propose the chemical composition and crystal structures for magnetically ordered materials with given parameters

- **Evaluation:** The student will be able to estimate the efficiency of magnetic materials based on their characteristics in magnetically ordered state

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – analysis of the chemical compositions of various magnetically ordered systems, relationships between the quantitative parameters of magnetic properties and chemical composition.

Discussion - encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

A.R. West. Basic Solid State Chemistry, 2nd Ed., John Wiley & Sons, Ltd, 1999.

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

#### 6. Additional notes

- The topics will be covered in one lecture



## Topics 3

### 1. The subject of the lecture

Magnetic structures. Magnetic phase diagrams

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The correlations between the crystal structure and the magnetic structure, and the application of the tool of phase diagrams to the magnetic systems will be the subject of this lecture. The definition of the magnetic structure will be introduced, the classification of the magnetic structures based on the dominating type of magnetic exchange interaction, the direction and mutual orientation of magnetic moments, the presence of modulations (commensurate or incommensurate) will be presented. The parameters for full description of magnetic structure will be named (temperature range, modulation wavevector, direction and magnitude of magnetic moment). Magnetic symmetry will be introduced. The rules to derive the magnetic point groups will be applied, the allowed types of magnetic order will be outlined. The magnetic space groups and Magnetic Group Tables will be introduced. The students will get familiar with the magnetic structures of the most common simple magnetic transition 3d metals (Fe, Co, Ni). It will demonstrate the reason for magnetocrystalline anisotropy. The mechanisms of magnetocrystalline anisotropy, the types (easy axis, easy plane, easy cone), and the quantitative parameters (energy, constants, and field of anisotropy) will be presented. The magnetic phase diagrams will be regarded in temperature-field coordinates, the representation of various magnetic phases and magnetic phase transitions will be illustrated. The analogies with conventional phase diagrams will be drawn.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define the magnetic space groups, the types of magnetic phase transitions
- **Comprehension:** The student will be able to find the correlation between the magnetic symmetry and bulk magnetic properties
- **Application:** The student will be able to use the magnetic symmetry operations to derive the magnetic structure and to interpret the magnetic phase diagrams for
- **Analysis:** The student will be able to find the optimal way to obtain the magnetic material with desired properties based on the magnetic phase diagram
- **Synthesis:** The student will be able to derive the hypothetical magnetic materials based on the magnetic symmetry and magnetic phase diagrams
- **Evaluation:** The student will be able to estimate the bulk magnetic properties of materials with given magnetic structure parameter

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – application of the magnetic symmetry operations, deriving the magnetic structures from the known set of symmetry operation.

Discussion - encouraging students to participate in the discussion on the issues actively.

**5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students are expected to read below texts related to the lecture:

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

**6. Additional notes**

- The topics will be covered in one lecture

## Topics 4

### 1. The subject of the lecture

Magnetism in materials

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

In this lecture the students will understand the relationship between the place of a chemical element in the periodic table and its ground magnetic properties. The first approach will be given using a “quasi-periodic” table for transition metals by Smith and Kmetko. The general trends will be outlined for the compounds of  $3d$ -elements,  $4f$ -elements, and the combination of  $3d$ - and  $4f$ -elements. The basic features for localized and band magnetism will be presented. The inconsistency between the Hund’s rules and ordered moments will be discussed in the case of  $3d$ -metals. The fundamentals of electronic structure of metallic systems will be reminded, the definitions of the density of states and Fermi level will be emphasized. The application of the electronic band theory to magnetically ordered systems will be demonstrated and the Stoner criteria will be introduced. Besides, the methods for the enhancement of magnetism will be discussed. The localized magnetism will be illustrated by the compounds of magnetic  $4f$ -elements. The definition of the de Gennes factor will be given. The peculiarities of the compounds containing both magnetic  $4f$ - and  $3d$ -metals will be discussed. The modified Curie-Weill law will be presented, the reasons for additional temperature-independent term will be discussed. The fundamentals of the  $5f$ -magnetism will be mentioned. The Hill limit for the occurrence of magnetism will be introduced. The role of orbital magnetic moments and giant magnetic anisotropy will be discussed.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define the peculiar features of the magnetic compounds of  $3d$ -,  $4f$ -,  $4f$ - $3d$ -,  $5f$ -elements
- **Comprehension:** The student will be able to explain different magnetic behaviour of the compounds of  $3d$ -,  $4f$ -,  $4f$ - $3d$ -,  $5f$ -elements
- **Application:** The student will be able to define the qualitative and quantitative parameters required for magnetic materials
- **Analysis:** The student will be able to discuss the efficiency of given compounds with respect to their potential application as magnetic materials
- **Synthesis:** The student will be able to derive the combination of the magnetic atoms of different origin to satisfy the requirement to efficient magnetic materials, including ordering temperatures and magnitude of magnetic moments
- **Evaluation:** The student will be able to compare various groups of magnetic materials and to outline the areas of their application

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – the typical representatives of the  $3d$ -,  $4f$ -,  $4f$ - $3d$ -,  $5f$ -magnets will be presented, the parameters of the magnetic properties will be analyzed.

Discussion - encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

A.R. West. Basic Solid State Chemistry, 2nd Ed., John Wiley & Sons, Ltd, 1999.

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

#### 6. Additional notes

- The topics will be covered in one lecture

## Topics 5

### 1. The subject of the lecture

Experimental methods in magnetism

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will cover the main experimental methods to study the magnetic properties of the materials, and the students will be able to develop their skills in the interpretation of experimental data. For better understanding of the applied experimental techniques, a common classifications will be given: (i) direct and indirect methods; (ii) macroscopic (or bulk) and microscopic methods. The conventional direct methods to measure the magnetization and susceptibility will be introduced, including force, induction, rotation and SQUID magnetometers. The general principles for each type of magnetometer will be presented, their advantages and drawbacks will be discussed, the quantum phenomena in SQUID magnetometers will be presented, practical application of SQUID detectors will be outlined. The microscopic direct method to measure local magnetic moments and fields will be represented by neutron diffraction and Mössbauer spectroscopy. The fundamental properties of neutrons will be described, the methods to produce neutrons will be analysed, the advantages of neutrons over other sources of radiation will be outlined, the fundamentals of elastic neutron scattering will be explained, the major research facilities offering the tools for neutron diffraction experiments will be named. The students will get familiar with the interpretation of neutron diffraction patterns for magnetic compounds, what information can be extracted, what software is applicable. The role of  $\gamma$ -rays in the solid state research will be demonstrated on the example of Mössbauer spectroscopy. The students will get familiar with the Mössbauer effect and the main quantitative parameters of Mössbauer spectra: isomer shift, quadrupole splitting, and Zeeman splitting. The definition of Mössbauer isotopes will be provided. The examples of Mössbauer spectra for various magnetic compounds will be analysed. The indirect methods of the magnetic properties' studies will include electric resistivity, magnetoresistance, and specific heat measurements. The magnetic contribution to the resistivity will be discussed in the terms of Matthiessen rule. The interplay between the resistivity and magnetism will be studied in the context of Hall effect and magnetoresistance. The general theory of specific heat will be provided for better understanding of the effect of magnetic phase transitions on the shape of specific heat curve and its role in the development of magnetocaloric materials which will be the subject of the next lecture.

### 3. Learning outcomes

- **Knowledge:** The student will learn the principles of the direct and indirect, bulk and microscopic methods of the experimental studies of the magnetic properties of materials
- **Comprehension:** The student will be able to describe the requirements and the outcome of various experimental methods in magnetism
- **Application:** The student will be able to draw an algorithm for the most informative studies of magnetism of given compounds
- **Analysis:** The student will be able to discuss the experimental results of the magnetic measurements and to compare them to those of other known materials

- **Synthesis:** The student will be able to combine the results of various complementary experimental methods to provide the most full and reliable description of magnetism in a material
- **Evaluation:** The student will be able to extract the parameters of the magnetic properties of materials

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – to propose an algorithm for the full cycle of the studies of magnetism of a given compound.

Discussion - encouraging students to participate in the discussion on the issues actively.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

N.W. Ashcroft, N.D. Mermin. Solid State Physics, Saunders, 1976.

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

#### 6. Additional notes

ASSESSMENT: to provide a full description of magnetic behaviour of a given compound based on a set of experimental data

- The topics will be covered in two lectures

## Topics 6

### 1. The subject of the lecture

Magnetic materials

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The survey of magnetic materials within this lecture will be provided with respect to various groups of applications of magnetic materials. At the beginning an attention will be paid to the production of permanent magnetic. The basic characteristics of Fe, Co, Ni will be given, as well as the most important commercial magnetic alloys based on 3d-metals. The impact of element substitutions on the magnetization value, Curie temperature, anisotropy constants, anisotropy *etc* will be discussed. The group of rare-earth containing magnets will be represented primarily by  $\text{SmCo}_5$  and  $\text{Nd}_2\text{Fe}_{14}\text{B}$  compounds, commercially accessible hydrides, but also by intermetallic compounds  $R_2T_{17}$ ,  $RT_2$  which can be tuned by various substitutions. For each compound, specific area of application will be defined. The magnetoresistance materials will cover thin films (Fe/Cr) and the family of perovskite manganites. The complex magnetic phase diagrams of magnetic perovskites will be analysed. The magnetocaloric materials will be presented with respect to their performance (working temperatures and relative cooling power), various  $\text{Gd}_5(\text{Ge,Si})_4$  phases will be discussed.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define various application of magnetic materials and their typical representatives
- **Comprehension:** The student will be able to describe the functional magnetic properties of various classes of magnetic materials based on their chemical compositions and crystal structures
- **Application:** The student will be able to predict the area of application of given magnetic materials and vice versa, choose an appropriate material for given application
- **Analysis:** The student will be able to draw a system of relationships composition-structure-property
- **Synthesis:** The student will be able to predict new classes of materials for various areas of application
- **Evaluation:** The student will be able to estimate the efficiency of various groups of compounds with respect to their application

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – specific groups of magnetic materials, their crystal structures.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

A.R. West. Basic Solid State Chemistry, 2nd Ed., John Wiley & Sons, Ltd, 1999.

## 6. Additional notes

- The topics will be covered in one lecture

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## Topics 7

### 1. The subject of the lecture

Unconventional magnetism

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will give an insight into the materials with exotic magnetic behaviour. The systems with strong electron correlations will be presented, including heavy fermion systems and Kondo lattice. The compounds demonstrating the coexistence of magnetism and superconductivity will be introduced. The peculiarities of magnetic nanoparticles and low dimension (0D-, 1D-, 2D-) will be discussed. The concept of superparamagnetism will be introduced, the effects of size distributions on the magnetic characteristics will be considered. The properties and applications of thin magnetic layers will be presented. The quantum materials will be discussed, including topological quantum materials, magnetic skyrmions etc. The peculiarities of the crystal structures of the quantum materials will be analysed.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define the magnetic properties beyond the classical conventional approach
- **Comprehension:** The student will be able to describe the factors causing the evolution of unconventional magnetic phenomena
- **Application:** The student will be able to find the areas of application of unconventional magnets
- **Analysis:** The student will be able to discuss the difference between conventional and unconventional magnetism
- **Synthesis:** The student will be able to find the tool to tune the parameters of magnetic materials in unconventional regime
- **Evaluation:** The student will be able to estimate the qualitative and quantitative parameters for unconventional magnets, to specify the range, i.e. concentration, temperature, field, where these properties are manifest

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Multimedia presentation - the use of PowerPoint presentations for discussed issues and examples.

Case study – specific groups of magnetic materials, their crystal structures.

Discussion - encouraging students to participate in the discussion on the issues actively.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

### 6. Additional notes

- ASSESSMENT: an essay (the list of topics will be provided)
- The topics will be covered in one lecture

## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

Introductory lesson. Safety techniques in laboratories

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory class is to get familiar with the laboratory. The students are obliged to learn the rules and the safety precautions related to the work in the laboratory of magnetic studies. Afterwards, the students get familiar with the equipment and perform the calibration of the Faraday magnetometer.

The preparation of the sample includes the characterization of the sample (elemental analysis and X-ray phase analysis). Finally, the mounting of the sample must be performed for further measurements.

#### 3. Learning outcomes

After completing the course, students:

- are aware of the safety precautions required to work in the laboratory of magnetic properties measurements;
- are aware of requirements to the sample for magnetic measurements, including its purity, weight, shape etc,
- can prepare the sample for magnetic measurements.

#### 4. Necessary equipment, materials, etc

- laboratory equipped with X-ray fluorescent spectrometer
- laboratory equipped with X-ray diffractometer
- computer laboratory with installed crystal structure database
- laboratory equipped with magnetometer

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- Quiz - summarized the essential information
- The main topic will be implemented during 4-hour classes in the form of a project task, in which students will design the assumptions and plan of the experiment in a group.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

-

#### 7. Additional notes

- The topics will be covered during 4-hour classes.

#### 8. Optional information

The safety precautions test should be passed

## Topics 2

### 1. The subject of the laboratory classes

Susceptibility of Curie-Weiss paramagnet

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory classes is to collect the magnetic susceptibility data in paramagnetic range, to convert the quantitative values obtained to a conventional system of magnetic unit, to extract the paramagnetic parameters and to analyse the obtained values. The students perform the susceptibility measurements, plot the data in the representation of direct and inverse magnetic susceptibility, based on the shape of the curve choose the proper equation to describe the dependence (Curie, Curie-Weiss, or modified Curie-Weiss fit), and extract the paramagnetic parameters (effective moment, paramagnetic Curie temperature, temperature-independent susceptibility term). The student make a conclusion which atom carries the magnetic moment and compare the obtained value with the calculated. In case the atom can exist with different valence states, a conclusion should be made about the valence state of the atom. Based on the value of paramagnetic Curie temperature, a conclusion on the exchange interactions must be drawn.

### 3. Learning outcomes

After completing the course, students:

- are aware of the construction of magnetometer;
- can perform the measurements of the temperature dependence of magnetic susceptibility and present the data in conventional format;
- can find the proper fit to describe the temperature dependence and extract the values of the effective moment and the paramagnetic Curie temperature;
- can interpret the obtained values in terms of defining the magnetic atoms and the type of magnetic exchange interactions;
- can determine the valency of the atoms of elements exhibiting mixed valency.

### 4. Necessary equipment, materials, etc

- laboratory equipped with magnetometer
- computer laboratory with the software for plotting graphs and fitting curves

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- During laboratory classes, students perform the calculations and prepare the laboratory report on their own.

- The main topic will be implemented during 8-hour classes in the form of a project task, in which students will design the assumptions and plan of the experiment in group and analyze the results on their own.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

Students are obliged to prepare a theoretical background as the introduction part to the laboratory report.

#### 7. Additional notes

- ASSESSMENT: laboratory report should be submitted
- The topics will be covered during 8-hour classes.

#### 8. Optional information

Exercise manuals will be available

## Topics 3

### 1. The subject of the laboratory classes

Magnetically ordered systems

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the studies of the magnetically ordered systems. The students will collect the susceptibility data from paramagnetic range down to the lowest available temperatures. In the magnetically ordered state ( $T < T_c$  ( $T_N$ )) the field dependences of magnetization will be obtained. The experimental data will be processed. The conclusions on the type of magnetic order must be drawn. The quantitative values of the ordered magnetic moments will be compared to calculated one. The assumptions on the magnetic structure can be drawn with respect to the crystal structure and considering of the complexity of magnetic behaviour.

### 3. Learning outcomes

After completing the course, students:

- are aware how to choose a proper sequence for measuring the magnetic properties of magnetically ordered systems;
- are able to distinguish the difference between the shapes of susceptibility and magnetization curves from various types of magnetically ordered systems;
- are able to estimate the quantitative parameters of magnetically ordered systems (e.g. ordering temperature, saturation moment, spontaneous magnetization, metamagnetic field);
- can interpret the obtained results with respect to the theoretical values of magnetic moments.

### 4. Necessary equipment, materials, etc

- laboratory equipped with magnetometer
- computer laboratory with the software for plotting graphs and fitting curves

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- During laboratory classes, students perform the calculations and prepare the laboratory report on their own.
- The main topic will be implemented during 8-hour classes in the form of a project task, in which students will design the assumptions and plan of the experiment in group and analyze the results on their own.

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

Students are obliged to prepare a theoretical background as the introduction part to the laboratory report.

## 7. Additional notes

- ASSESSMENT: laboratory report should be submitted
- The topics will be covered during 8-hour classes.

## 8. Optional information

Exercise manuals will be available

## Topics 4

### 1. The subject of the laboratory classes

Magnetic susceptibility of multi-phase alloys

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory classes is related to the magnetic studies of paramagnetic compounds in the presence of ferromagnetic impurity. The students will have to draw an algorithm how to separate the contributions from two phases. They will get a set of experimental data, process the data, separate two contributions and evaluate the parameters for each phase. The students will evaluate the intrinsic paramagnetic parameters of the main phase and will estimate the signal from the impurity phase. Knowing the composition of the impurity phase, the students will estimate the content of the impurity phase and, subsequently, will make a conclusion of the sensibility of magnetic measurements.

### 3. Learning outcomes

After completing the course, students:

- are aware to separate the signals from paramagnetic and ferromagnetic phases in a double phase alloy;
- can evaluate the intrinsic paramagnetic parameters of the paramagnetic phase;
- can estimate the content of a spurious ferromagnetic phase;
- can compare the sensibility of the magnetic measurements and other available techniques in case of ferromagnetic impurity.

### 4. Necessary equipment, materials, etc

- computer laboratory with the software for plotting graphs and fitting curves

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- During laboratory classes, students perform the calculations and prepare the laboratory report on their own.
- The main topic will be implemented during 6-hour classes in the form of a project task, in which students will design the assumptions and plan of the experiment in group and analyze the results on their own.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

Students are obliged to prepare a theoretical background as the introduction part to the laboratory report.

#### 7. Additional notes

- ASSESSMENT: laboratory report should be submitted
- The topics will be covered during 6-hour classes.

#### 8. Optional information

Exercise manuals will be available



## Topics 5

### 1. The subject of the laboratory classes

Arrott plots

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topic of the laboratory classes is related to the application of the Landau theory of the second order ferromagnetic phase transition. The students will get a chance to check the validity of the theory experimentally. The students will get a set of magnetization curves measured in the vicinity of the ferromagnetic phase transition. They will have to process the experimental data, draw the corresponding plot in the coordinates  $M = f(H)$  and Arrott's plot  $M^2 = f(H/M)$ . Based on the latter isotherms, the data for the precise estimation of the Curie temperature can be extracted. The students will draw a conclusion on the application of Arrott's plot for ferromagnets and will characterize the given material.

### 3. Learning outcomes

After completing the course, students:

- can apply the Landau theory of the second order phase transition for experimental determination of the Curie temperature;
- can plot the Arrott plots allowing precise determination of the Curie temperature;
- can demonstrate the validity of the quantum approach to the description of bulk properties of a material;
- can determine the Curie temperature precisely

### 4. Necessary equipment, materials, etc

- computer laboratory with the software for plotting graphs and fitting curves

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- During laboratory classes, students work in a group, sharing tasks and working together to establish a work plan, analyze the results and draw conclusions.
- During the laboratory classes, presentations of experiments illustrating the discussed topics are made.
- During laboratory classes, students perform the calculations and prepare the laboratory report on their own.
- The main topic will be implemented during 8-hour classes in the form of a project task, in which students will design the assumptions and plan of the experiment in group and analyze the results on their own.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

K.H.J. Buschow, F.R. de Boer, Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

Students are obliged to prepare a theoretical background as the introduction part to the laboratory report.

#### 7. Additional notes

- ASSESSMENT: laboratory report should be submitted
- The topics will be covered during 6-hour classes.

#### 8. Optional information

Exercise manuals will be available

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**DATABASES FOR MACHINE LEARNING**

**Code: DBML**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

Scientific information retrieval systems

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to present the common information search systems:

- ✓ **Scirus** (The first comprehensive search engine dedicated to science that was launched in April 2001. This product does a decent job of filtering out sources in its customized crawl of over 250 million, journal, and database sources);
- ✓ **BASE: Bielefeld Academic Search Engine** (One of the most comprehensive search engines in the world, especially for academic web resources, providing more than 340 million documents from more than 11 000 content providers, access to the full texts of about 60% of indexed documents for free (Open Access). BASE is managed by the Bielefeld University Library);
- ✓ **WorldWideScience** (A global science search engine (Academic databases and search engines) designed to accelerate scientific discovery and progress by accelerating the sharing of scientific knowledge);
- ✓ **FindArticles** (A website which provided access to articles previously published in over 3 000 magazines, newspapers, journals, business reports and other sources. The site offered free and paid content through the HighBeam Research database);
- ✓ **Science Research Portal** (A scientific search engine that performs full-text search in the journals of many scientific publishers, such as Elsevier, Highwire, IEEE, Nature, Taylor & Francis, etc. Searches for articles and documents in open scientific databases: Directory of Open Access Journals, Library of Congress Online Catalog, Science.gov, Scientific News etc.);
- ✓ **Chemical Abstracts Service (CAS)** (A division of the American Chemical Society, has provided the most comprehensive repository of research in chemistry and related sciences for over 100 years. CAS innovations have fueled chemical research through development of the CAS Registry<sup>SM</sup> and CAS databases which contain invaluable information for chemical scientists, including SciFinder<sup>®</sup> and STN<sup>®</sup>);
- ✓ **ScienceDirect** (A website that provides access to a large bibliographic database of scientific and medical publications of the Dutch publisher Elsevier. It hosts over 18 million pieces of content from more than 4 000 academic journals and 30 000 e-books of this publisher);
- ✓ **Scopus** (A source-neutral abstract and citation database curated by independent subject matter experts who are recognized leaders in their fields. Scopus puts powerful discovery and analytics tools in the hands of researchers, librarians, research managers and funders to promote ideas, people and institutions. Scopus indexes content from 7 000+ publishers and includes 91+ million records, 94 000+ affiliation profiles and 17+ million authors);
- ✓ **Web of Science** (A platform consisting of several literature search databases designed to support scientific and scholarly research);

- ✓ **Google Scholar** (Search for scholarly literature across many disciplines and sources: articles, theses, books, abstracts and court opinions, from academic publishers, professional societies, online repositories, universities and other web sites)

### 3. Learning outcomes

- ✓ Students will know common information search systems such as Scirus, BASE: Bielefeld Academic Search Engine, WorldWideScience, FindArticles, Science Research Portal, Chemical Abstracts Service (CAS), ScienceDirect, Scopus, Web of Science, Google Scholar.
- ✓ Students will become familiar with the capabilities of databases, search tools.
- ✓ Students will be able to search for scientific literature using various search services.
- ✓ Students will understand the importance using modern databases.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

<https://www.elsevier.com/>

<http://www.scirus.com> (Scirus) НЕ ПРАЦЮЄ

<https://www.base-search.net/> (BASE: Bielefeld Academic Search Engine)

<https://worldwidescience.org/> (WorldWideScience)

<http://www.findarticles.com/> (FindArticles)

<https://www.scienceresearch.com> (Science Research Portal) НЕ ПРАЦЮЄ

<https://www.cas.org/> (Chemical Abstracts Service (CAS))

<https://www.sciencedirect.com/> (ScienceDirect)

<https://www.scopus.com/> (Scopus)

<https://www.webofscience.com/> (Web of Science)

<https://scholar.google.com/> (Google Scholar)

### 6. Additional notes

The topics will be covered in one lecture

## Topics 2

### 1. The subject of the lecture

#### Crystallographic databases

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to present the crystallographic databases:

- ✓ **Pearson's Crystal Data (PCD)** (A crystallographic database contains crystal structures of a large variety of inorganic materials and compounds. The current release 2023/24 contains about 395 000 structural data sets (including atom coordinates and displacement parameters, when determined) for about 180 000 different chemical formulas, roughly 21 700 experimental powder diffraction patterns and about 375 000 calculated patterns (interplanar spacings, intensities, Miller indices). In addition over 62 000 figure descriptions for such as cell parameters as a function of temperature, pressure or concentration are given. To reach this result, scientific editors have critically analyzed and processed over 128 000 original publications.);
- ✓ **Crystallography Open Database (COD)** (Open-access collection of crystal structures of organic, inorganic, metal-organic compounds, and minerals, excluding biopolymers. All data in the COD and the database itself are dedicated to the public domain and licensed);
- ✓ **Bilbao Crystallographic Server (BCS)** (Web site with crystallographic programs and databases freely available on-line);
- ✓ **Powder Diffraction File (PDF)** (Database contains 1 186 076 material data sets (release 2024), each of them contains diffraction, crystallographic, and bibliographic data, as well as experimental, instrument, and sampling conditions, and select physical properties in a common standardized format);
- ✓ **NIMS Inorganic Materials Database (AtomWork)** (Database covers all basic crystal structure, x-ray diffraction, property and phase diagram data of inorganic and metallic materials from main literature sources);
- ✓ **Inorganic Crystal Structure Database (ICSD)** (One of the largest database for completely identified inorganic crystal structures, includes structure data (unit cell, space group, complete atomic parameters, site occupation factors, Wyckoff sequence, molecular formula and weight, ANX formula, mineral group, etc.), around 12 000 new structures are added every year);
- ✓ **Cambridge Structural Database (CSD)** (A collection of over 1 000 000 small-molecule organic and organometallic crystal structures that can be visualised and downloaded, around 50 000 new structures are added every year);
- ✓ **Protein Data Bank (PDB)** (a structure database that contains the three-dimensional crystal structure of macromolecules (experimental data sets of X-ray crystallography, NMR spectroscopy and cryo-electron microscopy));
- ✓ **IMA Database of Mineral Properties** (Database contains the list of all the IMA CNMNC minerals recognized as valid species with accessory information and links and its functions);



- ✓ **Database of Zeolite Structures** (Database contains structural information on all of the Zeolite Framework Types that have been approved by the Structure Commission of the International Zeolite Association (IZA-SC).)
- ✓ **TYPIX** (Database contains over 3200 compounds representative of the structure types found among inorganic compounds (crystal chemical information about individual structure types as well as an extensive chapter on the crystal chemistry of particular structure families)

### 3. Learning outcomes

- ✓ Students will know crystallographic databases such as Pearson's Crystal Data (PCD), Crystallography Open Database (COD), Bilbao Crystallographic Server (BCS), Powder Diffraction File (PDF), NIMS Inorganic Materials *Database* (AtomWork), Inorganic Crystal Structure Database (ICSD), Cambridge Structural Database (CSD), Protein Data Bank (PDB), IMA Database of Mineral Properties, Database of Zeolite Structures, TYPIX.
- ✓ Students will become familiar with the capabilities of crystallographic databases, search tools.
- ✓ Students will be able to search information using various crystallographic databases.
- ✓ Students will understand the importance using crystallographic databases.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

<https://www.crystalimpact.com>

<http://www.crystallography.net/cod/> (Crystallography Open Database (COD))

<https://www.cryst.ehu.es/> (Bilbao Crystallographic Server (BCS))

<https://www.icdd.com/> (Powder Diffraction File (PDF))

<https://crystdb.nims.go.jp/> (NIMS Inorganic Materials *Database* (AtomWork))

<https://icsd.products.fiz-karlsruhe.de/> (Inorganic Crystal Structure Database (ICSD))

<https://www.ccdc.cam.ac.uk/> (Cambridge Structural Database (CSD))

<https://www.rcsb.org/> (Protein Data Bank (PDB))

<https://rruff.info/ima/> (IMA Database of Mineral Properties)

<http://www.iza-structure.org/databases/> (Database of Zeolite Structures)



Villars P., Cenzual K. Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds // ASM International: Materials Park, Ohio, USA, Release 2023/24.

Parthé E., Gelato L., Chabot B., Penzo M., Cenzual K., Gladyshevskii R. TYPIX Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types. Vol. 1–4. Springer-Verlag : Heidelberg, 1993. 1596 p.

## 6. Additional notes

The topics will be covered in one lecture

## Topics 3

### 1. The subject of the lecture

**Pauling File Inorganic Materials Database and Design System and ASM Alloy Phase Diagram Database. Phase diagrams of chemical systems**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture is devoted to Pauling File Inorganic Materials Database and description of phase diagrams.

Binary alloy phase diagrams are the graphical representations of the physical states of a substance under different conditions of temperature and pressure that used by chemists and metallurgists to understand the behavior of mixtures of two elements by relating composition to temperature (pressure) and structure. Knowledge of phase equilibria is necessary in chemical processes, engineering, mineralogy and material science.

The database Pauling File is a relational database for materials scientists, grouping crystallographic data, phase diagrams, and physical properties of inorganic crystalline substances under the same frame. Focus is on experimental observations, and the data are processed from the original publications, covering world literature from 1900 to present date. Each individual crystal structure, phase diagram, or physical properties database entry contains data from a particular publication, but the linkage of the different data sets is achieved via the distinct phases concept, considering the chemical system and the crystal structure, or domain of existence, of different phases.

The phase diagram section of the Pauling File contains temperature-composition phase diagrams for binary systems, as well as horizontal and vertical sections and liquidus/solidus projections for ternary and multinary systems. Both experimentally determined and calculated diagrams are processed. All the diagrams have been converted to at.% and °C and redrawn in a standardized version, so that different reports for the same chemical system can easily be compared. Each phase diagram is linked to a database entry, which contains the following database fields: classification: chemical system; type of diagram; investigation: experimental/calculated; calculation; technique; APDIC/non-APDIC; remark; bibliographic data: data source; authors (affiliation); language; title; original diagram (figure number in the original publication); borders; scales; original size; redrawn diagram: concentration range; temperature (range); conversion of concentration; list of phases present on the diagram: standardized phase name, name used in the original publication; structure prototype assigned by the editor; structural; information given in the original publication; link to a representative Pauling File crystal structure entry. For binary systems also the temperature and reaction type for the upper and/or lower limit of existence of the phase are stored.

### 3. Learning outcomes

- ✓ Students will become familiar with the search tools of Pauling File Inorganic Materials Database.
- ✓ Students will be able to description of phase diagrams of the binary systems.
- ✓ Students will be able critically analyze information about phase equilibria of the binary systems.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Villars P., Cenzual K., Daams J.L.C., Hulliger F., Massalski T.B., Okamoto H., Osaki K., Prince A., Iwata S. (Eds.), PAULING FILE, Binaries Edition, Materials Park: ASM International, 2002.

P. Villars, K. Cenzual, R. Gladyshevskii, S. Iwata. Pauling File: Towards a Holistic View. Materials Informatics: Methods, Tools, and Applications. Eds. O. Isayev, A. Tropsha, S. Curtarolo. Weinheim: Wiley-VCH. – 2019. – P. 55–106.

#### 6. Additional notes

The topics will be covered in one lecture

## Topics 4

### 1. The subject of the lecture

**Pauling File Inorganic Materials Database and Design System. Crystal structures and physical properties of binary compounds**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture is devoted to Pauling File Inorganic Materials Database and description of crystal structures and physical properties of binary compounds.

Crystallographic data include atom coordinates, (an)isotropic displacement parameters and experimental diffraction lines, and are accompanied by information concerning preparation, experimental conditions, characteristics of the sample, phase transitions, dependence of the cell parameters on temperature, pressure, and composition. In order to give an approximate idea of the actual structure, a complete set of atom coordinates and site occupancies is proposed for database entries where a prototype could be assigned (by the authors or by the editors), but atom coordinates were not refined. A feature of this base is that the crystallographic data are presented as they were published, and converted so that all representatives of the same structure type can be directly compared.

All data sets with published atom coordinates are in the Pauling File classified into structure prototypes, following the criteria defined in TYPIC. Isotypic compounds must crystallize in the same space group, have similar cell parameter ratios, and the same Wyckoff positions should be occupied in the standardized description, with the same or similar values of the atom coordinates. Each structure prototype is defined on a database entry in the crystal structure part of the Pauling File. These database entries are grouped in the so-called Structure Type Pool (STP). More than 36'000 different prototypes have up to date been identified and added to the Structure Type Pool. During the lecture, students will be taken through the classification of the binary compounds according to their crystal structure: classes perovskites, AIB<sub>2</sub> family, close-packed structures, rocksalt family, and high-T<sub>c</sub> cuprates, classes of zeolites etc.

The database Pauling File contains a broad range of different intrinsic properties (examples in parentheses) of single-phase samples: electronic and electrical properties (energy gap, resistivity, Hall coefficient, effective mass), ferroelectricity (Curie temperature, permittivity, polarization), magnetic properties (transition temperatures, susceptibility, magnetization, hysteresis, Mossbauer spectra), mechanical properties (hardness, bulk modulus, magnetostriction), optical properties (absorption coefficient, refractive index, luminescence, optical spectra), phase transitions (melting point, temperatures and pressures for structural transitions), superconductivity (T<sub>c</sub>, critical field, current density, energy gap), thermal and thermodynamic properties (thermal expansion, enthalpy, entropy, thermoelectric power). The physical properties section of the Pauling File stores experimental and simulated data for a broad range of intrinsic physical properties of inorganic compounds in the solid crystalline state. Focus is on the characterization of inorganic substances (single-phase samples). When published, the entries also contain information about synthesis and sample preparation, as well as information that helps to establish the links to phase diagram and crystal structure

entries, such as colloquial names, crystallographic data, limits of stability of the phase with respect to temperature, pressure, or composition.

During the lecture, students will be taken through the classification of the binary compounds according to their physical properties: antiferromagnet, ferroelectric, metal, semiconductor, ionic conductor, superconductor, etc.

### 3. Learning outcomes

- ✓ Students will become familiar with the search tools of Pauling File Inorganic Materials Database.
- ✓ Students will be able to classify compounds by classes: compound classes (sulfate, nitrate, carbonate, fulleride, intermetallics, oxides, sulfides, hydrates, etc.), structure classes (classes perovskites,  $AlB_2$  family, close-packed structures, rocksalt family, and high-Tc cuprates, classes of zeolites etc.), property classes (antiferromagnet, ferroelectric, metal, semiconductor, ionic conductor, superconductor, etc.)
- ✓ Students will be able critically analyze information about crystal structures, and basic physical properties of substances formed in binary systems.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Villars P., Cenzual K., Daams J.L.C., Hulliger F., Massalski T.B., Okamoto H., Osaki K., Prince A., Iwata S. (Eds.), PAULING FILE, Binaries Edition, Materials Park: ASM International, 2002.

P. Villars, K. Cenzual, R. Gladyshevskii, S. Iwata. Pauling File: Towards a Holistic View. Materials Informatics: Methods, Tools, and Applications. Eds. O. Isayev, A. Tropsha, S. Curtarolo. Weinheim: Wiley-VCH. –2019. – P. 55–106.

### 6. Additional notes

The topics will be covered in one lecture

## Topics 5

### 1. The subject of the lecture

**Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds. Phase analysis of samples of inorganic compounds**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture is devoted to Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds and phase analysis of samples of inorganic compounds.

The Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds is the world's largest database containing critically evaluated crystallographic and derived data for intermetallics, oxides, halides, minerals, and other inorganic materials and compounds. This allows users to check data against crystallographic rules and therefore interpret the properties of chemical compounds quickly and efficiently. It is an essential tool for scientists and engineers working with inorganic crystalline matter.

During the lecture, students will be introduced to the basic principles of phase analysis. X-ray phase analysis is based on the property of X-rays to penetrate inside matter and be diffracted by the particles of the crystals (atoms, ions, molecules), which are periodically repeated in space. Advantages of X-ray powder diffraction for phase analysis are simplicity, speed, economy, non destructive method, small quantities of material required, polymorphic compounds can be distinguished.

Crystal Structure Database for Inorganic Compounds provides tools in the form of calculated powder patterns for phase analysis based on diffraction methods.

### 3. Learning outcomes

- ✓ Students will become familiar with the search tools of Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds Database.
- ✓ Students will be able to compare of observed X-ray powder diffraction pattern with calculated pattern.
- ✓ Students will be able to build theoretical patterns using different radiations.
- ✓ Students will be able critically analyze information, obtained from powder diffraction patterns.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

#### 6. Additional notes

The topics will be covered in one lecture



## Topics 6

### 1. The subject of the lecture

**Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds. Crystal chemistry of inorganic substances**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture is devoted to Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds and description of crystal chemistry of inorganic substances.

The lecture will contain a description of basic crystallographic characteristics of compounds: structure type, symmetry, Pearson symbol, cell parameters, atomic environment, interatomic distances.

Crystallographic data in Pearson's Crystal Data include atom coordinates, (an)isotropic displacement parameters and experimental diffraction lines, information about preparation, experimental conditions, characteristics of the sample, phase transitions, dependence of the cell parameters on temperature, pressure, and composition. A feature of this base, as well as database Pauling File, is that the crystallographic data are presented as they were published, and converted so that all representatives of the same structure type can be directly compared. Students will be introduced to search tools such as search on chemical composition, structure type, symmetry, Pearson symbol, unit cell parameters and on atomic environment.

Derived data in Pearson's Crystal Data include atomic environments of individual atom sites. One of the important characteristics for describing the structure is atomic environment. Atomic environment (coordination polyhedron) is defined using the method of Brunner and Schwarzenbach. According to this method the interatomic distances between an atom and its neighbors are plotted in a next-neighbor histogram. In most cases a clear maximum gap is revealed and the atoms situated at distances to the left of the maximum gap are considered to belong to the atomic environment of the central atom. An additional rule is "maximum-convex-volume rule". This rule is defined as the maximum volume around the central atom delimited by convex faces, with all the atoms of the atomic environment lying at the intersection of at least three faces. Coordination polyhedra also constitute a tool for the classification of crystal structures into geometrically similar types. In 1994 the Atomic-Environment principle said: "The vast majority of all atoms (point sets) in intermetallic compounds have as Atomic Environment one or several of the following 14 AETs: tetrahedron, octahedron, cube, tricapped prism, fourcapped trigonal prism, icosahedron, cuboctahedron, bicapped pentagonal pyramid, anticuboctahedron, pseudo Frank-Kasper (CN13), 14-vertex Frank-Kasper, rhombic dodecahedron, 15-vertex Frank-Kasper, and 16-vertex Frank-Kasper". Among the most popular coordination polyhedras there are also single atom (CN = 1), collinear (CN = 2), non-collinear (CN = 2), coplanar triangle (CN = 3), non-coplanar triangle (CN = 3), and square antiprism (CN = 8).

### 3. Learning outcomes

- ✓ Students will become familiar with the search tools of Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds Database.



- ✓ Students will be able analyze interatomic distances and coordination polyhedra of inorganic substances.
- ✓ Students will be able critically analyze information about crystal structures of inorganic substances.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

#### 6. Additional notes

The topics will be covered in one lecture

## Topics 7

### 1. The subject of the lecture

#### Holistic view on inorganic compounds

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to present holistic view on inorganic compounds.

To get a holistic view on materials is the ultimate goal of not only materials scientists, but also materials users. Deep insight into materials has been enhanced through continuous interaction between observation, experiment, data compilation, theoretical modeling, and calculation, as illustrated through history by prominent scientists such as Dmitri Mendeleev and Linus Pauling. Now, when moving into the "Data Era", such interactions can be carried out on a large scale and relatively easily by building up procedures using digitized logics and data.

There are two general approaches/concepts to obtain a holistic view on materials. The first one is the bottom-up approach (BUA), based on materials data. The second one is the top-down approach (TDA), for which guidelines and logics are taken from outside, from models (mathematics, physics, chemistry, and biology) and surrounding environments (nature and artifacts). TDA can be developed into a combination of powerful sets of scientific disciplines and/or market needs, based on logics, which requires networking of multi-facet knowledge models, bridging gaps and tuning mismatches. Logics described by explicitly digitized scientific knowledge (i.e. not tacit knowledge) have been used in simulation programs with embedded algorithms, rules in Artificial Intelligence (AI) systems and inspiring interfaces

The lecture will present also the historical aspect of the attempt to create the first databases, among which: structure-property correlations for organic materials (E.J. Corey, 1960s); phase diagrams based on thermodynamics (NIST & ASM, since 1970s); structure maps based on crystallography and/or quantum mechanics (D.G. Pettifor, 1980s); deformation/fracture mechanism maps based on defect theory (M.F. Ashby, 1970s).

### 3. Learning outcomes

- ✓ Students will become familiar with two general approaches/concepts to obtain a holistic view on materials.
- ✓ Students will become familiar with historical aspect of the attempt to create the first databases.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

**5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

P. Villars, K. Cenzual, R. Gladyshevskii, S. Iwata. Pauling File: Towards a Holistic View. Materials Informatics: Methods, Tools, and Applications. Eds. O. Isayev, A. Tropsha, S. Curtarolo. Weinheim: Wiley-VCH. –2019. – P. 55–106.

**6. Additional notes**

The topics will be covered in one lecture

## Topics 8

### 1. The subject of the lecture

**Searching for materials with predefined properties**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to present the common some prerequisites for searching for materials with predefined properties.

Several factors must be taken into consideration for the development of new materials and it is essential to build up a holistic view on inorganic substances by giving rapid access to different kinds of critically evaluated experimental data published in the world literature over the last 100 years.

The linkage between the three different groups of data (crystal structures, phase diagrams, physical properties) is a basis for synthesizing materials with predefined properties.

The underlying quantum mechanical laws can be parameterized using elemental-property parameters of the constituent chemical elements. An appropriate choice of parameters leads to relatively simple maps with well-defined stability domains, offering excellent overviews of experimentally known inorganic substances. The maps provide, as a direct consequence, some possibilities to predict features of not yet known compounds.

### 3. Learning outcomes

- ✓ Students will become familiar with some prerequisites for a holistic view.
- ✓ Students will become familiar with several examples, which show possible to gain a better view on inorganic substances, effective or potential materials, by looking at large amounts of different data in an appropriate way.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Informative lecture – a systematic course in a specific scientific discipline in a synthetic manner, the implementation implies the passive reception of the provided information.

Conversational lecture – delivered content that considers the interaction with the lecture's audience; discussion related to the lecture is one of its elements or its continuation.

Multimedia presentation – the use of a multimedia presentation, such as Microsoft PowerPoint, to visualize the discussed issues.

Explanation/classification – an explication involving the derivation of a pre-recognised statement from others already known in a number of steps determined by the lecturer.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

P. Villars, K. Cenzual, R. Gladyshevskii, S. Iwata. Pauling File: Towards a Holistic View. Materials Informatics: Methods, Tools, and Applications. Eds. O. Isayev, A. Tropsha, S. Curtarolo. Weinheim: Wiley-VCH. –2019. – P. 55–106.

### 6. Additional notes

The topics will be covered in one lecture

## Course content – laboratory classes

### Topics 1 – Lab 1

#### 1. The subject of the laboratory classes

##### Materials for heterogeneous catalysis

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

In heterogeneous catalysis, the catalyst is in a different phase from the reactants. At least one of the reactants interacts with the solid surface. An example of heterogeneous catalysis is the interaction of hydrogen gas with the surface of a metal, such as Ni, Ru, Pd, or Pt. For example, palladium is better known in chemistry as a universal catalyst in many chemical processes. Catalysts based on intermetallic palladium compounds are becoming increasingly used for reactions of oil cracking, hydrogenation and dehydrogenation of organic compounds. For instance, the catalytic activity of the compound  $\text{GaPd}_2/\text{SiO}_2$  in the process of synthesis of methanol from carbon dioxide and hydrogen at much lower pressures and temperatures than with the usual catalyst  $\text{Cu}/\text{ZnO}/\text{Al}_2\text{O}_3$  has been proven. The compound  $\text{Pd}_2\text{Ga}_{0.85}\text{Sb}_{0.15}$  is another great example of the catalytic activity of palladium alloys. It shows high activity and selectivity in the semi-hydrogenation of acetylene in excess of ethylene. The better catalytic activity of intermetallic compounds in hydrogenation processes, compared with pure palladium, is explained by the unique mechanism of the reaction. For example, in the semi-hydrogenation reaction of acetylene to ethylene, when used as a pure metal catalyst, the close arrangement of palladium atoms relative to each other significantly complicates the isolation of atoms and the formation of active centers. As a result, strong di- $\sigma$ -bonding is realized, which leads to the producing a considerable amount of unwelcome ethane. At the same time, in intermetallic compounds there are a decrease in the number of Pd–Pd bonds in the crystal structure of the compounds and an increase in interatomic distances. Consequently, palladium compounds, in which the active centers are isolated properly, have a weak  $\pi$ -binding of the acetylene molecule to the palladium atom.

In addition, the introduction into the system of less electronegative elements than palladium leads to the transfer of a partially negative charge to the Pd atom and greater filling of the electronic configuration of its d-orbital. As a consequence, increasing the energy of the active centers greatly improves the absorption properties of palladium. Moreover, the use of palladium alloys as catalysts allows not only to increase the efficiency of the process, but also to ensure its economy by reducing the consumption of precious metals.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties of the phase Ni, Pt, Pd,  $\text{Pd}_2\text{Ga}_{0.85}\text{Sb}_{0.15}$ .

#### 3. Learning outcomes

- ✓ Students will be able to search information on heterogeneous catalysts using databases and scientific articles.

- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of intermetallic compounds in heterogeneous catalysis.
- ✓ Students will be able to search for regularities.

#### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

##### *Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

Matselko O., Zimmermann R.R., Ormeci A., Burkhardt U., Gladyshevskii R., Grin Yu., Armbrüster M. Revealing Electronic Influences in the Semihydrogenation of Acetylene / J. Phys. Chem. – 2018. – Vol. 122. – P. 21891-21896.

<https://doi.org/10.1021/acs.jpcc.8b05732>

##### *Addition*

Fiordaliso E.M., Sharafutdinov I., Carvalho H.W.P., Kehres J., Grunwaldt J-D., Chorkendorff I., Damsgaard C.D. Evolution of intermetallic GaPd<sub>2</sub>/SiO<sub>2</sub> catalyst and optimization for methanol synthesis at ambient pressure // Sci. Technol. Adv. Mater. – 2019. – Vol. 20. – P. 521–531.

<https://doi.org/10.1080/14686996.2019.1603886>

Fleischer L.R. Intermetallic Compounds for High-Temperature Structural Use. Unique Iridium and Ruthenium Compounds // Platinum Met. Rev. 1992. – Vol. 36 (3). – P. 138–145.

<https://doi.org/10.1595/003214092x363138145>

Schriber T.J. The low temperature oxidation of ammonia over a supported ruthenium catalyst // Chem. Eng. Sci. – 1967. – Vol. 22 (8). – P. 1067–1078.

[https://doi.org/10.1016/0009-2509\(67\)80171-4](https://doi.org/10.1016/0009-2509(67)80171-4)

Manjunatha R., Schechter A. Electrochemical synthesis of ammonia using ruthenium–platinum alloy at ambient pressure and low temperature // *Electrochem. Commun.* – 2018. – Vol. 90. – P. 96–100.

<https://doi.org/10.1016/j.elecom.2018.04.008>

#### 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project “Proposals for potential catalysts”.

#### 8. Optional information

The necessary software and instructions for the work will be available.



## Topics 2 – Lab 2

### 1. The subject of the laboratory classes

#### Magnetic materials

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

All types of materials and substances possess some kind of magnetic properties: ferromagnetism, antiferromagnetism, ferrimagnetism, diamagnetism, paramagnetism.

Ferromagnetic materials are strongly attracted by a magnetic field or magnet. These include the elements iron, nickel and cobalt and their alloys, some alloys of rare-earth metals, and some naturally occurring minerals such as lodestone.

Antiferromagnetic materials occur commonly among transition metal compounds, especially oxides. Examples include hematite  $\text{Fe}_2\text{O}_3$ , alloys such as  $\text{FeMn}$ ,  $\text{MnF}_2$ , and oxides such as  $\text{NiO}$ ,  $\text{MnO}$ ,  $\text{CoO}$ ,  $\text{FeO}$ ,  $\text{Cr}_2\text{O}_3$ .

Ferrimagnetic materials contain atoms with opposing magnetic moments, as in antiferromagnetism, but these moments are unequal in magnitude, so a spontaneous magnetization remains. The best example of a ferrimagnetic mineral is magnetite  $\text{Fe}_3\text{O}_4$  with  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  ions.

Diamagnetic materials - non-magnetic materials such as silver, carbon, zinc, bismuth, gold, antimony, copper, etc. They are not attracted to any magnetic field.

Paramagnetic materials tend to get weakly magnetized in the direction of the magnetizing field when placed in a magnetic field.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties of the pure elements Fe, Co, Ni, Gd, and compounds  $\text{MnSb}$ ,  $\text{EuO}$ ,  $\text{EuS}$ ,  $\text{GdNi}_2$ ,  $\text{GdNi}$ ,  $\text{GdCl}_3$ ,  $\text{SmCo}_5$ ,  $\text{Nd}_2\text{Fe}_{14}\text{B}$ ,  $\text{Fe}_{65}\text{Co}_{35}$ ,  $\text{Fe}_{20}\text{Ni}_{80}$  (ferromagnetic materials);  $\text{MnF}_2$ ,  $\text{MnO}$ ,  $\text{CoO}$ ,  $\text{FeO}$ ,  $\text{Cr}_2\text{O}_3$ ,  $\alpha\text{-Fe}_2\text{O}_3$  (antiferromagnetic materials);  $\text{Fe}_3\text{O}_4$ ,  $\text{CoFe}_2\text{O}_4$ ,  $\text{NiFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ ,  $\text{Y}_3\text{Fe}_5\text{O}_{12}$ ,  $\text{Gd}_3\text{Fe}_5\text{O}_{12}$ ,  $\text{Dy}_3\text{Fe}_5\text{O}_{12}$ ,  $\text{Ho}_3\text{Fe}_5\text{O}_{12}$ , (ferrimagnetic materials).

### 3. Learning outcomes

- ✓ Students will be able to search information on magnetic materials using databases and scientific articles.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of the compound that possesses some kind of magnetic properties.
- ✓ Students will be able to search for regularities.

### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection



- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

### *Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

Blundell S. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.

### *Addition*

Buschow K.H.J., de Boer FR Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

## 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project "Proposals for potential magnetic materials".

## 8. Optional information

The necessary software and instructions for the work will be available.

## Topics 3 – Lab 3

### 1. The subject of the laboratory classes

#### High-density materials

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The density of a substance is its mass per unit volume. It is a unique physical property of an object that shows how tightly matter is packed.

The highest density elements are osmium with density 22.61 g/cm<sup>3</sup>, iridium (22.56 g/cm<sup>3</sup>), platinum (21.46 g/cm<sup>3</sup>), rhenium (21.20 g/cm<sup>3</sup>), uranium (20.20 g/cm<sup>3</sup>).

High density materials are used in various applications due to their unique properties, some of them: radiation shields, and armor-piercing means, in aerospace and defense due to strength and durability, used as counterweights in various machinery and equipment to provide balance and stability, ballast in ships.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra, physical properties density of the pure elements Os, Ir, Pt, Re, U, Fe.

### 3. Learning outcomes

- ✓ Students will be able to search information on high-density materials using databases and scientific articles.
- ✓ Students will be able to analyse of chemical composition and physical properties of high-density materials.
- ✓ Students will be able to search for regularities.

### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

*Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

#### 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project "Proposals for potential high-density materials".

#### 8. Optional information

The necessary software and instructions for the work will be available.

## Topics 4 – Lab 4

### 1. The subject of the laboratory classes

#### Superhard ceramic materials

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Superhard materials find wide application in various industries. These materials, characterized by their exceptional hardness and durability, are in demand due to their suitability in the production of cutting tools, protective coatings, and other industrial applications where high mechanical resistance is required. The production of novel, high-tech, superhard materials based on new compounds or new composites is one of the priority tasks of modern industry.

Ceramics is based on valence compounds with very strong covalent bonding. Thus, their hardness is the highest. Ceramics can be classified into three distinct material categories: oxides (alumina, beryllia, ceria, zirconia); non-oxides (carbide, boride, nitride, silicide); composite materials (particulate reinforced, fiber reinforced, combinations of oxides and nonoxides). The advanced ceramic materials consist of highly pure compounds of aluminum oxide ( $\text{Al}_2\text{O}_3$ ), silicon carbide ( $\text{SiC}$ ), and silicon nitride ( $\text{Si}_3\text{N}_4$ ).

Advanced ceramics, due to their unique properties, can be used for civil, military and industrial applications at room and high temperatures and in extreme conditions.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties of  $\text{B}_4\text{C}$ ,  $\text{SiC}$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{Si}_3\text{N}_4$ ,  $\text{B}_{13}\text{C}_2$ ,  $\text{VB}_2$  phase

### 3. Learning outcomes

- ✓ Students will be able to search information on superhard ceramic materials using databases and scientific articles.
- ✓ Students will be able to understand of the basic chemical and physical phenomena of superhard ceramic materials in order to obtain materials with desired structural features and properties.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of intermetallic compounds of superhard ceramic materials.
- ✓ Students will be able to search for regularities.

### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis

- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

### *Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

### *Addition*

Babizhetskyy V. Bauer J., Gautier R., Hiebl K., Simon A., Halet J.-F. Structural, Electronic and Physical Properties of Solid-State Rare-Earth Boride Carbides // Handbook on the Physics and Chemistry of the Rare Earths including Actinides [Eds. J. C. Bünzli, V. Pecharsky]. – Amsterdam : Elsevier – 2018. – Vol. 53, Ch. 302. – P.145–269.

<https://doi.org/10.1016/bs.hpcr.2018.05.001>

Yamada S., Hirao K., Yamauchi Y., Kanzaki S. Densification behaviour and mechanical properties of pressureless-sintered  $B_4C-CrB_2$  ceramics / // J. Mater. Sci. – 2002. – Vol. 37. – P. 5007–5012.

<https://doi.org/10.1023/A:1021027430338>

Song Q., Zhang Z. H., Hu Z. Y. Microstructure and mechanical properties of super-hard  $B_4C$  ceramic fabricated by spark plasma sintering with  $(Ti_3SiC_2+Si)$  as sintering aid // Ceram. Int. – 2019. – Vol. 45 (7). – P. 8790–8797.

<https://doi.org/10.1016/j.ceramint.2019.01.204>

## 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project “Proposals for superhard ceramic materials”.

## 8. Optional information

The necessary software and instructions for the work will be available.

## Topics 5 – Lab 5

### 1. The subject of the laboratory classes

#### High-entropy alloys

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

High-entropy alloys (HEAs) are alloys with five or more principal elements. These alloys are named 'High-entropy alloys' because their liquid or random solid solution states have significantly higher mixing entropies than those in conventional alloys. Experimental results show that the higher mixing entropy in these alloys facilitates the formation of solid solution phases with simple structures. Due to the distinct design concept, these alloys often exhibit unusual and advantageous properties compared with other systems as a result of their chemistry and crystal structure. Properties such as competitive hardness, corrosion resistance, wear resistance, fatigue behavior are characteristic of high-entropy alloys. Some of these properties are not seen in conventional alloys, making high-entropy alloys attractive in many fields.

Basic aspects of high-entropy alloys:

- ✓ High-Entropy Effect. The high-entropy effect states that the higher mixing entropy in high-entropy alloys lowers the free energy of solid solution phases and facilitates their formation, particularly at higher temperatures.
- ✓ Sluggish Diffusion Effect. It was proposed that the diffusion and phase transformation kinetics in high-entropy alloys are slower than those in their conventional counterparts.
- ✓ Severe-Lattice-Distortion Effect. The lattice in high-entropy alloys is composed of many kinds of elements, each with different size. These size differences inevitably lead to distortion of the lattice.
- ✓ Cocktail Effect. The properties of high-entropy alloys are certainly related to the properties of its composing elements.

Because of the wide composition range and the enormous number of alloy systems in HEAs, the mechanical properties of high-entropy alloys can vary significantly. In terms of hardness/strength, the most critical factors are: hardness/strength of each composing phase in the alloy (it is largely determined by the crystal structure and bonding of each phase); relative volume ratio of each composing phase (the general rule to estimate the hardness/strength of an high-entropy alloy is straight forward: the harder the phase (and the higher the fraction of the hard phase), the harder the alloy); morphology/distribution of the composing phases.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra, valence electron concentration and physical properties of phase in the Al-Co-Cr-Fe-Ni, Al-Co-Cr-Cu-Fe-Ni, Mo-Nb-Ta-V-W, Co-Cr-Fe-Mn-Ni, Cr-Cu-Fe-Mn-Ni, Ca-Mg-Zn-Sr-Yb systems.

### 3. Learning outcomes

- ✓ Students will be able to search information on high-entropy alloys using databases and scientific articles.

- ✓ Students will understand the importance of current challenges and important future directions for high-entropy alloys.
- ✓ Students will become familiar with some critical aspects of high-entropy alloys, including core effects, phases and crystal structures, mechanical properties, high-temperature properties, structural stabilities, and corrosion behaviors.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of high-entropy alloys.
- ✓ Students will be able to search for regularities.

#### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

##### *Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

Tsai M.H, Yeh J.W. High-entropy alloys: a critical review // Matr. Res. Lett. – 2014. – Vol. 2. – No. 3. – P. 107–123.

<http://dx.doi.org/10.1080/21663831.2014.912690>

##### *Addition*

King D.M., Middleburgh S.C., Edwards L., Lumpkin G.R., Cortie M. Predicting the crystal structure and phase transitions in high-entropy alloys // JOM. – 2015. –Vol. 67. – No.10. – P. 2375–2380.

[https:// doi: 10.1007/s11837-015-1495-4](https://doi.org/10.1007/s11837-015-1495-4)

Wang X.F., Zhang Y., Qiao Y., Chen G.L. Novel microstructure and properties of multicomponent CoCrCuFeNiTi<sub>x</sub> alloys // Intermetallics. – 2007. – Vol. 15. – P. 357–362.

doi:10.1016/j.intermet.2006.08.005

Yeh J.W., Chen S.K., Lin S.J., Gan J.Y., Chin T.S., Shun T.T., Tsau C.H., Chang S.Y. Nanostructured high-entropy alloys with multiple principal elements: novel alloy design concepts and outcomws // Adv. Eng. Mater. – 2004. – Vol. 6.– No. 5. – P. 299–303.

<https://doi.org/10.1002/adem.200300567>

Zhang Y., Zhou Y.J., Lin J.P., Chen G.L., Liaw P.K. Solid-solution phase formation rules for multi-component alloys // Adv. Eng. Mater. – 2008. – Vol. 10.– No. 6. – P. 534–538.

DOI:[10.1002/ADEM.200700240](https://doi.org/10.1002/ADEM.200700240)

#### 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project “Proposals for high-entropy alloys”.

#### 8. Optional information

The necessary software and instructions for the work will be available.



## Topics 6 – Lab 6

### 1. The subject of the laboratory classes

#### Semiconductors

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

A semiconductor is a type of material that has an electrical resistance which is between the resistance typical of metals and the resistance typical of insulators. Semiconductors are essential materials for manufacturing smart phones, computers, cars, refrigerators, really any electronic device. Common semiconductor materials include antimony, arsenic, boron, carbon, germanium, selenium, silicon, sulfur and tellurium, gallium arsenide, indium antimonide and the oxides of most metals. Silicon is the best known of these, forming the basis of most ICs. One of their most interesting characteristics is that their electrical properties can be modified through a process called doping.

Depending on their purity, semiconductors are classified into two groups:

Intrinsic semiconductors - natural materials that can be used directly in devices. They are made of one single type of atom, arranged to impede free movement of the electrons around the molecule.

Extrinsic semiconductors. In order to use them in devices, they must first be doped, which involves adding a small amount of atoms from other elements, such as antimony, arsenic, or phosphorus, that transforms the intrinsic semiconductors into extrinsic.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties of silicon, germanium, gallium arsenide.

### 3. Learning outcomes

- ✓ Students will be able to search information on semiconductors using databases and scientific articles.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of semiconductors.
- ✓ Students will be able to search for regularities.

### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work

- ✓ Communication on specialist topics
- ✓ Work with computer

## 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

*Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

## 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project "Proposals for semiconductors".

## 8. Optional information

The necessary software and instructions for the work will be available.

## Topics 7 – Lab 7

### 1. The subject of the laboratory classes

#### Intermetallic hydrides

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Intermetallic hydrides are attractive for applied research as potential candidates for on-board vehicular use (engines, batteries, etc.). Among the 92 stable elements of the periodic table, nearly fifty combine with hydrogen in large quantities. This makes them to play a role of “hydrogen sponge”. Therefore there is, in principle a large choice of candidates for hydrogen storage.

In the case of intermetallic hydrides, certain positions for hydrogen atoms are preferred. There are only two types of interstitial sites – octahedral (O) and tetrahedral (T) sites, which they are practically the only ones that are occupied by hydrogen atoms.

On the fundamental side, the interaction of hydrogen with the atoms of the host crystal structure leads to different phenomena as the modification of the long-range structural order, the chemical bonding of hydrogen and its binding energy within the metallic lattice, the volume expansion effects such as those influencing the magnetic order and the valence state of the rare earth (mainly cerium), etc.

There are some criteria, which are to be fulfilled to make the hydride formation favourable:

- ✓ Hydrogen absorption by intermetallics at hydrogen pressure below 100 bar at room temperature requires the presence of hydride-forming element (no exception is known to this “rule”).
- ✓ Geometrical requirements include sufficient size for the interstitials and their arrangement in space. The well-known Westlake’s criterion states that available interstitial sites must have a spherical volume with radius  $\geq 40$  pm. The minimum H-H distance should be 210 pm. Besides, according to the “Shoemaker’s exclusion rule” two tetrahedra sharing the same face cannot be occupied simultaneously.

Despite the simplicity of these rules they provide good ground for the preliminary estimate of the probability of the formation of stable hydride. However one should keep in mind that there are always some exceptions from these rules due to the fact that the stability of the hydride is determined by many factors and none of them predominates in all cases.

For example, it was shown that UPd<sub>3</sub>, which fulfils all the requirements listed above, absorbs just a negligible amount of hydrogen. The correlation between the bonding strength in the intermetallic lattice and the corresponding hydrogen absorption capacities was analysed and it was shown that besides the geometrical considerations, the stabilities of the parent intermetallic compounds is another factor which determines the possibility of hydrogen absorption.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties of the compounds ZrNi, UPd<sub>3</sub>, PdH<sub>2</sub>, UH<sub>3</sub>, LaNi<sub>5</sub>

### 3. Learning outcomes

- ✓ Students will be able to search information on intermetallic hydrides using databases and scientific articles.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of intermetallic hydrides.
- ✓ Students will be able to search for regularities.

### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:

#### *Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

Westlake D.G. Stoichiometries and interstitial site occupation in the hydrides of ZrNi and other isostructural intermetallic compounds // J. Less-Common Met. – 1980. – Vol. 75. – P. 177–185.

Samir F. Matar Intermetallic hydrides: A review with ab initio aspects // Prog. Solid State Chem. – 2010. – Vol. 38. – P. 1–37.

<https://doi.org/10.1016/j.progsolidstchem.2010.08.003>

#### *Addition*

Feenstra R., de Groot D.G., Griessen R., Burger J.P., Menovski A. Absorption of hydrogen in Pd-Co and Pd-U alloys. J. Less-Common Met. – 1987. – Vol. 130. – P. 375–386.

[https://doi.org/10.1016/0022-5088\(87\)90132-9](https://doi.org/10.1016/0022-5088(87)90132-9)

### 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project “Proposals for intermetallic hydrides”.

### 8. Optional information

The necessary software and instructions for the work will be available.

## Topics 8 – Lab 8

### 1. The subject of the laboratory classes

#### Superconductors

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Superconductivity is the property of the materials to conduct direct current electricity without energy loss when they are cooled below a critical temperature ( $T_c$ ). In general, superconductors are divided into low-temperature superconductors (with a critical temperature  $< 77$  K) and high-temperature superconductors, the existence of which was established only in 1986.

Classical (low-temperature) superconductors are such substances as Hg, Pb, Nb, etc.); borides, carbides, nitrides, hydrides, oxides ( $MgB_2$ ,  $\alpha$ -MoC,  $\delta$ -NbN, etc.); intermetallic compounds ( $Nb_3Sn$ ,  $V_3Ga$ ,  $Cr_3Si$ , etc.).

The composition of high-temperature superconductors necessarily includes layers of Cu and O atoms. It is believed that high-temperature superconductivity occurs precisely in these layers. These are usually the cuprates with layered structures. Their structures are built by stacking four types of atomic layers. In all layers, cations form square grids. One of the four types of layers is built exclusively of metal atoms, while the rest also contain oxygen atoms located in the centers of the squares, which are built by metal atoms or in the centers of the sides of the squares. Layers are stacked only in a strictly defined order.

Families of high-temperature superconductors are usually classified by the cation present in the additional layers. For example, it is possible to distinguish cuprates based on Bi ( $Bi_2Sr_2CuO_{6+\delta}$ ,  $Bi_2Sr_2CaCu_2O_{8+\delta}$ ); Pb-based cuprates ( $Pb_2Sr_2ACu_3O_{8+\delta}$  ( $A = Y, Nd$ )); C-based cuprates ( $CSr_2CuO_5$ ,  $C_{0,9}Ba_{1,1}Sr_{0,9}Cu_{1,1}O_{4,9+\delta}$ ); Hg-based cuprates ( $HgBa_2CuO_{4+\delta}$ ,  $HgBa_2CaCu_2O_{6+\delta}$ ); Tl-based cuprates ( $Tl_2Ba_2CuO_6$ ,  $Tl_2Ba_2CaCu_2O_8$ ), cuprates containing Ba and Y ( $Ba_2YCu_3O_{7-\delta}$  - YBCO); cuprates of rare earth and alkaline earth elements ( $Sr_{0,86}Nd_{0,14}CuO_2$ ,  $La_{1,6}Sr_{0,4}CaCu_2O_6$ ), halogen-containing cuprates ( $(Ca,Na)_2CuO_2Cl_2$ ,  $Sr_2CuO_2F_{2,57}$ ). The most promising for practical application are the superconducting phases in the Bi-Sr-Ca-Cu-O and Tl-Sr-Ca-Cu-O systems, which have a high critical temperature and critical current density in the grains.

Structures are designated by four-digit codes, which are derived from the general formula  $A_kB_lC_mD_nO_{k+l+2m+2}$ , taking into account the number of layers of each type in the stacking element  $klmn$ . For example, the structure  $Tl_{1,64}Ba_2Ca_3Cu_4O_{12}$  ( $A_2B_2C_3D_4O_{12}$ ) is denoted by 2234. To distinguish chemical classes, cation symbols in additional layers precede the Tl-2234 code.

Tasks for students:

search information and analysis of crystal structure, interatomic distances, coordination polyhedra and physical properties such compounds as  $Bi_2Sr_2CuO_{6+\delta}$ ,  $Bi_2Sr_2CaCu_2O_{8+\delta}$ ,  $Pb_2Sr_2ACu_3O_{8+\delta}$  ( $A = Y, Nd$ ),  $CSr_2CuO_5$ ,  $C_{0,9}Ba_{1,1}Sr_{0,9}Cu_{1,1}O_{4,9+\delta}$ ,  $HgBa_2CuO_{4+\delta}$ ,  $HgBa_2CaCu_2O_{6+\delta}$ ,  $Tl_2Ba_2CuO_6$ ,  $Tl_2Ba_2CaCu_2O_8$ ,  $Ba_2YCu_3O_{7-\delta}$ ,  $Sr_{0,86}Nd_{0,14}CuO_2$ ,  $La_{1,6}Sr_{0,4}CaCu_2O_6$ ,  $(Ca,Na)_2CuO_2Cl_2$ ,  $Sr_2CuO_2F_{2,57}$ .

### 3. Learning outcomes

- ✓ Students will be able to search information on superconductors using databases and scientific articles.
- ✓ Students will be able to analyse of chemical composition, crystal structure, physical properties of superconductors.
- ✓ Students will be able to search for regularities.

#### 4. Necessary equipment, materials, etc

- ✓ Personal computer or laptop.
- ✓ Internet connection.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- ✓ Data collection
- ✓ Conversion and standardization
- ✓ Materials design
- ✓ Discussion/debate (brainstorm)
- ✓ Critical analysis
- ✓ Individual and team work
- ✓ Communication on specialist topics
- ✓ Work with computer

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts to prepare a theoretical introduction to the classes:  
*Main*

P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.

P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.

Gladyshevskii R., Galez Ph. Crystal Structures of High- $T_c$  Superconducting Cuprates // Handbook of Superconductivity, Ed. Ch. Poole, Jr.- San Diego, USA: Academic Press. – 2000. – Ch. 8. – P. 267–431.

*Addition*

R. Flükiger, G. Grasso, B. Hensel, M. Däumling, R. Gladyshevskii, A. Jeremie, J.C. Grivel, A. Perin. Thermodynamics, Microstructure, and Critical Current Density in Bi,Pb(2223) Tapes. Bismuth-Based High-Temperature Superconductors. Eds. H. Maeda, K. Togano. New-York: Marcel Dekker. – 1996. – Ch. 15. – P. 319–367.

R.E. Gladyshevskii, R. Flükiger. Modulated structure of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+d}$ , a high- $T_c$  superconductor with monoclinic symmetry. Acta Crystallogr. – 1996. – Vol. B52. – P. 38–53.

<https://doi.org/10.1107/S0108768195007075>

R. Gladyshevskii, N. Musolino, R. Flükiger. Structural origin of the low superconducting anisotropy of  $\text{Bi}_{1.7}\text{Pb}_{0.4}\text{Sr}_2\text{Ca}_{0.9}\text{Cu}_2\text{O}_8$ . Phys. Rev. B. – 2004. – Vol. 70. – 184522.

<https://doi.org/10.1103/PhysRevB.70.184522>

## 7. Additional notes

The topic will be covered in one laboratory class (4 h)

The student is obliged to prepare a project “Proposals for superconductors”.

## 8. Optional information

The necessary software and instructions for the work will be available.

matsci.us.edu.pl

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv



**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

The Teachers' Guide is a supplement to the information  
contained in the course syllabus

**PEROVSKITE-BASED MATERIALS**

**Code: PBM**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

Review of the perovskite family. The crystal structure of perovskite and its derivatives.

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture is set to provide a comprehensive overview of a specific group of compounds that fall under the perovskite family. During the discourse, students will be taken through the history of the discovery of perovskite and its derivatives, as well as the classification of these compounds (according crystal structure: cubic  $\text{CaTiO}_3$ , orthorhombic  $\text{GdFeO}_3$ , hexagonal  $\text{BaMnO}_3$  and so on; according cation valence:  $\text{A}^+\text{B}^{5+}\text{O}_3$  (1,5),  $\text{A}^{2+}\text{B}^{4+}\text{O}_3$  (2,4), and  $\text{A}^{3+}\text{B}^{3+}\text{O}_3$  (3,3); single perovskite ( $\text{ABO}_3$ ) and double perovskite ( $\text{A}_2(\text{BB}')\text{O}_6$ ), hybrid organic–inorganic perovskites, antiperovskites, etc.). The crystal structure peculiarities of ideal perovskite  $\text{CaTiO}_3$  and its derivatives, octahedral tilting, symmetry relationships will also be explored in detail, providing students with a deeper understanding of the fundamental principles that govern these compounds. One of the key concepts that will be discussed during the lecture is the tolerance factor, which plays a crucial role in determining the structure, stability and properties of perovskite compounds. Additionally, the lecture will touch on the flexibility of the unique perovskite structure, which allows for the incorporation of a wide range of different elements that provides easy compositional modification and tuning, accordingly, affects the properties. Overall, this lecture promises to be an engaging and informative session that will provide students with a solid foundation in the principles of perovskite materials science. By the end of the lecture, students will have a deeper appreciation for the importance of perovskite compounds in modern materials science and the potential applications that these materials hold for the future.

#### 3. Learning outcomes

- Students will gain an appreciation for the importance of perovskite compounds in modern materials science, including their diverse applications and potential impact on various technological fields.
- Students will be able to describe the discovery and historical background of perovskite family.
- Students will know the different approaches to classification of compounds within the perovskite family, providing a comprehensive overview of their categorization.
- Students will gain an in-depth understanding of the unique crystal structure peculiarities of perovskite and its derivatives, including the arrangement of atoms and other factors that contribute to their exceptional properties.
- Students will be introduced to the concept of the tolerance factor and its significance in determining the stability and characteristics of perovskite structures, enabling them to analyze and predict the behavior of different perovskite phases.

- Students will be familiarized with the flexibility and adaptability of the perovskite structure that allows to appreciate the diverse possibilities for tailoring perovskite materials to specific applications and the potential for innovation in materials design.
- Students will be equipped with the knowledge and understanding necessary to apply the concepts learned to real-world materials science and engineering challenges, fostering critical thinking and problem-solving skills.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the crystal structure description. Also, they are recommended to read first chapter at R. J. D. Tilley. Perovskites Structure–Property Relationships, John Wiley & Sons, Ltd., UK, 2016 as well as S. Thomas, A. Thankappan. Perovskite Photovoltaics. Basic to Advanced Concepts and Implementation, Academic Press, Elsevier, 2018 and M. Borowski. Perovskites: Structure, Properties and Uses, Nova Science Publishers, 2011.

#### 6. Additional notes

The topics will be covered in one lecture.

## Topics 2

### 1. The subject of the lecture

Methods of synthesis of perovskites and their characteristics.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The aim of the lecture is to present an in-depth review of the various techniques used to synthesize compounds with a perovskite structure, along with their key characteristics and required equipment. The audience will gain insights into the solid-state reaction, sol-gel method, and the production of perovskites in different forms such as single crystals, thin films, etc. The lecture will elucidate the solid-state reaction method for synthesizing polycrystalline samples of perovskite compounds, emphasizing the underlying chemical processes, reaction conditions, starting reagents and the resulting material properties. This will provide the audience with a fundamental understanding of this widely used synthesis approach. The sol-gel method, another prominent technique for perovskite synthesis, will be thoroughly discussed. The audience will be guided through the intricacies of sol-gel chemistry, precursor selection, gel formation, and the subsequent heat treatment to obtain perovskite materials with tailored properties. The sol-gel technique is a beneficial procedure for the synthesis of perovskite-type materials to develop a single-phase material with comparatively high surface area and great uniformity. In this technique, the sol successively forms a gel-like dipole mode, which consists of a liquid and a solid phase. The disintegration of desiccated gel precursor substances during calcination produces the preferred perovskite. This process exhibits large improvements such as lower temperature, greater homogeneity, higher flexibility in fabricating thin layers, enhanced reactivity, distinct structures, and greater control of stoichiometry, particle size, and accuracy. The lecture will cover the diverse forms in which perovskite compounds can be synthesized, including single crystals and thin films. This segment will shed light on the specific challenges and applications associated with each form, offering the audience a comprehensive perspective on the versatility of perovskite materials. In conclusion, the main advantages and disadvantages of the considered synthesis methods will be discussed.

### 3. Learning outcomes

- Students will obtain knowledge about variety of methods for synthesizing perovskites, including solid-state reactions, sol-gel methods, obtaining them in the form of single crystals, thin films, etc.
- Students will understand the principal advantages and disadvantages of various techniques employed for the synthesis of perovskite-based materials.
- Students will be equipped with skills to evaluate the suitability of different synthesis methods for specific applications.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and

description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the manufacturing of ceramics. Also, they are expected to read corresponding chapters at S. Thomas, A. Thankappan. Perovskite Photovoltaics. Basic to Advanced Concepts and Implementation, Academic Press, Elsevier, 2018 as well as I. Khan, A. Khan, M. M. A. Khan, S. Khan, F. Verpoort, A. Umar. Hybrid Composite Perovskite Materials: Design to Applications, Woodhead Publishing, 2020, P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, Phys. Status Solidi A, 2017, Vol. 214(9), 1700394 and C. Moure, O. Pena. Recent advances in perovskites: Processing and properties, Progress in Solid State Chemistry, 2015, Vol. 43(4), 123-148.

#### 6. Additional notes

The topics will be covered in one lecture.

## Topics 3

### 1. The subject of the lecture

Application of perovskites as catalysts.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will delve into the critical significance of advancing catalysts for chemical and electrochemical reactions, which serve as the fundamental drivers of numerous facets of modern technology and industry. These reactions play a pivotal role in various domains, including energy storage and conversion, as well as in addressing pressing environmental concerns related to harmful emissions. The discourse will shed light on the promising potential of environmentally sustainable, cost-effective, and easily adjustable catalysts based on perovskites. These catalysts are positioned as a compelling alternative to the prevailing expensive catalysts that incorporate noble metals. Subsequently, the discussion will pivot towards the examples of exploration of perovskite-based catalysts, their unique properties, including remarkable catalytic activity, abundance, and potential for tailored design. At the same time existing limitations and challenges will be marked. So, since the 80s of the last century it was pointed out that a variety of perovskites (cobaltites, manganites, chromites, and ruthenates) have high potential as catalysts to oxidize CO and to reduce NO<sub>x</sub> in automotive exhaust gases. Today, this is a crucial topic given the increasingly stricter exhaust regulations and the limited resources of precious metals used in mass fabricated three-way catalysts (TWC's) that are also able to convert unburnt hydrocarbons. According literature the mechanism of the oxidation of CO on a perovskite is a suprafacial reaction starting with the dissociation of O<sub>2</sub> from the gas phase into two O atoms that adsorb at B-site cations of the perovskite surface. Next, CO adsorbs to the surface and forms unstable CO<sub>3</sub>, which decomposes finally to an adsorbed O atom while CO<sub>2</sub> is released back to the gas phase. The mechanism of the intrafacial reactions involved in the reduction of NO<sub>x</sub> to N<sub>2</sub>: NO molecules adsorb at the surface containing vacancies in the oxygen lattice. There, NO dissociates in a way that O atoms fill the vacancies while N atoms recombine to N<sub>2</sub> that leaves the surface. As a downside, perovskite catalysts undergo activity loss under ageing, especially due to sulphur residues in the exhaust gas. Moreover, their surface-to-volume ratio is inferior to classical TWC's in which precious-metal particles are finely dispersed over a honeycomb-shaped network of alumina, ceria or silicates. An interesting option is the palladium-modified perovskite LaFe<sub>0.57</sub>Co<sub>0.38</sub>Pd<sub>0.05</sub>O<sub>3</sub> for which it was shown that Pd migrates reversibly in and out of the perovskite lattice under oxidizing and reducing gas conditions. Here, Pd stays catalytically active either as a B-site cation or as dispersed Pd nanoparticles with 1–3 nm diameter on top of the perovskite surface. Besides, there are also considerable efforts to synthesize perovskite catalysts with a textured structure in order to enhance their surface-to-volume ratio. Using hydrothermal synthesis routes from precursor solutions in combination with organic or inorganic templates resulted in mesoporous LaCoO<sub>3</sub> and LaMnO<sub>3</sub> specimens, three-dimensionally ordered macroporous LaCo<sub>x</sub>Fe<sub>1-x</sub>O<sub>3</sub> networks, and hollow LaMnO<sub>3</sub> spheres. A more straightforward technique to enlarge the active area of La<sub>0.9</sub>Ce<sub>0.1</sub>CoO<sub>3</sub> was reported also. The perovskite was found to catalyze the flameless combustion of hydrocarbons (e.g., methane) at comparatively low temperatures (800°C), thus avoiding formation of CO and NO<sub>x</sub>.

as noxious by-products. Perovskites can moreover catalyze the oxidative dehydrogenation of ethane ( $C_2H_6$ ) to ethane ( $C_2H_4$ ) and halogen-substituted perovskites such as  $La_{1-x}Sr_xFeO_{3-d}X_d$  turned out to be most efficient. The materials are synthesized with an oxygen deficiency  $d$ , which is replenished by fluorine or chlorine ( $X$ ) thus underpinning the relevance of oxygen vacancies for the catalytic mechanism. So, in case of catalysis, however, perovskites may soon play an important role due to limited resources of precious metals such as platinum and increasing needs in purification of exhaust gases and environmentally friendly energy storage and conversion. In essence, the lecture will encapsulate the imperative need to augment catalysts for chemical and electrochemical reactions, while spotlighting the promise of perovskite-based catalysts as a compelling and sustainable alternative.

### 3. Learning outcomes

- Students will understand the significance of catalysts improvement in chemical and electrochemical reactions for various modern technological and industrial applications, in particular environmental remediation.
- Students will gain insights into the available examples of perovskites as catalysts in addressing environmental challenges, such as reducing harmful emissions and promoting sustainable industrial processes.
- Students will acquire knowledge about the advantages and limitations of perovskite-based catalysts.
- Students will recognize the potential of perovskite-based catalysts as environmentally friendly, cost-effective, and easily tunable alternatives to existing catalysts containing noble metals and will appreciate their prospects in advancing green technology and contributing to the development of sustainable and efficient industrial practices.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the catalytic processes, known industrial catalytic reactions, etc. Also, they are recommended to read an articles P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, *Phys. Status Solidi A*, 2017, Vol. 214(9), 1700394; H. Arandiyana, P. Sudarsanam, S. K. Bhargava, A. F. Lee, and K. Wilson. Perovskite Catalysts for Biomass Valorization, *ACS Catal*, 2023, Vol. 13(12), 7879; J. A. Onrubia-Calvo, B. Pereda-Ayo, and J. R. González-Velasco. Perovskite-Based Catalysts as Efficient, Durable, and Economical NO<sub>x</sub> Storage and Reduction Systems, *Catalysts*, 2020, Vol. 10(2), 208; K. Wang, C. Han, Z. Shao, J. Qiu, S. Wang, S. Liu. Perovskite Oxide Catalysts for Advanced Oxidation Reactions, *Adv. Funct. Mater.*, 2021, Vol. 31(30), 2102089.

### 6. Additional notes

The topics will be covered in one lecture.



## Topics 4

### 1. The subject of the lecture

Perovskite piezoelectrics and ferroelectrics.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture aims to provide students with a comprehensive understanding of today's fields of application and future potential of piezoelectric/ferroelectric perovskites. Over the two hours, students will delve into the structural peculiarities that cause remarkable properties of perovskite piezoelectrics and ferroelectrics, and the impact of these advanced materials to revolutionize various areas, including electronics, energy, sensing technologies, etc. Piezoelectricity is the ability of certain materials to generate an electric charge in response to mechanical stress or pressure. Ferroelectricity is a characteristic of some substances that have a spontaneous electric polarization that can be reversed by the application of an external electric field. Perovskite compositions are one of the best known and the largest family of ferroelectric and piezoelectric materials. The piezoelectric properties of perovskites arise from their crystal structure, which consists of a three-dimensional network of metal cations and nonmetal anions. When a mechanical force is applied to the crystal, it causes a distortion in the lattice structure, which results in the separation of positive and negative charges, generating an electric field. Perovskites have been studied extensively for their piezoelectric properties, they exhibit high piezoelectric coefficients, which is a measure of the strength of the piezoelectric effect, and good thermal stability. In addition, perovskites have been shown to have good mechanical properties, such as high stiffness and low density, which make them suitable for use in various applications. Among the main fields of application of perovskite-based piezoelectrics are sensors for detecting pressure, strain, and vibration, environmental monitoring, healthcare as well as energy harvesting devices that convert mechanical energy into electrical energy; ultrasound transducers; analytical microbalances; actuators, which are devices that convert electrical energy into mechanical motion, for instance, actuators for the precision positioning of cantilevers in scanning tunnelling- and atomic force microscopy, so on). The interrelationship between the crystal structure of perovskites and their ferroelectric properties lies in the unique arrangement of ions and the resulting electric dipole moments within the perovskite lattice. The ferroelectric behavior is primarily attributed to the displacement of the B-site cations (usually a larger, more polarizable cation) relative to the A-site cations (usually a smaller, less polarizable cation) within the octahedral sites. This displacement leads to the formation of electric dipole moments along specific directions within the crystal lattice. As a result, the perovskites possess varying properties, such as high dielectric constants, large remnant polarization, and low coercive fields. These properties make perovskites attractive for a wide range of implementation, including energy storage devices, sensors, and piezoelectric transducers. During the lecture the best-known piezoelectric and ferroelectric perovskite materials will be discussed, among them  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  (PZT),  $\text{Pb}(\text{La,Zr,Ti})\text{O}_3$ ,  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $\text{PbTiO}_3$ ,  $\text{Pb}(\text{Sc,Ta})\text{O}_3$ ,  $(\text{K,Na})\text{NbO}_3$ ,  $\text{BaTiO}_3$ ,  $\text{BiFeO}_3$ ,  $\text{SrTiO}_3$ ,  $\text{SrZrO}_3$ ,  $\text{SrHfO}_3$  and others. In conclusion, it will be emphasized that despite the fact that PZT and its analogues are still the most widely used materials due to its outstanding performance



and commercial availability, there is an active and ongoing search for lead-free perovskites as potential replacements to explore new perovskites with improved properties and performance for emerging applications. The lecture will highlight the potential of piezoelectric/ferroelectric perovskites for the development of advanced material science.

### 3. Learning outcomes

- Students will be informed about the unique piezoelectric and ferroelectric properties of perovskites related to the peculiarities of their crystal structure and the latest research and developments in this field.
- Students will be familiarized with the advantages and limitations of perovskite piezoelectrics and ferroelectrics, as well as their potential to overcome existing challenges in current technologies.
- Students will gain insights into how perovskites can be leveraged to enhance the efficiency and performance of electronics, energy, and sensing technologies, including actuators, memory devices, energy harvesting, and sensors, contributing to the advancement of sustainable energy and technology solutions.
- Students will develop an ability to critically analyze and evaluate the future prospects of perovskite piezoelectrics and ferroelectrics in various applications, as well as their role in driving innovation across different sectors.
- Students will be equipped with skills to apply their theoretical knowledge to real-world problems and potential solutions.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the piezoelectricity and ferroelectricity. Also, they are recommended to read Ch. 6 at R. J. D. Tilley. Perovskites Structure–Property Relationships, John Wiley & Sons, Ltd., UK, 2016; K. Uchino. Glory of piezoelectric perovskites, Sci. Technol. Adv. Mater., 2015, Vol. 16(4), 046001; H. Park, C. Ha, and J.-H. Lee. Advances in piezoelectric halide perovskites for energy harvesting applications, J. Mater. Chem. A, 2020, Vol. 8(46), 24353; corresponding paragraph at P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, Phys. Status Solidi A, 2017, Vol. 214(9), 1700394.

### 6. Additional notes

The topics will be covered in one lecture.

## Topics 5

### 1. The subject of the lecture

Superconducting materials based on perovskites.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The aim of the lecture is to reveal the discovery and development of superconducting perovskites, current state-of-the-art research in this field and prospects of their practical application. The phenomenon of superconductivity has been a topic of interest for scientists for over a century. Superconducting materials exhibit zero electrical resistance and exclude magnetic fields, making them highly desirable for a range of applications, including power transmission, medical imaging, energy storage and quantum computing. The first perovskite material for which superconductivity was reported in 1975 is the cubic  $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$  with  $T_c = 13$  K. In recent years, perovskite-based superconductors have emerged as a promising area of research due to their potential for high-temperature superconductivity. Perovskites are a class of materials with a specific crystal structure, and they have been found to exhibit superconductivity when doped with certain elements. During the discussion, the unique properties of perovskite-based superconductors, including high critical temperatures and strong electron-phonon coupling, which are essential for achieving high-temperature superconductivity, will be considered. The students will have a possibility to familiarize with most promising examples of perovskite-based superconductors. Additionally, the audience will also examine the challenges facing researchers in this field, including the difficulty in synthesizing high-quality perovskite materials, their stability, need for a better understanding of the underlying physics, environmental safety, etc. For instance, famous organic-inorganic hybrid perovskite, such as methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ), that is well-known as a material for solar cells, LEDs, photodetectors, so on, have also shown superconductivity at low temperatures. Researchers are exploring ways to increase the  $T_c$  of these materials and make them more stable. Today the perovskite superconductors are still in the early stages of development and much work is needed to improve their superconducting characteristics. However, the potential for high-temperature superconductivity in perovskite materials is an exciting area of research that could lead to significant advancements in superconducting technology.

### 3. Learning outcomes

- Students will receive in-depth knowledge about superconducting perovskite-based materials, their properties and promising branches of implementation, in particular in energy storage and transmission, medical imaging, and quantum computing.
- Students will be familiarized with the existing challenges and limitations of perovskite superconductors and potential solutions to overcome them.
- Students will develop skills of critical thinking connected with evaluation of the perovskite's potential for future advancements and breakthroughs in the field of superconductivity.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the superconductivity. Also, they are recommended to read corresponding paragraph at P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, *Phys. Status Solidi A*, 2017, Vol. 214(9), 1700394; R. Kleiner, W. Buckel, and R. Huebener. *Superconductivity: An Introduction*, Wiley-VCH, 2015; D. Pelc, Z. Anderson, B. Yu, C. Leighton, and M. Greven. Universal superconducting precursor in three classes of unconventional superconductors, *Nat. Commun.*, 2019, Vol. 10, 2729.

#### 6. Additional notes

The topics will be covered in one lecture

## Topics 6

### 1. The subject of the lecture

Exploitation of perovskites in the solar cell development

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Perovskite solar cells (PSCs) are a relatively new and promising technology in the field of photovoltaics, offering potential advantages over traditional silicon-based solar cells. The most common perovskite material used in solar cells is methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ), also known as  $\text{MAPbI}_3$ . As of now, perovskite solar cells have achieved power conversion efficiencies of over 25%, which is comparable to the best silicon-based solar cells. The exploitation of perovskites in solar cell development is a rapidly growing field that has the potential to revolutionize the way we produce and store energy. This lecture will provide an in-depth overview of this exciting area of research, highlighting the advantages of perovskites over traditional materials and their potential (high sunlight absorption coefficient, tunable bandgap, high charge carrier mobility, low-cost fabrication) to drive sustainable and efficient sources of energy as well as currently existing problems (exclusion of toxic elements, improvement the stability and scalability of perovskite solar cells). In general, perovskites are a class of materials that have a unique crystal structure, which makes them highly efficient at converting sunlight into electricity. They are also relatively inexpensive and easy to produce, which makes them an attractive alternative to traditional solar cell materials like silicon. In recent years, researchers have made significant progress in improving the efficiency and stability of perovskite solar cells, making them a promising candidate for large-scale energy production. During the lecture, the questions about fundamental properties of perovskites and how they can be optimized for use in solar cells will be explored. The challenges associated with perovskite solar cell development, including stability issues and the need for improved manufacturing processes will also be discussed. In addition, one of the key benefit of perovskites – their ability to be used in tandem with other materials, such as silicon, to create highly efficient solar cells – will be underlined. This approach, known as tandem solar cells, has the potential to significantly increase the efficiency of solar energy conversion and reduce the cost of solar energy production. We will discuss the latest research in this area and the limitations associated with integrating perovskites into tandem solar cells. Finally, the potential impact of perovskite solar cells on the renewable energy industry and the broader energy landscape will be examined. We will discuss the economic and environmental benefits of perovskite solar cells and the role they could play in reducing our dependence on fossil fuels. Overall, this lecture will provide a comprehensive understanding of the exploitation of perovskites in solar cell development, highlighting the potential of this exciting field to drive sustainable and efficient sources of energy production and storage. Attendees will gain a deep knowledge about fundamental properties of perovskites, the advantages and disadvantages associated with their development, and the potential impact of perovskite solar cells on the renewable energy industry.

### 3. Learning outcomes

- Students will gain an understanding of the unique crystal structure of perovskites and their potential for efficient solar-to-electricity conversion.
- Students will be familiarized with the best and latest research regarding the development of solar cells on perovskite-based materials.
- Students will recognize the advantages of perovskites over traditional solar cell materials, such as high sunlight absorption coefficient, tunable bandgap, high charge carrier mobility, and low-cost fabrication, so on.
- Students will examine the challenges associated with PSC development, including stability issues, the need for improved manufacturing processes, environmental friendliness, etc.
- Students will explore the ability of perovskites to be used in tandem with other materials, such as silicon, to create highly efficient solar cells.
- Students will be able to analyze and evaluate the economic and environmental benefits, impact of PSCs on the renewable energy industry.
- Students will be capable to discuss the potential of perovskite materials to revolutionize the way we produce and store energy and their role in reducing our dependence on fossil fuels.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the sources of energy production and storage. Also, they are recommended to read S. Thomas, A. Thankappan. Perovskite Photovoltaics. Basic to Advanced Concepts and Implementation, Academic Press, Elsevier, 2018; corresponding chapters at R. J. D. Tilley. Perovskites Structure–Property Relationships, John Wiley & Sons, Ltd., UK, 2016; M. Borowski. Perovskites: Structure, Properties and Uses, Nova Science Publishers, 2011.

### 6. Additional notes

The topics will be covered in one lecture

## Topics 7

### 1. The subject of the lecture

Testing of perovskites in lithium-ion batteries.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Lithium-ion batteries are commonly used in portable electronic devices, such as smartphones, laptops, and tablets, as well as in electric vehicles and energy storage systems. Improving of Li-ion accumulators is a critical and ongoing endeavor to address the growing demand for energy storage, particularly in the context of renewable energy and electric vehicles. Recently, in the realm of lithium-ion batteries, perovskite materials are being explored for their potential to improve battery efficiency, capacity, and stability. During the lecture, the most prominent and innovative applications of perovskite materials in the field of lithium-ion batteries, focusing on both electrode and solid-state electrolyte components will be discussed in details. The thematic scope of this lecture will encompass the following key aspects: a brief consideration of the perovskite crystal structure from the point of view of its potential for enhancing lithium-ion battery performance; a thorough overview of the most promising perovskite-based cathode and anode materials, including their advantages, such as enability to rapid and efficient transfer of lithium ions during the charging and discharging processes that can lead to enhanced battery performance, shorter charging times, and increased energy density; highlighting of the unique properties of perovskite-based solid-state electrolytes, such as their high ionic conductivity, excellent mechanical and thermal stability, and potential for eliminating the safety concerns associated with liquid electrolytes; a discussion of the current challenges and limitations associated with the integration of perovskite electrodes and solid-state electrolytes; an inspection of the state-of-the-art perovskite-based lithium-ion batteries, including their performance, safety, and scalability. A summary of the key findings and future perspectives for perovskite materials in lithium-ion batteries, highlighting the potential for significant advancements in energy storage technology, will be formulated. In sum, the lecture will provide participants with a comprehensive understanding of the most recent developments and future prospects of perovskite-based materials in lithium-ion batteries, equipping them with the knowledge and skills necessary to contribute to the advancement of this rapidly evolving field.

### 3. Learning outcomes

- Students will be familiarized with the current state in Li-ion battery industry, including the latest achievements in this field related to the exploitation of ceramics, in particular most prominent examples of already used perovskite-based materials.
- Students will obtain a comprehensive understanding of the relationship between crystal structure and electrochemical properties of perovskite materials in the context of Li-ion batteries.
- Students will evaluate the existent advantages and limitations of perovskite cathode and anode materials as well as solid-state electrolytes in comparison with conventional Li-ion battery materials.



- Students will realize the potential perspectives of advancing and refining perovskite-based materials in Li-ion battery development. Their further optimization obviously will lead to enhanced energy density, improved safety, increased environmental friendliness, heightened stability, and expanded cycling and scalability capabilities, etc. Consequently, these advancements will have a profound impact on energy storage technology and the creation of next-generation energy storage and conversion systems.
- Students will improve their communicative and collaborative skills as well as encouraging innovative thinking and problem-solving abilities in discussing the latest research and development in perovskite materials for Li-ion batteries.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the modern energy storage and transformation systems, in particular Li-ion batteries. Also, they are recommended to read corresponding chapter at R. J. D. Tilley. Perovskites Structure–Property Relationships, John Wiley & Sons, Ltd., UK, 2016; corresponding paragraph at P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, Phys. Status Solidi A, 2017, Vol. 214(9), 1700394 as well as G. R. Monama, K. E. Ramohlola, E. I. Iwuoh, K. D. Modibane. Progress on perovskite materials for energy application, Results in Chemistry, 2022, Vol. 4, 100321.

#### 6. Additional notes

The topics will be covered in one lecture

## Topics 8

### 1. The subject of the lecture

Perovskite-based magnetic materials.

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Perovskite materials exhibit a broad spectrum of magnetic properties, including ferromagnetism, antiferromagnetism, ferrimagnetism, and paramagnetism. These properties can be tuned by modifying their chemical composition, structure, and external conditions, making them promising candidates for many today and tomorrow magnetic technologies. For instance, some perovskites, such as  $\text{LaFeO}_3$  and  $\text{SrFeO}_3$ , exhibit ferromagnetic behavior, where the magnetic moments of neighboring ions are aligned in the same direction, resulting in a net magnetic moment. This property is particularly interesting for potential applications in spintronics and magnetic storage devices. In antiferromagnetic perovskites, the magnetic moments of neighboring ions are aligned in opposite directions, canceling out the net magnetic moment. However, this property can be tuned by applying external factors, such as pressure or electric fields, which can lead to the emergence of ferromagnetism or other magnetic states. Ferrimagnetism is observed in perovskites where the magnetic moments of different ions are aligned in opposite directions, but their magnitudes are not equal. The net magnetic moment results from the difference in the magnitudes of the magnetic moments, leading to a ferrimagnetic state. In paramagnetic perovskites, the magnetic moments of the ions are randomly oriented, and they align with an external magnetic field. This property is observed in perovskites with unpaired electrons, such as those containing transition metal ions. This lecture aims to provide a comprehensive overview of perovskite-based magnetic materials. It will shed light on the wide range of magnetic properties and corresponding fields of practical application of perovskite-based materials. A special attention will be focused on the phenomenon of colossal magnetoresistance (CMR), which is predominantly observed in perovskite manganites. CMR refers to the dramatic change in electrical resistance of these materials in response to an external magnetic field. This effect is particularly intriguing due to its potential for applications in magnetic sensors, data storage, spintronic devices, etc. Despite the fact that mechanisms responsible for CMR in perovskite manganites is complex and is not yet fully understood, an attempt to discuss it will be done. Understanding these mechanisms is essential for optimizing the performance of ceramic magnetic phases and their utilizations. The study of CMR in perovskites represents an exciting frontier in materials science with the potential to drive innovation in the design of advanced functional materials and devices. In addition, the lecture will highlight actual challenges standing on the way of perovskite-based materials improvement (sensitivity to temperature, humidity, oxygen vacancies, etc), possible ways to solve them, and future prospects for perovskite-based magnetic materials to revolutionize the development of future magnetic technologies.

### 3. Learning outcomes

- Students will gain a comprehensive understanding of the diverse magnetic properties exhibited by perovskite materials, their connect to unique crystal structure and flexibility of perovskite chemical composition that opens wide opportunities for their tuning in



accordance with the needs of practical implementation, especially CMR and its potential for applications in magnetic sensors, data storage, and spintronic devices.

- Students will be capable of recognizing the obstacles impeding the advancement of perovskite-based materials and propose viable solutions to overcome these challenges.
- Students will be able to realize the future prospects and potential impact of perovskite-based magnetic materials on the advancement of future and emerging magnetic technologies.

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Lecture (informative/monographic/conversational) will be conducted with the use of multimedia (PowerPoint presentation) or interactive board to provide the coverage and description of key concepts and examples illustrating the discussed topic. During the lecture, the discussions and conversations with the students will take place.

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should review and refresh knowledge about the magnetic materials. Also, they are recommended to read corresponding chapter at R. J. D. Tilley. Perovskites Structure–Property Relationships, John Wiley & Sons, Ltd., UK, 2016 as well as M. Borowski. Perovskites: Structure, Properties and Uses, Nova Science Publishers, 2011; B. Raveau, A. Maignan, C. Martin, and M. Hervieu. Colossal Magnetoresistance Manganite Perovskites: Relations between Crystal Chemistry and Properties, Chem. Mater., 1998, Vol. 10(10), 2641-2652; J. Dho, W.S. Kim, E.O. Chi, N.H. Hur, S.H. Park, H.-C. Ri. Colossal magnetoresistance in perovskite manganite induced by localized moment of rare earth ion, Solid State Commun., 2003, Vol. 125(3-4), 143-147; corresponding paragraphs at P. Wagner. From Colossal Magnetoresistance to Solar Cells: An Overview on 66 Years of Research into Perovskites, Phys. Status Solidi A, 2017, Vol. 214(9), 1700394 and C. Moure, O. Pena. Recent advances in perovskites: Processing and properties, Progress in Solid State Chemistry, 2015, Vol. 43(4), 123-148.

#### 6. Additional notes

The topics will be covered in one lecture

## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory class

Pre-experimental preparation – literature data analysis.

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

This laboratory class aims to develop students' expertise in search and analysis of literature data from numerous resources and databases to optimize synthetic approaches on the example of ceramic materials with a perovskite structure. In particular, the students will be familiarized with various databases for processing relevant literature on perovskite ceramics, their properties, and synthesis methods (Pearson's Crystal Data, Scopus, Web of Science, Google Scholar, etc) and search strategies for locating pertinent information. They will be prompted to carry out critical analyze of the research articles and data, extract valuable insights from them, identify gaps in existing knowledge and propose innovative solutions based on current findings. The participants will gain hands-on practice in selecting appropriate synthesis techniques and parameters for specific applications. Over four hours, participants will engage in an immersive learning experience that emphasizes critical thinking, evidence-based decision making, and practical application of scientific knowledge.

#### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to identify key characteristics, ways to obtain and properties of perovskite ceramics.
- to locate and evaluate relevant literature using specialized databases and search engines.
- to analyze research articles and interpret results effectively.
- to apply critical thinking skills for assess the experimental designs and outcomes.
- to select suitable synthesis routes and parameters based on available literature data.
- to propose improvements or modifications to existing synthesis protocols of proposed perovskites.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

#### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory class will carry out with the use of specialized software (databases).
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.

d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 1 and 2.

#### **7. Additional notes**

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary software and instructions for practical work will be available.

## Topics 2

### 1. The subject of the laboratory classes

Producing of perovskite ceramics.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory course will be focused on the producing of perovskite ceramics. The students will engage in a hands-on exploration of solid-state reaction method to synthesize advanced multicomponent perovskite-based materials that contain alkali-earth, rare-earth, and 3d-metals. Students will obtain in-depth knowledge about the principles behind solid-state reaction methods, including phase diagrams, diffusion mechanisms, and kinetics. They gain insight into how these factors influence the formation of perovskite phases. Students will explore various  $ABO_3$  compositions, focusing on the impact of A- and B- cations on the resulting structure and (in future) material's properties. This thematic scope encompasses both fundamental and applied aspects of material science, with an emphasis on practical skills development. This laboratory course provides students with essential knowledge and skills that are transferable across multiple disciplines, fostering their growth as independent researchers capable of addressing complex challenges in modern material science research.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to deepen their knowledge of safety protocols at working with chemicals and equipment involved in the production of ceramic materials.
- to master their practical skills regarding common techniques used during the synthesis process, such as mixing powders, heat treatment, etc.
- to prepare high-quality samples of multicomponent perovskite using solid-state reaction method.
- to improve their own communication skills by performing group tasks.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- Powders of starting materials (oxides or carbonates of alkali-earth, rare-earth, and 3d-metals), solvents.
- Laboratory electronic balance.
- Agate mortars, corundum crucibles, press-forms, and other laboratory equipment.
- Muffle and tube furnaces.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory class will carry out with the use of specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.

c. Besides, during laboratory class, students will receive an individual task and perform it independently.

d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 1 and 2.

#### **7. Additional notes**

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary software and instructions for practical work will be available.

## Topics 3

### 1. The subject of the laboratory classes

Surface morphology and composition control.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

During the laboratory class students will be familiarized with advanced analytical techniques for characterizing surface morphology and chemical composition of different types of materials, among which perovskite-based ceramics. Over a span of four hours, students will engage in hands-on experiments using state-of-the-art instrumentation such as Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray Spectroscopy (EDX), and X-Ray Fluorescence spectroscope (XRF). These methods are essential tools for confirmation of qualitative and quantitative chemical composition of samples and phases, understanding or predict material properties, correction and optimization of performance for various applications, etc. Students will learn about the peculiarities of preliminary preparation, investigation and interpretation of experimental results on the example of ceramic samples. By mastering these techniques, they will acquire valuable skills applicable not only to perovskite ceramics but also to other functional materials systems across diverse fields of science and engineering.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand the basic principles of operation of a scanning electron microscope and X-ray fluorescence analyzer.
- to recognize common pitfalls associated with each method.
- to interpret images and spectra generated during analysis.
- to apply knowledge gained from the lab to predict material behavior based on observed characteristics.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- Scanning electron microscope and X-ray fluorescence analyzer.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory class will carry out with the use of specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students should prepare a theoretical introduction to the laboratory class.

Students are recommended to read A. Ul-Hamid. A Beginners' Guide to Scanning Electron Microscopy, Springer Cham, 2018; H. Ait Bouh. X-ray fluorescence analysis techniques: Principles and instrumentations, LAP LAMBERT Academic Publishing, 2020.

#### **7. Additional notes**

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary software and instructions for practical work will be available.



## Topics 4

### 1. The subject of the laboratory classes

X-ray phase analysis.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The laboratory class on X-ray phase analysis offers students a comprehensive introduction to the methodology and software utilized for phase identifying within polycrystalline ceramic samples, including multiphase materials. This practical session aims to equip students with the necessary skills and knowledge to analyze diffraction data obtained from an automated diffractometer. They will learn about the interaction of X-rays with crystalline samples and how diffraction patterns can be used to identify different phases present in a sample. Students will gain an understanding of the principles behind X-ray diffraction and its application in determining the crystal structure. Through hands-on experience, they will learn the step-by-step process of analyzing diffraction data to identify perovskite phases within polycrystalline samples. Students will be introduced to specialized software tools commonly used in X-ray phase analysis. They will learn how to input diffraction data, perform data processing, and interpret results to determine the composition of the sample in terms of different phases present. The class will cover the analysis of complex samples containing multiple phases. Students will explore strategies for distinguishing between overlapping peaks, quantifying phase fractions, and interpreting results accurately in the context of multiphase materials. By working with real data acquired on an automated diffractometer, students will have the opportunity to apply their theoretical knowledge in a practical setting. They will learn how to optimize experimental parameters, troubleshoot common issues, and validate their phase identification results. By engaging with actual experimental data and software tools, students will develop proficiency in conducting phase identification within polycrystalline ceramic samples, thereby enhancing their understanding of material characterization techniques in the field of solid-state chemistry and materials science.

### 3. Learning outcomes

- to understand the methodology for phase identification within polycrystalline ceramic samples.
- to carry out preliminary preparation of the sample before diffraction experiment.
- to operate with specialized equipment and typical software used in X-ray phase analysis.
- to interpret diffraction patterns acquired on an automated diffractometer.
- to gain and develop practical experience in analyzing multiphase materials (including perovskite phases) using diffraction data.
- to cultivate critical thinking skills by comparing theoretical knowledge with practical results obtained during the analysis.
- to foster teamwork and collaboration through group discussions and sharing of findings.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop.



- Internet connection.
- Automated diffractometer.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory class will carry out with the use of specialized software.
- Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- Besides, during laboratory class, students will receive an individual task and perform it independently.
- At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Students are recommended to read B.D. Cullity, S.R. Stock. Elements of X-Ray Diffraction, Pearson Education Limited, 2014; B. E. Warren. X-Ray Diffraction, Dover Publications Inc., 2003; W. Clegg. X-Ray Crystallography, Oxford Chemistry Primers, 2015.

#### 7. Additional notes

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### 8. Optional information

The necessary software and instructions for practical work will be available.

## Topics 5

### 1. The subject of the laboratory classes

Crystal structure characterization.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The thematic scope of the laboratory class on crystal structure characterization is centered around providing students with a deep understanding of the fundamental concepts and principles involved in solving and refinement of crystal structure of the chemical substances. The focus of this laboratory class will be on perovskite structures, which are a class of materials with a unique crystal structure that has been extensively studied due to their potential applications in various fields. During the laboratory class, students will have the opportunity to develop practical skills in utilizing specialized software for the determination, refinement, and crystal chemical analysis of perovskite-like structures. The audience will be introduced to the theoretical concepts of crystal structure solving and will be provided with hands-on experience in using specialized software for crystal structure analysis. It will cover a range of topics related to crystal structure characterization, including crystal symmetry, crystallographic databases, crystal structure determination, and refinement techniques. Students will also learn about crystal chemical analysis, which involves the analysis of the chemical composition, bonding, atomic surrounding, etc. The laboratory class will be conducted in a state-of-the-art laboratory equipped with advanced X-ray diffraction instruments and software. It will be led by experienced instructors who are experts in the field of crystal structure characterization. The laboratory class will equip students with practical skills in utilizing specialized software for crystal structure analysis, which will be invaluable in their future careers in various fields, including materials science, chemistry, and physics.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand the basic principles of crystal structure determination.
- to demonstrate knowledge of perovskite structures, their crystal structure peculiarities and diversity.
- to enhance practical skills in operating crystal structure characterization equipment.
- to apply commonly used specialized software for determination, refinement, and crystal chemical analysis of perovskite-like structures.
- to Interpret and analyze data obtained from crystal structure characterization experiments effectively.
- to use theoretical knowledge to real-world scenarios involving crystal structure analysis.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- Automated diffractometer.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory class will carry out with the use of specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Students are recommended to read B.D. Cullity, S.R. Stock. Elements of X-Ray Diffraction, Pearson Education Limited, 2014; B. E. Warren. X-Ray Diffraction, Dover Publications Inc., 2003; W. Clegg. X-Ray Crystallography, Oxford Chemistry Primers, 2015; V. Pecharsky, P. Zavalij. Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer, 2009.

#### 7. Additional notes

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### 8. Optional information

The necessary software and instructions for practical work will be available.

## Topics 6

### 1. The subject of the laboratory classes

Examination of mechanical properties.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The thematic scope of the laboratory class revolves around delving into the realm of mechanical properties through hands-on exploration and theoretical understanding. The practical work on the examination of mechanical properties focuses on familiarizing students with the basic principles and techniques involved in measuring mechanical properties, with a specific emphasis on the Vickers microhardness testing method as it pertains to ceramic perovskite materials. It uses a diamond indenter and a light load to produce an indentation on the material being tested, is widely used for measuring the hardness of different types of materials, including ceramics. The size or depth of the indentation caused by the indenter on the ceramic material is measured to determine its hardness. In addition, students will be introduced to the advantages and limitations of applying this method to ceramics. The Vickers test is renowned for its high precision and accuracy, ensuring consistent and reliable hardness measurements. One major limitation is that the surface of the ceramic specimen must be well-prepared, as the quality of the surface finish affects the precision of the measurement. This practical session is designed to equip students with a thorough comprehension of the methodologies and tools essential for evaluating the mechanical characteristics of materials. Through a blend of theoretical knowledge and practical experience, participants will emerge with a deeper appreciation for the role of mechanical properties in material science and engineering, equipped with valuable skills that can be applied across various industries and research domains.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand and explain about the Vickers microhardness testing method, its main principles, applications, and relevance to ceramic materials.
- to operate the equipment utilized in assessing mechanical properties, gaining hands-on experience with tools essential for conducting tests and measurements.
- to develop the skills necessary to accurately perform and interpret results from Vickers hardness measurements.
- to deepen a holistic understanding of how mechanical properties are evaluated and interpreted in real-world scenarios.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- equipment for hardness measurement by Vickers method.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory class will carry out with the use of specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### **6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Students should prepare a theoretical introduction to the laboratory class.

Students are recommended to read K. Herrmann. Hardness Testing: Principles and Applications, ASM International, 2011; H. Chandler. Hardness Testing, ASM International, 1999; D. Medlin, H. Kuhn. Mechanical Testing and Evaluation, ASM International, 2000.

#### **7. Additional notes**

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary software and instructions for practical work will be available.

## Topics 7

### 1. The subject of the laboratory classes

Electrochemical behavior study.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

This laboratory class aims to introduce students to the design principles and experimental analysis of lithium-ion energy storage systems, focusing on the electrochemical behavior of perovskite materials as potential battery electrodes. Over four hours, students will engage in hands-on experiments that foster their understanding of the following thematic areas: designing lithium-ion energy storage systems, perovskite materials as battery electrodes, investigating electrochemical properties and data analysis and interpretation. Students will learn about the key components and factors involved in designing an efficient Li-ion battery, including cell architecture, safety considerations, and performance metrics such as energy density, cycle life, and cost. They will apply this knowledge when analyzing existing literature and discussing the advantages and limitations of various cathode and anode materials. Students will explore the unique characteristics of perovskite materials, particularly those based on  $ABO_3$  compositions, which have promising prospects as high-performance cathodes for Li-ion batteries due to their high capacity and environmental stability. Throughout the lab session, students will perform experiments aimed at investigating the electrochemical properties of perovskite materials using techniques such as galvanostatic charge–discharge measurements. This will help students to understand how these materials interact with lithium ions during charging and discharging processes, ultimately enabling them to evaluate the suitability of perovskite materials as battery electrodes. By completing this laboratory course, participants will acquire essential skills in experiment planning, execution, data interpretation, and critical thinking within the field of electrochemistry and energy storage technology. Additionally, they will develop a deeper appreciation for the importance of interdisciplinary collaboration between chemists, physicists, engineers, and materials scientists in advancing sustainable energy solutions.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand the design principles and algorithms for developing energy storage systems.
- to enhance knowledge of the fundamental concepts underlying the operation of Li-ion batteries and their components.
- to gain the hands-on experience for producing Li-ion battery prototype and measurement of electrochemical properties.
- to evaluate the electrochemical behavior of perovskite materials as potential battery electrodes.
- to develop the problem-solving and critical thinking skills by analyzing data obtained from experiments.
- to improve teamwork and communication abilities while working collaboratively during the lab session.

- to draw up the obtained results and conclusions in the form of a report.

#### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- Galvanostat.
- 2-electrode prototype “Swagelok-cell” for electrochemical lithiation.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory class will carry out with the use of specialized software.
- Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- Besides, during laboratory class, students will receive an individual task and perform it independently.
- At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 7 and 8. Students are also recommended to read R. Korthauer. Lithium-Ion Batteries: Basics and Applications, Springer, 2018.

#### 7. Additional notes

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### 8. Optional information

The necessary software and instructions for practical work will be available.



## Topics 8

### 1. The subject of the laboratory classes

Magnetic properties measurements.

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

This laboratory class is designed to enhance students' practical competencies in investigation of magnetic properties within the context of ceramic materials. By engaging in this hands-on learning environment, participants will not only acquire essential technical abilities but also deepen their comprehension of fundamental theories pertinent to magnetism and materials science. The laboratory course aims to develop students' proficiency in measuring magnetic characteristics specifically related to perovskite ceramic materials. By participating in this lab course, students will have access to facilities that alleviate the study of these actual and needed objects. They will be familiarized with the equipment and methodology to measure magnetic susceptibility of perovskite-based materials at different temperatures or applied field using Faraday method. Participants will be able to observe firsthand how different parameters influence the magnetic response of perovskite ceramics, thereby developing a deeper appreciation for the interconnection between structure, composition, and properties of the materials. This immersive educational experience provides an opportunity for students to apply theoretical knowledge to real-world scenarios, fostering critical thinking and problem-solving capabilities. It will equip them with the tools needed to excel in the rapidly evolving field of materials science, particularly in areas involving magnetic perovskite materials. As they progress through the course, students will become adept at designing experiments, analyzing results, and drawing conclusions based on scientific evidence. In addition to acquiring practical skills, students will benefit from the guidance of experienced instructors who can provide valuable insights into current research trends and applications of perovskite ceramics in fields such as energy storage, sensors, and data storage devices. Overall, this laboratory class offers a unique opportunity for students to engage with cutting-edge technologies and concepts in magnetism and materials science, preparing them for careers in academia or industry where they may contribute to advancing our understanding of perovskite ceramics and their potential applications.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to master the basic knowledge and principles relating to magnetic phenomena, in particular in perovskite ceramics.
- to plan and carry out the experiments that yield reliable and reproducible results.
- to skillfully use of equipment for measurement of magnetic properties.
- to gain the abilities necessary to critically evaluation and interpretation of experimental findings.
- to apply acquired knowledge to solve problems that will encounter during research activities in future.
- to enhance teamwork capabilities due to collaborative efforts required during the lab.



- to draw up the obtained results and conclusions in the form of a report.

#### 4. Necessary equipment, materials, etc

- Personal computer or laptop.
- Internet connection.
- Equipment for magnetic susceptibility measurements by Faraday method.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- Laboratory class will carry out with the use of specialized software.
- Students will labor in a group, sharing tasks and working together to create a strategic plan, carry out an experiment, analyze and discuss the results and draw conclusions.
- Besides, during laboratory class, students will receive an individual task and perform it independently.
- At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 8. Students are also recommended to read D. Jiles. Introduction to magnetism and magnetic materials, CRC Press, 2015.

#### 7. Additional notes

The topic will be covered in 4 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### 8. Optional information

The necessary software and instructions for practical work will be available.

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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv

**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**SCANNING ELECTRON MICROSCOPY  
AND ENERGY DISPERSIVE X-RAYS ANALYSIS  
FOR MATERIALS SCIENCE**

**Code: SEM**

## Course content – lecture

### Topics 1

#### 1. The subject of the lecture

**Introduction to Microscopy. The theoretical principle of the method. Types of microscopes**

#### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to present the theoretical foundations of physical effects and phenomena, which are the basis of the principle of operation of various types of microscopes (laboratory light, electronic scanning (SEM), and electronic transmission (TEM)).

The lecture will include the general theory of obtaining electron flows for surface analysis (types of electron beam generation, methods of accelerating the electron flow, features of interaction with the surface). Also schematic diagram of different types of microscopes (light, atomic force, scanning and transmission) will be considered and analyzed in the lecture to define and specify the set scientific tasks (aim and purpose of the research, type of sample, size of crystallites, etc.)

#### 3. Learning outcomes

- **Knowledge:** The student will be able to define scientific task for SEM-investigation, selection of research objects and selection of the type of microscopy for analysis
- **Comprehension:** The student will be able to describe the schematic diagram of different types of microscopes with theoretical explanation of physical effects and phenomena
- **Application:** the student will be able to choose the studied materials in new and specific situations related to the study of the surface morphology, analysis of different inclusions, measurement of crystallite sizes, etc.
- **Analysis:** The student will be able to discuss the role of Scanning electron microscopy as an indispensable modern method of control and research of materials
- **Synthesis:** The student must create a conclusion about the fields of use and peculiarities of the study of various objects
- **Evaluation:** The student will be able to judge the value of theoretical and practical knowledge for setting real specific tasks

#### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

**A classic lecture** with repetition of previously studied material in physics and related courses

#### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

[https://imf.ucmerced.edu/sites/imf.ucmerced.edu/files/documents/sem\\_manual\\_06102019.pdf](https://imf.ucmerced.edu/sites/imf.ucmerced.edu/files/documents/sem_manual_06102019.pdf)

## Topics 2

### 1. The subject of the lecture

**Types of cathodes and detectors for image acquisition in microscopy. Practical requirements and preparation of samples for analysis.**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lectures will consider methods of generating electron flows and main types of materials for thermal emission (W-cathode, LaB<sub>6</sub>-cathode etc.). Also we will consider the main aspects for the preparation, installation and studying conditions of various type samples.

The lecturer pays special attention to the fundamental difference between ceramic cathode materials of field emission and thermocathode, in particular, the emission time, which is significantly different, and the price of the materials. It is also relevant why the system should be evacuated and how the presence of micro impurities such as oxygen negatively affects the life of the cathode. The lecturer together with the students will discuss the main requirements for samples for SEM research. The conversation with the students will be about the diversity of the nature of samples for research: powders, crystals, solids, bacteria, viruses, finished products, electronic elements, power sources, catalysts, etc.

### 3. Learning outcomes

- **Knowledge:** The student will be able to identify the method of sample analysis depending on its electrical conductivity and type (fragment, bulk body, powder, film, crystal)
- **Comprehension:** The student will be able to indicate technological features regarding the type of electron beam generation.
- **Application:** The student will propose a mechanism or algorithm for preparing samples for analysis and predict the expected results.
- **Analysis:** The student will be able to compare preparation and research methods for different types of samples.
- **Synthesis:** The student will be able to discuss how the conditions of examination of the samples affect the results of the analysis, in particular, preliminary sanding - polishing, sputtering of a conductive layer, cleaning with ultrasound, blowing with inert gas and connecting contacts to improve the electrical conductivity of the system.
- **Evaluation:** The student will be able to evaluate the profitability of using different types of cathodes and the complexity of researching real objects, in particular industrial products.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Interactive lecture: Lecture with two- to fifteenminute breaks for student activities (such as answering a multiple-choice objective item, solving a problem, comparing and filling in lecture notes

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

[https://courses.minia.edu.eg/Attach/10131Fundamentals%20of%20Scanning%20Electron%20Microscopy%20\(SEM\).pdf](https://courses.minia.edu.eg/Attach/10131Fundamentals%20of%20Scanning%20Electron%20Microscopy%20(SEM).pdf)

## Topics 3

### 1. The subject of the lecture

**Energy dispersive X-ray spectrum. Overlapping lines of the energy spectrum**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

At the beginning of the lecture, we will consider the main effects that occur during the interaction of matter with electrons or X-ray waves. In the following, we will discuss the relationship between the electronic configuration of elements and the number of series of peaks in the spectrum. Also we will explain the methods of calculating the composition in the cases when overlapping of lines in the spectra is occurred (Na/Zn; Gd/Ge; Hf/Re).

### 3. Learning outcomes

- **Knowledge:** The student will be able to determine the effects that occur during the interaction of an X-ray beam or an electron beam with a substance.
- **Comprehension:** The student will be able to describe primary and secondary phenomena during the interaction of electromagnetic radiation with matter.
- **Application:** The student will be able to select specific spectrum lines of various elements to determine the composition of a substance.
- **Analysis:** The student will be able to compare the appearance of the energy dispersion spectrum for different elements.
- **Synthesis:** The student will be able to predict the appearance of the spectrum for a specific composition of the substance
- **Evaluation:** The student will be able to evaluate the value of this material from the point of view of application for the analysis of complex objects

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with two- to fifteenminute breaks for student activities (such as answering a multiple-choice objective item, solving a problem, comparing and filling in lecture notes, debriefing a minicase, doing a thinkpair-share exercise).

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

C.E. Lyman, D.E. Newbury, J.I. Goldstein, D.B. Williams, A.D. Romig, J.T. Armstrong, P. Echlin, C.E. Fiori, D.C. Joy, E. Lifshin and Klaus-Ruediger Peters, Scanning Electron Microscopy, X-Ray Microanalysis and Analytical Electron Microscopy: A Laboratory Workbook, (Plenum Press. New York, N.Y., 1990).

<https://www.rigakuedxrf.com/nex-cg/>

Scimeca, M., Bischetti, S., Lamsira, H. K., Bonfiglio, R., & Bonanno, E. (2018). Energy Dispersive X-ray (EDX) microanalysis: A powerful tool in biomedical research and diagnosis. European Journal of Histochemistry, 62(1). <https://doi.org/10.4081/ejh.2018.2841>

## Topics 4

### 1. The subject of the lecture

**Analysis of objects of metal systems (bulk, polycrystalline and films) synthesized methods of electric arc and induction fusion, powder metallurgy etc.)**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture includes information about the conditions and peculiarities of researching metal objects that do not require sputtering of conductive applications. In the following, it will be shown how the method of synthesis of samples affect on the differs in size, shape of crystals and the presence of defects in the sample.

At the beginning of the lecture teacher will be devoted to various methods of synthesis of single-phase and multiphase metal objects, in particular, emphasis will be placed on the appearance of the surface morphology of samples of single composition and different methods of production (during melting and solid-phase reactions). Students will propose a method of synthesis and heat treatment for bulk samples, polycrystals, films, etc.

### 3. Learning outcomes

- **Knowledge:** The student will be able to distinguish the method of synthesis of the metallic type of the sample by the morphology of its surface.
- **Comprehension:** The student will be able to understand the meaning of the analysis of real objects for metallurgy or industrial products, in particular, how the shape and size of the grains affect the physical and chemical properties of the material.
- **Application:** The student will be able to apply the studied materials in new and specific situations related to the analysis of different types and compositions of samples student will be able to choose learned materials in new and concrete situations related to various types of water electrolysis
- **Analysis:** The student will be able to discuss the method of preparation and the peculiarity of the analysis of specific metal objects.
- **Synthesis:** The student will be able to discuss the sequence of operations during the examination of samples and the situation when it is necessary to involve the results of other methods for a competent interpretation of the results.
- **Evaluation:** The student will be able to assess the importance of the research for controlling the chemical composition and purposeful synthesis of new materials.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with two- to fifteenminute breaks for student activities (such as answering a multiple-choice objective item, solving a problem, comparing and filling in lecture notes).

**5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)**

Argast, Anne and Tennis, Clarence F., III, 2004, A web resource for the study of alkali feldspars and perthitic textures using light microscopy, scanning electron microscopy and energy dispersive X-ray spectroscopy, *Journal of Geoscience Education* 52, no. 3, p. 213-217.



## Topics 5

### 1. The subject of the lecture

**Quantitative analysis of objects with different chemical composition (oxides, chalcogenides, pnictides, borides etc.)**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The beginning of the lecture will include the theoretical and practical foundations of the synthesis of non-metallic objects (borides, oxides, chalcogenides, and nitrides). The lecturer will focus on the practical use of thin films of chalcogenides and oxide ceramics, in particular in photovoltaics. During the lecture, the necessity of obtaining monocrystalline, polycrystalline and thin films without defects and included impurities for high-quality physicochemical properties of materials will be discussed. To obtain a high-quality image and precise composition, it is necessary to apply a conductive thin layer of gold or carbon. Often, the thickness of such layers does not exceed 5-10 nm and has a positive effect on the quality of research. The lecture will be devoted to the study of weakly conductive and non-conductive surfaces of samples containing oxygen, phosphorus, sulfur or boron. Methods of applying conductive applications to improve conductivity for obtaining quality results will also be considered.

### 3. Learning outcomes

- **Knowledge:** The student will be able to define features of **chemical composition** of the different non-metallic objects (oxides, chalcogenides, pnictides, borides).
- **Comprehension:** The student will be able to describe the factors of the practical application of monocrystal, polycrystals and thin films of chalcogenides, and ceramics and the importance of controlling the chemical composition and homogeneity of surfaces to obtain high performance of the materials/
- **Application:** The student will be able to choose the learned knowledge and skills in new and specific situations related to the study of various types of non-metallic objects.
- **Analysis:** The student will be able to analyze and simulate the algorithm of preparation and research of real samples of materials.
- **Synthesis:** The student will be able to discuss the most important differences between types of non-metallic materials.
- **Evaluation:** The student will be able to evaluate the value of this material from the point of view of the possibility of practical application to control the composition and surface morphology of monocrystalline, polycrystalline, and thin films.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with 5-10 min breaks for student activities (such as answering a multiple-choice objective item, repetition of material from previously studied related courses, solving a problem) every twelve to twenty minutes.

## 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

Heslop-Harrison, J.S. (1990). Energy Dispersive X-Ray Analysis. In: Linskens, HF., Jackson, J.F. (eds) *Physical Methods in Plant Sciences. Modern Methods of Plant Analysis*, vol 11. Springer, Berlin, Heidelberg. [https://doi.org/10.1007/978-3-642-83611-4\\_9](https://doi.org/10.1007/978-3-642-83611-4_9)

## Topics 6

### 1. The subject of the lecture

#### Quantitative analysis of multiphase samples

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

This lecture aims to familiarize students with current trends in the SEM- and EDX- researching. The lecture discusses the multiphases materials (alloys, minerals, composites). The lecture will cover theoretical and applied aspects of the SEM- and EDX-analysis of multiphase samples (alloys, polycrystals, films, powders, bulk samples, minerals).

The researching algorithm for the investigation of concentration polymorphism, the study of composition of impurities, domains, and inclusions will be analyzed separately. For specific cases, the lector will analyze the elemental mapping and the composition of different phases by contrast using a BSE-detector.

### 3. Learning outcomes

- **Knowledge:** The student will be able to provide a list of real materials in industry or energy, where it is important to control the chemical and phase composition of the substance.
- **Comprehension:** The student will be able to describe the technological features of the analysis of complex multiphase samples.
- **Application:** The student will be able to use the learned materials and skills in new and non-standard situations related to the study of multiphase samples or composites.
- **Analysis:** The student will be able to discuss trends in the integration of methods of sample preparation and their research, in particular those close in composition (concentration polymorphism).
- **Synthesis:** The student will be able to independently formulate conclusions about the technological state of the surface of material samples, give a qualitative assessment of the chemical and phase composition.
- **Evaluation:** The student will be able to evaluate the usefulness and importance of scientific information for the complex analysis of the surfaces of multiphase samples

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with 5-10 min breaks for student activities (such as answering a multiple-choice objective item, repetition of material from previously studied related courses, solving a problem) every twelve to twenty minutes.

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

Students are expected to read below texts related to the lecture:



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Heslop-Harrison, J.S. (1990). Energy Dispersive X-Ray Analysis. In: Linskens, HF., Jackson, J.F. (eds) *Physical Methods in Plant Sciences. Modern Methods of Plant Analysis*, vol 11. Springer, Berlin, Heidelberg. [https://doi.org/10.1007/978-3-642-83611-4\\_9](https://doi.org/10.1007/978-3-642-83611-4_9)

## Topics 7

### 1. The subject of the lecture

**Analysis of composite systems (catalysts, electrocatalysts, electrodes, functional surfaces)**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

The lecture will be devoted to an overview of various composite objects (catalysts, electrocatalysts, layered compounds, compounds with a developed surface, electrode materials, and modified functional surfaces).

The beginning of the lecture will contain information on the features of electrodeposition of particles of different composition, surfaces for the formation of catalysts or electrocatalysts, in particular, a reminder of the features of electrolytic deposition of metals on the cathode or oxides such as TiO<sub>2</sub> (anatase, rutile) or PbO<sub>2</sub>. The lecture will also include an analysis of the quantitative composition of catalysts or functional surfaces

### 3. Learning outcomes

- **Knowledge:** The student will be able to determine the need for homogeneous doping and electrodeposition and to control the shape and size of particles for the best characteristics of catalysts and composites.
- **Comprehension:** The student will be able to describe the algorithm for preparing and examining samples and the aspects that need to be paid attention to in the first place during the examination of multiphase samples.
- **Application:** The student will be able to apply scientific information to interpret the obtained results and predict the effectiveness of materials, taking into account the uniformity, size and shape of particles and the presence of impurities or defects in the material.
- **Analysis:** The student will be able to analyze the obtained results and possible ways to improve the characteristics of the functional materials.
- **Synthesis:** The student will be able to formulate the sequence and algorithm of surface analysis, research of the chemical and phase composition of catalysts, composites and functional surfaces, sorbents, etc.
- **Evaluation:** The student will be able to analyze the effectiveness of functional materials depending on the type, shape, thickness and particle size.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with two- to fifteenminute breaks for student activities (such as answering a multiple-choice objective item, solving a problem, comparing and filling in lecture notes).

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

An FIB-SEM Study on Correlations between PEFC Electrocatalyst Microstructure and Cell Performance Makito Okumura *et al* 2016 *ECS Trans.* 75, 347

<https://doi.org/10.1149/07514.0347ecst>



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## Topics 8

### 1. The subject of the lecture

**Nanoscale systems. Methods and technologies of formation and analysis of nanostructures.**

### 2. Thematic scope of the lecture (abstract, maximum 500 words)

Methods of synthesis and stabilization of nano-sized particles and preparation samples for analysis will be considered in the lecture. Study conditions and interpretation of surface morphology will be discussed. The lecture is devoted to the study of nanoscale objects of various morphologies and sizes (0-D, 1-D, 2-D, 3-D). Spherical particles of perovskites obtained by the sol-gel method, anatase and carbon nanotubes by the electrochemical method, and thin films of metals obtained by epitaxy will be presented as examples. The lecturer will also consider the effect of the surface of the substrate on the shape and orientation of the particles. As a result, we will conduct statistical data processing, construct distribution diagrams, determine the average size of crystallites and compare these results using empirical methods, in particular, the Debye-Scherrer method.

### 3. Learning outcomes

- **Knowledge:** The student will be able to determine the morphology (spherical, rod, octagons, irregular, needles, plates etc.) and size of nanosized particles.
- **Comprehension:** The student will be able to analyze the methods of synthesis and research of nano-sized particles and the aspects that must be addressed to control uniformity and morphology.
- **Application:** The student will be able to apply scientific information to interpret the obtained results and predict the performance of materials, taking into account the uniformity, size and shape of particles.
- **Analysis:** The student will be able to analyze the obtained results, carry out statistical data processing, and determine the average particle size.
- **Synthesis:** The student will be able to formulate a sequence of research on the surface, chemical and phase composition of nanosized particles.
- **Evaluation:** The student will be able to analyze and evaluate the morphological and dimensional characteristics of the particles, their homogeneity, and the thickness of the synthesized layers.

### 4. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

#### Interactive lecture:

Lecture with two- to fifteenminute breaks for student activities (such as answering a multiple-choice objective item, solving a problem, comparing and filling in lecture notes).

### 5. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students are expected to read below texts related to the lecture:

D. B. Williams and C. B. Carter, *Transmission Electron Microscopy*, Springer, 2009.

W. Zhou, R. Apkarian, Z. L. Wang and D. Joy, "Fundamentals of Scanning Electron Microscopy (SEM)," in *Scanning Microscopy for Nanotechnology*, Springer, 2007, pp. 1-40.

## Course content – laboratory classes

### Topics 1-2 – Lab 1

#### 1. The subject of the laboratory classes

Preparation of metal samples for analysis (film and bulk sample). Image acquisition, interpretation of results.

EDX and XRF analysis for general sample composition.

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Laboratory works include methods of preparing samples for analysis, applying and attaching samples to conductive tables, blowing with inert gas applied powdered samples, choosing research conditions to obtain qualitative results at different magnifications (voltage, working distance, electron beam intensity). The beginning of the laboratory work will include a visual introduction to scientific equipment and auxiliary equipment for sample preparation. SEM images of the samples will be obtained using SE-, and BSE-detectors, and the total composition of the samples will be obtained by the methods of EDX (area mapping and composition in the point) and XRF.

#### 3. Learning outcomes

- **Knowledge:** The student will be able to choose the preconditions for preparation and examination of samples using SEM-, EDX- and XRF- methods.
- **Comprehension:** The student will be able to explain the need to prepare samples for analysis, and the obtained results of experiments
- **Application:** The student will be able to use the accessory for cutting, grinding and polishing and applying samples for researching work.
- **Analysis:** The student will be able to determine and compare the conditions of shooting samples, the selection of optimal operating parameters for obtaining quality results.
- **Synthesis:** The student will be able to describe a step-by-step algorithm for sample preparation and research
- **Evaluation:** The student will be able to evaluate the quality of the SEM image depending on the operating parameters; also will be able to analyze which parameters need to be controlled, which corrections need to be made in order to obtain qualitative results of the chemical composition of the samples.

#### 4. Necessary equipment, materials, etc

- Samples: steel-stainless metallic plates, metallic bulk sample.
- Apparatus: electron microscope with EDX-analyzer, XRF-analyzer with cells, grinding and polishing machine, compressed gases in cylinders.
- Solutions for cleaning the surfaces, abrasive papers and suspension, C-coating films.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

Teaching methods used:



*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

**Laboratory course outline:**

1. Introduction

- Presentation of rules at the hydrogen technology laboratory.
- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

2. Course of exercise

- Presentation of instructions on the use of equipment.
- Carrying out of the experimental research.

3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.

4. Summary and conclusions

- Comparison of experimental results from EDX-method with results from XRF-method.

5. Organizing positions and ending

- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 3-4 – Lab 2

### 1. The subject of the laboratory classes

Examination of metal samples after thermal structuring, annealing or modified. Analysis of solid phase reactions and eutectics.

Research of non-conductive samples. Application of conductive surfaces (C- or Au-nanofilms)

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study of the metal and non-metal samples. The first part of the laboratory work will include the study of metal objects of different crystallization methods: rapid quenching from the liquid state, in particular with eutectics-reaction, after annealing in an inert environment and in air. This is necessary to see the different microstructure of the material, as well as to trace the microcrystallization of oxide particles on the metal surface. The second part of the laboratory will include the study of non-metallic objects (non-conductive samples) with mandatory preliminary preparation, namely, applying a conductive layer or making contacts using conductors.

### 3. Learning outcomes

- **Knowledge:** The student will be able to choose specific experimental conditions of research and preparation of samples for metallic samples (for example, eutectic alloys of the Cu-Pb system) and non-metallic samples for example, ceramic powders of the Ca-R-{Fe,Mn}-O or TiO<sub>2</sub>-Nb<sub>2</sub>O<sub>5</sub> system.
- **Comprehension:** The student will be able to explain the need to apply a conductive layer for non-conductive samples.
- **Application:** The student will be able to apply knowledge about the appearance of the microstructure of samples to explain and interpret the technological conditions of their production (tempering, annealing, etc.)
- **Analysis:** The student will be able to determine the type of metallic alloy or non-metallic sample, analyze the microstructure and phase composition by morphology.
- **Synthesis:** The student will be able to interpret the obtained results, analyze the chemical and phase composition of the samples, and formulate the conclusions.
- **Evaluation:** The student will be able to evaluate the importance of information for analyzing samples of real materials.

### 4. Necessary equipment, materials, etc

- Samples: metallic pieces (Cu-Pb), non-metallic ceramic powders of the Ca-R-{Fe,Mn}-O or TiO<sub>2</sub>-Nb<sub>2</sub>O systems.
- Apparatus: electron microscope with EDX-analyzer, grinding and polishing machine, compressed gases in cylinders.
- Solutions for cleaning the surfaces, abrasive papers and suspension, C-coating films.

## 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

### Teaching methods used:

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data (chemical and phase composition) and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn (in particular, conclusions about obtaining results and ensuring the application of a layer of carbon or gold on non-conductive samples to obtain electrically conductive objects.)
- Comparison of experimental results with theoretical expectations (eutectic alloys etc.).

#### 5. Organizing positions and ending

- Tips for organizing work stations and proper storage of materials and chemical reagents used.
- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 5-6– Lab 3

### 1. The subject of the laboratory classes

**Analysis of single crystals and polycrystalline. Determination of amounts of impurities.**

**Analysis of electrodeposited surfaces and modified catalysts.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Laboratory work will be devoted to the study of the chemical and phase composition of complex multiphase objects and non-conductive samples containing light elements (boron, carbon, nitrogen, phosphorus, oxygen, etc.).

During laboratory work, students will be able to prepare one metal polycrystalline and sample and one composite ceramic sample for research. At the end of the lesson, the overall composition of the sample (obtained from the elemental mapping-distribution) and the composition of individual phases will be analyzed.

Electrocatalysts are products for various industries, so it is necessary to control the thickness, composition and shape of electrodeposited coatings.

### 3. Learning outcomes

- **Knowledge:** The student will be able to choose working parameters for the analysis of single-crystalline and polycrystalline metallic and non-metallic samples.
- **Comprehension:** The student will be able to explain the importance of the conductivity of objects and the precise determination of chemical composition on flat areas (perpendicular to the electron beam) of the sample.
- **Application:** The student will be able to apply knowledge to research materials for electrocatalysts, photovoltaics and electronics.
- **Analysis:** The student will be able to analyze the surface condition, presence of impurities and chemical composition in mono and polycrystalline samples.
- **Synthesis:** The student will be able to evaluate the dimensional characteristics and shape of crystallites.
- **Evaluation:** The student will be able to evaluate the state of the surface of crystals, polycrystals for example, microelectronics and photovoltaics (mono- and polycrystalline samples and films).

### 4. Necessary equipment, materials, etc

- Samples: metallic polycrystallines and crystals, non-metallic powders, Si-crystals, ZnO- thin films, Pt/TiO<sub>2</sub>-electrocomposites.

- Apparatus: electron microscope with EDX-analyzer, grinding and polishing machine, a device for sputtering gold or carbon, compressed gases in cylinders.

- Solutions for cleaning the surfaces, abrasive papers and suspension, C-coating films.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

**Teaching methods used:**

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.
- 

#### 3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn (the importance and necessity of spraying the conductive surface to obtain high-quality and precise results)
- Comparison of experimental results with theoretical expectations.
- Discussion of the relationship between theory and practice and the importance of results for materials engineering.

#### 5. Organizing positions and ending

- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 7-8 – Lab 4

### 1. The subject of the laboratory classes

**SEM in battery research. Morphology investigation of electrodes.**

**Analysis of multiphase samples.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

Laboratory work will include the analysis of electrode materials for lithium-ion and metal-hydride batteries. In order to explain the course of electrochemical processes, the starting material will be examined and after passing 50 or 100 charge-discharge cycles. It is important to show side processes, processes occurring on the surface of grains - surface passivation with the participation of SEI (solid-electrolyte interface). Samples of electrode materials are multiphase, so it is important to establish the composition of each phase of the electrode materials. The morphology of the surface of the electrode shows the resource of the battery or fuel cell.

### 3. Learning outcomes

- **Knowledge:** The student will be able to analyze the importance of controlling the surface condition, chemical and phase composition of battery materials to ensure the best performance.
- **Comprehension:** The student will be able to explain the principle of the structure of batteries and fuel cells, the importance of controlling the morphology, particle size and phase composition of the material
- **Application:** The student will be able to apply knowledge to find ways to improve the efficiency of current sources by knowing the mechanisms of processes at the micro level.
- **Analysis:** The student will be able to determine the size of the polycrystallines and the composition and thickness of the passivating film ( )
- **Synthesis:** The student will be able to evaluate the stability of the material of the chemical source of electrical energy (accumulators, fuel cells) and formulate the requirements for the morphology and grain sizes of the electrode material
- **Evaluation:** The student will be able to evaluate the changes in the dimensional characteristics of the grains of the electrode material and the phase and composition changes during electrochemical processes.

### 4. Necessary equipment, materials, etc

- Samples: as-cast electrode materials for Li-ion battery and nickel metalhydride battery and electrodes after 50 or 100 cycles of charge/discharge, electrolytes.
- Apparatus: electron microscope with EDX-analyzer, a device for sputtering gold or carbon, compressed gases in cylinders.
- Solutions for cleaning the surfaces, C-coating films.

## 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

### Teaching methods used:

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn.
- Comparison of experimental results with theoretical expectations or earlier results.
- Discussion of the relationship between theory and practice and the importance of results for materials engineering, in particular energy materials.

#### 5. Organizing positions and ending

- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.



## Topics 9-10 – Lab 5

### 1. The subject of the laboratory classes

**Analysis of composites with polymers.**

**Investigation of the samples with concentration polymorphism.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study the different composites with organic and inorganic polymers. Most related objects show a small contrast at BSE-detector because of the particles have a similar composition. During the first part of the laboratory work, students will investigate the morphology and phase composition of multiphase samples containing polymers and a metal matrix. In the second part of the laboratory, students will set up a composition of the phases with a very similar composition by modifying the study conditions to increase phase contrast. Study of concentration polymorphism is an interesting phenomenon as a derivative of temperature polymorphism, when the material is sensitive to temperature changes. Concentration polymorphism is more characteristic of inorganic objects and occurs during a small change in chemical composition. As an example, consider alloys based on compounds of digermanides  $RGe_{2-x}$  or disilicides  $RSi_{2-y}$  which have a defective structure. Using SEM, EDX and XRD methods, we can interpret these multiphase alloys.

### 3. Learning outcomes

- **Knowledge:** The student will be able to choose the working parameters of the study taking into account the chemical composition of the studied objects to increase the phase contrast.
- **Comprehension:** The student will be able to explain the inverse dependence of the working voltage of the cathode and the wavelength of the electron beam and its effect on the quality of the obtained images.
- **Application:** The student will be able to apply correctly selected research conditions and interpret the research results, indicate the type of morphology, phase composition and crystallite sizes.
- **Analysis:** The student will be able to determine the main characteristics of composites and multiphase alloys.
- **Synthesis:** The student will be able to comprehensively analyze complex objects using the methods of SEM, EDX and powder XRD.
- **Evaluation:** The student will be able to formulate competent conclusions about the phase and chemical composition and crystal structure of multiphase samples or composites.

### 4. Necessary equipment, materials, etc

- Samples: polymer and metallic composites, multiphase alloys  $RGe_{2-x}$  and  $RSi_{2-y}$  or another.
- Apparatus: electron microscope with EDX-analyzer, a device for sputtering gold or carbon, compressed gases in cylinders, powder XRD diffractometer.
- Solutions for cleaning the surfaces, C-coating films.



## 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

### Teaching methods used:

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn.
- Comparison of experimental results with theoretical expectations or earlier results.
- Discussion of the relationship between theory and practice and the importance of results for materials engineering.

#### 5. Organizing positions and ending

- Tips for organizing work stations and proper storage of materials and chemical reagents used.
- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 11-12 – Lab 6

### 1. The subject of the laboratory classes

**Femtosecond laser-induced nano- and microstructuring.**

**SEM-investigation of biological objects and composite biosensors.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study of objects with the obligatory application of a conductive layer (nanolayer of Au), since the surface with nano-structures after laser treatment or biological objects (bacteria, viruses and biosensors) are not electrically conductive over the entire surface. LIPSS as a target product of femtosecond surface treatment of materials are interesting for fundamentally changing the properties of materials, in particular hydrophilicity-hydrophobicity. The study of biological objects is interesting for establishing the mechanisms of biochemical reactions and the study of selective sorption for the development of bio- or chemosensors

### 3. Learning outcomes

- **Knowledge:** The student will be able to model the sequence of actions for the preparation and analysis of biological samples and surfaces after femtosecond laser processing.
- **Comprehension:** The student will be able to characterize the investigated nano- and microstructures.
- **Application:** The student will be able to apply correctly selected research conditions and interpret the research results, indicate the type of morphology, phase composition and crystallite sizes.
- **Analysis:** The student will be able to determine the main characteristics of bio-composites and functional surfaces after femtosecond laser processing.
- **Synthesis:** The student will be able to comprehensively analyze complex bio-objects and functional surfaces after femtosecond laser processing.
- **Evaluation:** The student will be able to formulate competent conclusions about the morphology and size characterization of the bio-objects and functional surfaces after femtosecond laser processing.

### 4. Necessary equipment, materials, etc

- Samples: metallic polycrystalline plates after femtosecond-laser-induced, bio-material, bio-cells, commercial rapid tests for bioresearching.
- Apparatus: electron microscope with EDX-analyzer, grinding and polishing machine, a device for sputtering gold or carbon, compressed gases in cylinders.
- Solutions for cleaning the surfaces, abrasive papers and suspension, C-coating films.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

**Teaching methods used:**

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn.
- Comparison of experimental results with theoretical expectations or earlier results.
- Discussion of the relationship between theory and practice and the importance of results for materials engineering.

#### 5. Organizing positions and ending

- Tips for organizing work stations and proper storage of materials and chemical reagents used.
- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 13-14 – Lab 7

### 1. The subject of the laboratory classes

**Morphology of superhard materials. Investigation of microhardness of the samples.**

**Microstructure and phase analysis of MAX phases.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study the different superhard materials, composites carbides based on the Ti-alloys. The laboratory work will investigate and measure the dimensions of the diagonals after pressing a diamond pyramid into the surface of hard materials(determination of microhardness by the Vickers method), in particular titanium alloys, borocarbides and borosilicides.Using higher loads, it is possible to research of the crack resistance of the material. MAX-phases are interesting and promising layered materials for functional electronics. A sample of the MAX-alloy will be examined in cross-section to determine the thickness of the layers.

### 3. Learning outcomes

- **Knowledge:** The student will be able to prepare the surface of a super-hard sample for microhardness measurement and perform pyramid indentation measurements and determination of mechanical parameters.
- **Comprehension:** The student will be able to explain the obtained results.
- **Application:** The student will be able to qualitatively interpret the results of the study, indicate the type of morphology, sizes of cracks, mechanical properties.
- **Analysis:** The student will be able to determine the main mechanical characteristics of alloys, analyze the obtained results.
- **Synthesis:** The student will be able to analyze the state of the functional surface using SEM, EDX methods.
- **Evaluation:** The student will be able to formulate competent conclusions about phase and chemical composition, mechanical properties such as Vickers microhardness and crack resistance.

### 4. Necessary equipment, materials, etc

- Samples: Ti-based alloys, borocarbides, borosilicides.
- Apparatus: electron microscope with EDX-analyzer, device for measuring microhardness, compressed gases in cylinders.
- Solutions for cleaning the surfaces, C-coating films.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

**Teaching methods used:**

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained. It is important to maintain a balance between student activity and the lecturer's role to ensure interactivity and effective knowledge assimilation.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn.
- Comparison of experimental results with theoretical expectations (literature data) or earlier results.
- Discussion of the relationship between theory and practice and the importance of results for materials engineering.

#### 5. Organizing positions and ending

- Tips for organizing work stations and proper storage of materials and chemical reagents used.
- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

## Topics 15-16 – Lab 8

### 1. The subject of the laboratory classes

**Microstructure and composition of high-entropy alloys.**

**Microstructure and composition of the objects for micro- and nano-electronics.**

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The topics of the laboratory classes are related to the study high-entropy alloys and multiphases for micro- and nano-electronics. High-entropy alloys are not only promising structural materials, but also the basis of micro- and nano-electronics. Functional layered and high-entropy alloys coatings are the basis for boards, controllers and chips. The purpose of the work is to establish the thickness, size of contacts and chemical composition of coatings in real electronics objects. Since a large part of the electronics area consists of a non-conductive polymer, a conductive layer of carbon or gold is additionally applied.

### 3. Learning outcomes

- **Knowledge:** The student will be able to choose specific experimental conditions for research and preparation of real samples of micro- and nano-electronics, establish the thickness of the coating and the composition of the material.
- **Comprehension:** The student will be able to explain the need to establish the composition and dimensional characteristics of coatings and contacts.
- **Application:** The student will be able to apply knowledge to explain and interpret the technological conditions of production of electronic objects.
- **Analysis:** The student will be able to determine the type of metal coating, analyze the microstructure and phase composition by morphology and chemical composition.
- **Synthesis:** The student will be able to interpret the obtained results, analyze the chemical and phase composition of samples and formulate conclusions.
- **Evaluation:** The student will be able to assess the importance of a scientific approach to the analysis of samples of real materials of nano- and microelectronics.

### 4. Necessary equipment, materials, etc

- Samples: metallic multicomponent alloys, samples of chips or controllers.
- Apparatus: electron microscope with EDX-analyzer, grinding and polishing machine, device for sputtering gold or carbon, compressed gases in cylinders.
- Solutions for cleaning the surfaces, abrasive papers and suspension, C-coating films.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

**Teaching methods used:**

*Group work:* Students doing an exercise activity or creating a product in small groups of two to six in laboratory; exercise is carefully managed by the lecturer.

*Case method:* Students applying course knowledge to devise one or more solutions or resolutions to problems or dilemmas presented in a realistic story or situation.

### Lab course outline:

#### 1. Introduction

- Introduction to the topic of the laboratory.
- A short test or colloquium to see how well students understood the content of previous lectures and prepared for the laboratory. Questions may apply to both theory and practical aspects related to the experiment.
- Presentation of goals, procedures and expected results of the exercise.
- Division of students into groups and assigning appropriate positions. Individual groups are responsible for developing a research plan and determining the role of each group member in the exercise.

#### 2. Course of exercise

- Presentation of instructions on the use of equipment.

#### 3. Data analysis and interpretation

- Groups analyze the collected data (chemical and phase composition) and prepare appropriate charts, tables or reports.
- The lecturer conducts a discussion on the results received and helps students interpret the data obtained.

#### 4. Summary and conclusions

- A joint discussion about the results obtained and conclusions drawn (in particular, conclusions about obtaining results and ensuring the application of a layer of carbon or gold on non-conductive samples to obtain electrically conductive objects.)
- Comparison of experimental results with theoretical expectations (eutectic alloys etc.).

#### 5. Organizing positions and ending

- Tips for organizing work stations and proper storage of materials and chemical reagents used.
- End of the laboratory. The lecturer reminds students about the next date of laboratory classes.

#### 6. Preparing a report

- The lecturer discusses the requirements and rules for assessing the report.

<b>Reports:</b>	40%
<b>Quiz:</b>	10%
<b>Total</b>	100%

#### Grading Scale

89.5% - 100% = A
84.5% - 89.4% = B+
79.5% - 84.4% = B
74.5% - 79.4% = C+
69.5% - 74.4% = C
64.5% - 69.4% = D+
59.5% - 64.4% = D
0% - 59.4% = F



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**Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv**



**SUPPLEMENTARY MATERIALS**  
**FOR THE FOUR-SEMESTER MASTER'S DEGREE PROGRAM**  
**MATERIALS SCIENCE MA(S)TERS**

# **TEACHERS' GUIDE**

**The Teachers' Guide is a supplement to the information  
contained in the course syllabus**

**X-RAY DIFFRACTION**  
**ATOMIC STRUCTURE AND MICROSTRUCTURE**

**Code: XRDASM**

## Table of Contents

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- **Topic 7:** Microstructural analysis
- **Topic 8:** Short- and medium-range order analysis

### Laboratory Topics

- **Topic 1:** Applied crystallography
- **Topic 2:** Applied crystal chemistry
- **Topic 3:** XRD data collection
- **Topic 4:** XRD data proceedings
- **Topic 5:** Structure solution
- **Topic 6:** Structure refinement
- **Topic 7:** Microstructural analysis
- **Topic 8:** Short-range order analysis

## Course content – lecture

### Topic 1

#### Fundamentals of crystalline state: Part I

During the lecture, students will be familiarized with the concepts of crystalline state, which is characterized by the presence of both short-, medium-range, and long-range ordering of particles. Short-range order is an arrangement of atoms, which is repeated at distances commensurate with the distances between atoms, that is, a regularity in the arrangement of nearest neighbors. Long-range order is the periodicity of the arrangement of atoms in the entire crystalline body, regardless of the distances between atoms. The lecture will give the students knowledge about the symmetry operations, crystal systems, Bravais lattices, atomic coordinates, and space groups, and will allow to get an idea of ideal, real, and average structures. The real structure is responsible for the property, without explaining the crystal structure it will not be possible to explain why exactly the material functions. In real structures, there are various defects, that is, local changes in the arrangement of atoms that break the translational symmetry of the ideal structure. Students will also learn about the liquids and amorphous/semi-amorphous substances as examples of short- and medium-range order.

#### LEARNING OUTCOMES

- **Understanding** the general concept of crystalline state in modern science.
- **Knowledge:** the student will be known about the methodology for description of crystalline state: crystal lattice and crystal structure, symmetry operations and symmetry elements, fundamentals of group theory, crystal systems, Bravais lattices, atomic coordinates, space groups, non-conventional symmetry, radial distribution function.
- **Comprehension:** the student will understand the importance of the concept of the crystalline state as a foundation for explaining the properties of substances.
- **Application:** based on the data on the structure of the substance, the student will know which substances can be promising for practical use.
- **Analysis and Synthesis:** the student will be able to compare different substances and their properties depending on their structure and to select the necessary candidates or create a new one (based on known compounds with a similar structure) for following application.
- **Evaluation:** the student will be able to predict possible physical properties of known or new compounds having information about the structure of the substance.

#### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.
- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

## RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.

International Tables for Crystallography. <https://it.iucr.org>

Also, compact, complete and accessible information is presented on Wikipedia in the category Crystallography:

<https://en.wikipedia.org/wiki/Category:Crystallography>

## Topic 2

### Fundamentals of crystalline state: Part II

During the lecture, students will be familiarized with the concepts of crystal chemistry (types of crystal structures, atomic radii, interatomic distances and angles, close-packed structures, atomic coordination and polyhedra). Crystal chemistry is the study of the principles of chemistry behind crystals and their use in describing structure-property relations in solids, as well as the chemical properties of periodic structures. The principles that govern the assembly of crystal and glass structures are described, models of many of the technologically important crystal structures are studied, and the effect of crystal structure on the various fundamental mechanisms responsible for many physical properties are discussed. The main concept is crystal structure, which includes: chemical formula, crystal system, space group, cell parameters, number of formula units in the unit cell, calculated density, atom coordinates. Short range order refers to the regular and predictable arrangement (i.e. crystalline lattice) of atoms over a short distance, usually with one or two atom spacings. However, this regularity described by short-range order does not necessarily apply to a larger area. In addition, students will be familiar with ionic, covalent, molecular and metallic compounds, Valence Electron Concentration, hydrogen bonding, different kinds of defects. Students will be introduced to such concepts as structure types (specific arrangements of atoms (without taking into consideration the chemical nature of the components) with their standardization and classification, allotropic forms, polymorphism, nonstoichiometry, solid solutions, phase transitions, group-subgroup relationships, non-commensurate modulated and composite structures and quasicrystals, and superstructures.

### LEARNING OUTCOMES

- **Understanding** the general concepts of crystal chemistry.
- **Knowledge:** the student will be known about the methodology for description of crystalline state: crystal structure, structure types and their standardization; and will be known structures of ionic, covalent, molecular and metallic compounds.
- **Comprehension:** the student will understand the importance of the concept of the crystalline state as a foundation for explaining the properties of substances; factors that influence the crystal structure.
- **Application:** based on the data on the structure of the substance, the student will know which substances can be promising for practical use.
- **Analysis and Synthesis:** the student will be able to compare different substances and their properties depending on their structure and to select the necessary candidates or create a new one (based on known compounds with a similar structure) for following application.
- **Evaluation:** the student will be able to predict possible physical properties of known or new compounds having information about the structure of the substance.

### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.
- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons, Chichester, United Kingdom (1984) – 734 p.

E. A. Lord, A. L. Mackay, S. Ranganathan, New geometries for new materials, Cambridge University Press, Cambridge (2006) – 257 p.

E. Parthé, Elements of inorganic structural chemistry. Selected efforts to predict structural features, K. Sutter Parthé Publisher, Petit-Lancy (1996) – 170 p.

V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.

International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables.  
<https://it.iucr.org/C/>

Also, compact, complete and accessible information is presented on Wikipedia in the categories Crystallography, Materials Science:

<https://en.wikipedia.org/wiki/Category:Crystallography>

[https://en.wikipedia.org/wiki/Materials\\_science](https://en.wikipedia.org/wiki/Materials_science)

## Topic 3

### Fundamentals of diffraction: Part I

The lecture will be devoted to properties and sources of radiation, detections of X-rays, collimation and monochromatization, scattering process. Students will be introduced to nature, properties and production of x-rays, x-ray spectra, classification of detectors, scattering factor. Diffraction – coherent scattering of an object with a periodic arrangement of atoms (crystal). Atomic scattering (form) factor – the ratio of the amplitude of the wave scattered by an individual atom to the amplitude of the wave scattered by a single electron. The most commonly used is X-ray diffraction, other are electron, neutron diffraction. X-ray is a high-energy electromagnetic radiation with wavelengths ranging from 10 nm nanometers to 10 picometers, corresponding to photon energies in the range of 100 eV to 100 keV, respectively. X-ray analysis is based on the property of X-rays to penetrate inside matter and be diffracted by the particles of the crystals (atoms, ions, molecules), which are periodically repeated in space at short-, medium- or long-range order. To produce X-rays, it is necessary to: -obtain large quantities of free electrons; - force them to move in a certain direction with a high speed; - stop the electrons by an anode, which is the source of X-rays. An X-ray tube is the source of white and characteristic radiation; thus, it is necessary to use certain voltage, filters, monochromatization, etc. to obtain quality x-ray radiation ( $K\alpha_1$ ). X-ray detectors can be divided into two major categories: imaging detectors (such as photographic plates and X-ray film (photographic film), now mostly replaced by various digitizing devices like image plates or flat panel detectors) and dose measurement devices (such as ionization chambers, Geiger counters, and dosimeters used to measure the local radiation exposure, dose, and/or dose rate).

### LEARNING OUTCOMES

- **Understanding** the general concept of diffraction.
- **Knowledge:** the student will be known about the properties and sources of radiation, detections of X-rays, collimation and monochromatization, scattering process. Students will be introduced to nature, properties and production of x-rays, x-ray spectra, classification of detectors, scattering factor.
- **Comprehension:** the student will understand the importance of the concept of diffraction as one of the foundations for studying the structure of matter.
- **Application:** the student will know how and when diffraction is used, its possibilities, advantages and disadvantages for studying the structure of matter.
- **Analysis and Synthesis:** the student will be able to compare different diffraction methods and their experimental results depending on the research tasks, determine the range of order in matter.
- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data.

### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.

- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.

International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables.  
<https://it.iucr.org/C/>

B.D. Cullity, S.R. Stock, Elements of X-ray diffraction, Pearson New International Edition (2014) – 649 p.

Also, compact, complete and accessible information is presented on Wikipedia in the categories Diffraction, X-rays, X-ray instrumentation:

<https://en.wikipedia.org/wiki/Category:Diffraction>

<https://en.wikipedia.org/wiki/Category:X-rays>

[https://en.wikipedia.org/wiki/Category:X-ray\\_instrumentation](https://en.wikipedia.org/wiki/Category:X-ray_instrumentation)



## Topic 4

### Fundamentals of diffraction: Part II

This lecture will focus on geometry of diffraction by lattices and coordination spheres. Students will be introduced to Laue equations and Bragg's law, reciprocal lattice and Ewald's sphere, structure amplitude, atomic displacement and population parameters, origin and properties of the powder diffraction peaks, preferred orientation and microstructural parameters. Lattice plane – plane, which passes through three lattice points (owing to the periodicity of the lattice it contains an infinite number of lattice points). Families of (parallel) lattice planes are named by Miller indices ( $h k l$ ). Interplanar distance (spacing)  $d_{hkl}$  – distance between two neighboring lattice planes belonging to the same family. Diffraction can be considered as the reflection of the primary beam on the lattice planes. Constructive interference occurs when  $n\lambda = 2d_{hkl}\sin\theta$  (Bragg's law). Structure factor – amplitude of the wave, which is diffracted by the atoms in the unit cell. The Laue interference function depends on the translation lattice and is independent of the arrangement of the atoms within the cell. Diffraction is observed only in the directions that satisfy the 3 equations (Laue conditions). The thermal motions of the atoms in a crystal can be described as an oscillation around the equilibrium positions (atomic displacement parameters). In some polycrystalline specimens, the orientation of the crystallites is not random but certain orientations are predominant. This preferred orientation (or texture) may be due to geometric characteristics of the crystals, or to the method used to prepare the sample. Microstructural parameters are domain size (size of coherently diffracted domains) and internal strains (microstrains). The grain size causes a broaden of the peaks when less than 200 nm, while strain in the crystal causes displacements of the peaks from their ideal position.

### LEARNING OUTCOMES

- **Understanding** the general concept of diffraction.
- **Knowledge:** the student will be known about the Laue equations and Bragg's law, reciprocal lattice and Ewald's sphere, structure amplitude, atomic displacement and population parameters, origin and properties of the powder diffraction peaks, preferred orientation and microstructural parameters, etc.
- **Comprehension:** the student will understand the importance of the concept of diffraction as one of the foundations for studying the structure of matter.
- **Application:** the student will know how and when diffraction is used, its possibilities, advantages and disadvantages for studying the structure of matter.
- **Analysis and Synthesis:** the student will be able to compare different diffraction methods and their experimental results depending on the research tasks, determine the range of order in matter.
- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data.

### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.

- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.

International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables.  
<https://it.iucr.org/C/>

B.D. Cullity, S.R. Stock, Elements of X-ray diffraction, Pearson New International Edition (2014) – 649 p.

Also, compact, complete and accessible information is presented on Wikipedia in the categories Diffraction, X-rays, X-ray instrumentation:

<https://en.wikipedia.org/wiki/Category:Diffraction>

<https://en.wikipedia.org/wiki/Category:X-rays>

[https://en.wikipedia.org/wiki/Category:X-ray\\_instrumentation](https://en.wikipedia.org/wiki/Category:X-ray_instrumentation)

## Topic 5

### Crystal structure solution

This lecture will focus on standard and modern methods of crystal structure determination. Students will be introduced to single crystal and powder methods, phase problem (Patterson technique, direct methods), Fourier transformation, selection of experimental conditions, stages of data processing, software packages. The main concept is electron density  $\rho(x, y, z)$ , and the number of peaks in the  $\rho$  mapping corresponds to the number of atoms  $N$ . The main problem during a structure solution is to determine the phases  $\alpha_{hkl}$ . In the Patterson method the coordinates correspond to interatomic vectors. The number of peaks in the Patterson mapping is equal to  $N(N-1)+1$ . On the other side, using *ab initio* (direct) methods it is possible to derive the phases of the structure factors  $\alpha_{hkl}$  from the observed intensities using mathematical correlations based on probabilities. X-ray single crystal and X-ray powder diffraction methods will be analyzed.

### LEARNING OUTCOMES

- **Understanding** the general concept of crystal structure solution.
- **Knowledge:** the student will be known about the single crystal and powder methods, phase problem (Patterson technique, direct methods), Fourier transformation, selection of experimental conditions, stages of data processing, software packages.
- **Comprehension:** the student will understand the importance of the concept of crystal structure solution as the first and main step for studying the structure of matter.
- **Application:** The student will know how to perform the solution of structure, its possibilities, advantages and problems.
- **Analysis and Synthesis:** the student will be able to use and compare different crystal structure solution methods depending on the research tasks and experimental possibilities.
- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data.

### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.
- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*, Springer Science + Business Media, New York (2009) – 741 p.

International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables.  
<https://it.iucr.org/C/>

B.D. Cullity, S.R. Stock, Elements of X-ray diffraction, Pearson New International Edition (2014) – 649 p.

R.E. Gladyshevskii, Methods to Determine Crystal Structures, Textbook, Publishing Center of Ivan Franko National University of Lviv, Lviv (2015) – 135 p.

Also, compact, complete and accessible information is presented on Wikipedia in the categories Diffraction, Crystallography, Materials science stubs:

<https://en.wikipedia.org/wiki/Category:Diffraction>

<https://en.wikipedia.org/wiki/Category:Crystallography>

[https://en.wikipedia.org/wiki/Category:Materials\\_science\\_stubs](https://en.wikipedia.org/wiki/Category:Materials_science_stubs)

## Topic 6

### Crystal structure refinement

The lecture will discuss the positions, shapes and intensity of powder diffraction peaks, indexation and refinement procedures, Rietveld method, quality and quantitative X-ray phase analysis, using the databases, mathematical and crystal-chemical reliability factors. The determination of a crystal structure may be considered complete only when multiple pattern variables and crystallographic parameters of a model have been fully refined against the observed powder diffraction data. Obviously, the refined model should remain reasonable from both physical and chemical standpoints, indicated by mathematical reliability factors and crystal-chemical features. The refinement technique, most commonly employed today, is based on the idea suggested H. Rietveld. The essence of Rietveld's approach is that experimental powder diffraction data are utilized without extraction of the individual integrated intensities or the individual structure factors, and all structural and instrumental parameters are refined by fitting a calculated profile to the observed data. To a certain extent, the Rietveld method (also known as the full pattern or the full profile refinement) is similar to the full pattern decomposition using Pawley and/or Le Bail algorithms, except that the values of the integrated intensities are no longer treated as free least squares variables (Pawley) or determined iteratively after each refinement cycle (Le Bail). Significant attention will be paid to qualitative and quantitative X-ray phase analysis, which remains a powerful tool in materials science.

### LEARNING OUTCOMES

- **Understanding** the general concept of crystal structure refinement.
- **Knowledge:** the student will be known about the single crystal and powder methods, characteristics of diffraction peaks, indexation and refinement procedures, Rietveld method, quality and quantitative X-ray phase analysis, using the databases, stages of data processing, software packages.
- **Comprehension:** the student will understand the importance of the concept of crystal structure refinement as the final step for studying the structure of matter.
- **Application:** The student will know how to perform the refinement of structure, its possibilities, advantages and problems, together with quality and quantitative X-ray phase analysis, and how to work with the databases.
- **Analysis and Synthesis:** the student will be able to use and compare different crystal structure refinement methods depending on the research tasks and experimental possibilities, to perform selection of experimental conditions, treatment of diffraction data, profile analysis of diffraction peaks.
- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data, to perform phase identification with the databases.

### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.

- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.

R.A. Young (Ed.), The Rietveld Method, IUCr Monographs of Crystallography. N 5. International Union of Crystallography, Oxford University Press, 1993, 298 p.

International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables.  
<https://it.iucr.org/C/>

P. Villars, K. Cenzual, J.L.C. Daams, F. Hulliger, H. Okamoto, K. Osaki, A. Prince, S. Iwata, Pauling File. Inorganic Materials Database and Design System. Binaries Edition, Crystal Impact (Distributor), Bonn (2001).

P. Villars, K. Cenzual, Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds, ASM International, Materials Park (OH) (2023).

International Centre for Diffraction Data® (ICDD®) Home Page XRD Database. <https://www.icdd.com/>

Also, compact, complete and accessible information is presented on Wikipedia in the categories Diffraction, Crystallography:

<https://en.wikipedia.org/wiki/Category:Diffraction>

<https://en.wikipedia.org/wiki/Category:Crystallography>

## Topic 7

### Microstructural analysis

This lecture will focus in more detail on determining preferred orientation (texture), defects and microstructural parameters (size of coherently diffraction domains, microstrains) by diffraction methods. Analysis of the profile of diffraction peaks will be performed. Data from X-ray diffraction studies of solids can be used not only for X-ray phase and structural analyzes of polycrystals, elucidation of short-range order parameters for amorphous substances, but also for determining microstructural parameters, the so-called fine crystal structure of a substance. Fine crystal structure is understood as the real structure of polycrystals, mosaic crystals, films, etc., and its main parameters are the sizes of the coherent scattering domains (which can be approximated by the sizes of the phase grains), internal stresses (micro-strains) in the lattice, intra-grain angular misorientation for mosaic crystals and films, texture. Determination of microstructural parameters is of great importance for the successful practical application of substances and materials based on them. In some polycrystalline specimens, the orientation of the crystallites is not random but certain orientations are predominant. This preferred orientation (or texture) may be due to geometric characteristics of the crystals, or to the method used to prepare the sample. Different texture model descriptions will be described (ellipsoid, March-Dollase, Rietveld- Toraya functions). Microstructural parameters are domain size (size of coherently diffracted domains) and internal strains (microstrains). The grain size causes a broaden of the peaks when less than 200 nm, while strain in the crystal causes displacements of the peaks from their ideal position. Line broadening analysis provides information on the microstructure of the material. However, it is appropriate to note that most programs for structural analysis give only FWHM values, and to describe the effect of line broadening from crystallite sizes and microstrains, the integral width  $\beta$  should be used as a unit of measurement of the diffraction peak width. Simplified integral breadth methods, microstructural analysis by profile parameters during refinement of the crystal structure by the Rietveld method, Fourier methods and double Voigt methods will be described.

### LEARNING OUTCOMES

- **Understanding** the general concept of microstructural analysis.
- **Knowledge:** the student will be known about the sources of broadening of diffraction lines, and preferred orientation, methods of investigations, software packages.
- **Comprehension:** the student will understand the importance of the concept of microstructural analysis for studying the real structure of matter.
- **Application:** The student will know how to perform the determination of texture and microstructural parameters.
- **Analysis and Synthesis:** the student will be able to use and compare different methods depending on the research tasks and experimental possibilities, to perform selection of experimental conditions, treatment of diffraction data, profile analysis of diffraction peaks.
- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data, to perform microstructural analysis.

#### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.
- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

V.K. Pecharsky, P.Y. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*, Springer Science + Business Media, New York (2009) – 741 p.

R.A. Young (Ed.), *The Rietveld Method*, IUCr Monographs of Crystallography. N 5. International Union of Crystallography, Oxford University Press, 1993, 298 p.

R.L. Snyder, J. Fiala, H.J. Bunge, Eds., *Defect and Microstructure Analysis by Diffraction*, Oxford University Press, Oxford (1999) – 785 p.

T. Egami, S.J.I. Billinge, *Underneath the Bragg Peaks: Structural Analysis of Complex Materials*, Elsevier, Pergamon Materials Series (2012) – 422 p.

J. Rodriguez-Carvajal, T. Roisnel, *Line Broadening Analysis Using Fullprof\*: Determination of Microstructural Properties*. Mater. Sci. Forum. 2004, 443–444, 123–126.

Also, compact, complete and accessible information is presented on Wikipedia in the categories Diffraction, Crystallography:

<https://en.wikipedia.org/wiki/Category:Diffraction>

<https://en.wikipedia.org/wiki/Category:Crystallography>



## Topic 8

### Short- and medium-range order analysis

During the lecture, students will be introduced to the characterisation of the structure of solids (amorphous glasses, polymers) at short- and medium range order (radial distribution function, first sharp diffraction peak). X-ray studies of the structure of amorphous substances are based on the analysis of the angular distribution of the diffraction intensity of X-ray scattering. At the same time, the function that recognizes is the atomic amplitude of coherent X-ray scattering (atomic factor) depends on the electron density distribution. The atomic scattering function monotonically decreases with increasing wave vector, which corresponds to scattering by a system of non-interacting atoms with chaotic arrangement ("gas scattering"). However, for such disordered systems as amorphous alloys and liquids, some correlation can be traced in the space arrangement of atoms, which enables the appearance of a stable interference pattern during the scattering of X-rays. Unlike crystalline solids, in disordered systems there is no long-range order in the arrangement of atoms. As a result, a series of broad diffuse maxima can be traced on the diffraction spectra of substances. The orderly arrangement of atoms is observed at small distances (1–2 nm) relative to an arbitrarily selected atom (close order). Therefore, the relative arrangement of atoms is described by the function  $g(r)$ , which determines the probability of finding an atom at a distance  $r$  from the conventionally chosen central atom. The angular dependence of the average scattering intensity is related to the atomic distribution function. The radii of coordination spheres and coordination numbers – the number of atoms in radially distributed coordination spheres – are determined using the radial distribution function. At the same time, the maxima of the radial distribution function determine the set of the most probable interatomic distances, and the area under them is the number of nearest neighbors of the atom conventionally chosen as the central one. The first sharp diffraction peak (FSDP) is a distinct feature of many noncrystalline solids, which are characterized by the presence of a peak in the low wavevector region ( $0.1-0.2 \text{ nm}^{-1}$ ) of the structure factor of the solids.

### LEARNING OUTCOMES

- **Understanding** the general concept of X-ray atomic pair distribution function method for study short-range order.
- **Knowledge:** the student will be known about the atomic pair distribution function technique as a powerful approach to study the structures of materials at short-range order, methods of investigations, software packages.
- **Comprehension:** the student will understand the importance of the concept of the atomic pair distribution function for studying the structure of matter at nanoscale level.
- **Application:** The student will know how to perform the short-range order analysis.
- **Analysis and Synthesis:** the student will be able to use and compare different methods depending on the research tasks and experimental possibilities, to perform selection of experimental conditions, treatment of diffraction data.

- **Evaluation:** the student will be able to evaluate experimental X-ray diffraction data, to perform short-range order analysis.

#### DIDACTIC METHODS USED

- Lecture conducted with the use of multimedia: the use of PowerPoint presentations for discussed issues and examples.
- Case study: presentation of specific examples.
- Discussion: encouraging students to participate in the discussion on the issues actively.
- Quiz: summarized the essential information.

#### RECOMMENDED READING

Students are expected to read below texts related to the lecture:

T. Egami, S.J.I. Billinge, *Underneath the Bragg Peaks: Structural Analysis of Complex Materials*, Elsevier, Pergamon Materials Series (2012) – 422 p.

S. J. L. Billinge (2019) The rise of the X-ray atomic pair distribution function method: a series of fortunate events. *Phil. Trans. R. Soc. A* 377: 20180413.

<https://dx.doi.org/10.1098/rsta.2018.0413>

S. R. Elliot (1992) The origin of the first sharp diffraction peak in the structure factor of covalent glasses and liquids. *J. Phys.: Condens. Matter* 4 7661.

<https://dx.doi.org/10.1088/0953-8984/4/38/003>

## Course content – laboratory classes

### Topics 1

#### 1. The subject of the laboratory classes

Applied crystallography

#### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to introduce students to the basic concepts of applied crystallography. During laboratory work, students will know how to define the elements of symmetry, unit cells, planar and space symmetry groups. Students gain knowledge about definition of syngonies, Bravais lattice types, unit cell parameters, atomic coordinates. Also, some examples of short- and medium-range order will be considered. All this knowledge is basic for understanding the crystal structure of matter.

#### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to perform crystallographic analysis.
- to identify key characteristics, ways to obtain necessary information about crystal structure.
- to analyze research articles, database and interpret known results effectively.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

#### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connection.
- demonstration models of polyhedra, simple forms, crystal structures.

#### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

#### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 1. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration models, software and instructions for practical work will be available.

## Topics 2

### 1. The subject of the laboratory classes

Applied crystal chemistry

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to introduce students to the basic concepts of applied crystal chemistry. During laboratory work, students will know how to define the types of compounds and crystal structures, interatomic distances and angles, to analyze close-packed structures, atomic coordination and polyhedra. Also, the aim of the laboratory is to draw the projections of crystal structures, visualize of crystal structures of compounds, derivation of space symmetry groups. Some basic aspects of crystal chemical analysis will be studied. All this knowledge is basic for understanding the crystal structure of matter.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to define the types of compounds and crystal structures, interatomic distances and angles.
- to perform crystal chemical analysis. to draw the projections of crystal structures, visualize of crystal structures of compounds.
- to perform crystal chemical analysis.
- to identify key characteristics, ways to obtain necessary information about crystal structure.
- to analyze research articles, database and interpret known results effectively.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connection.
- demonstration models of polyhedra, simple forms, crystal structures.
- specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.

c. Besides, during laboratory class, students will receive an individual task and perform it independently.

d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 2. Students should prepare a theoretical introduction to the laboratories.

#### **7. Additional notes**

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary demonstration models, software and instructions for practical work will be available.

## Topics 3

### 1. The subject of the laboratory classes

XRD data collection

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to familiarize students with modern X-ray diffractometer system, its constituent parts: high-voltage generator, detector, X-ray tube, tools for collimation and monochromatization. Students will learn how to prepare different samples correctly for recording, then they will record and obtain raw diffraction data. Special attention will also be paid to safety techniques when working with ionizing radiation and high-voltage equipment.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to define the types of diffractometers and other X-ray equipment.
- to know main parts of X-ray diffractometer system.
- to prepare the samples based on the assigned tasks.
- to record and obtain X-ray raw diffraction data, to determine factors that affect data quality (texture, elemental composition of the samples and type of anode, absorption, etc.)
- to know the safety techniques when working with ionizing radiation and high-voltage equipment.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops.
- X-ray diffractometer system, other X-ray technique for familiarization (e.g., Laue and Debye-Scherrer cameras).
- Working samples and necessary equipment for their preparation (agate mortars, foils, glue, capillaries, etc.).
- Individual and general means of protection.
- Specialized software.

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 3. Students should prepare a theoretical introduction to the laboratories.

#### **7. Additional notes**

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

#### **8. Optional information**

The necessary demonstration and working equipment, software and instructions for practical work will be available.



## Topics 4

### 1. The subject of the laboratory classes

XRD data proceedings

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The purpose of the laboratory work is to familiarize students with corrections of raw XRD data, indexing of diffractograms, unit cell search, phase identification.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to correct raw XRD data (background, absorption, smoothing, etc.).
- to perform the indexing of diffractograms by different methods, search of the unit cell.
- to perform the X-ray qualitative phase analysis.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connections, databases.
- X-ray diffractometer system and specialized software.
- Raw X-ray diffraction data (previously recorded files).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.

c. Besides, during laboratory class, students will receive an individual task and perform it independently.

d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 4. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration and working equipment, software and instructions for practical work will be available.

## Topics 5

### 1. The subject of the laboratory classes

Structure solution

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory work is to teach students the basics of X-ray structural analysis: to solve the crystal structure of selected compounds: determine atomic coordinates, displacement parameters, and occupancies, and perform the quality crystal chemical test. Different methods and software packages will be tested.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to solve crystal structures at initial stage.
- to perform the X-ray structural analysis.
- to analyze the reliability of structures.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connections, databases.
- X-ray diffractometer system and specialized software packages.
- X-ray diffraction data (previously recorded files).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
  - b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
  - c. Besides, during laboratory class, students will receive an individual task and perform it independently.
  - d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.
- Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class.

Literature is related to Lecture 5. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration and working equipment, software and instructions for practical work will be available.

## Topics 6

### 1. The subject of the laboratory classes

Structure refinement

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory work is to teach students the basics of X-ray structural analysis using powder methods: to determine the positions, shapes and intensity of powder diffraction peaks, familiarize with indexation and refinement procedures, Rietveld method, quality and quantitative X-ray phase analysis, to refine the crystal structure of selected compounds (atomic coordinates, displacement parameters, and occupancies), to use the databases, to perform crystal-chemical test using mathematical and crystal-chemical reliability factors. Different methods and software packages will be tested.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to refine the crystal structures.
- to perform the quality and quantitative X-ray phase analysis.
- to analyze the reliability of structures.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connections, databases, specialized software packages.
- X-ray diffraction data (previously recorded files).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class. Literature is related to Lecture 6. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration and working equipment, software and instructions for practical work will be available.

## Topics 7

### 1. The subject of the laboratory classes

Microstructural analysis

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory work is to evaluate the preferred orientation (texture), defects and microstructural parameters (size of coherently diffraction domains, microstrains) by diffraction methods. Analysis of the profile of diffraction peaks will be performed. Different methods and software packages will be tested.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand the general concept of microstructural analysis.
- to understand the sources of broadening of diffraction lines, and preferred orientation.
- to perform the X-ray microstructural analysis.
- to understand the importance of the concept of microstructural analysis for studying the real structure of matter.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connections, databases, specialized software packages.
- X-ray diffraction data (previously recorded files).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

- a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.
- b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.
- c. Besides, during laboratory class, students will receive an individual task and perform it independently.
- d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class. Literature is related to Lecture 7. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration and working equipment, software and instructions for practical work will be available.

## Topics 8

### 1. The subject of the laboratory classes

Short-range order analysis

### 2. Thematic scope of the laboratory classes (abstract, maximum 500 words)

The aim of the laboratory work is to obtain radial and pair distribution functions, evaluate other parameters for amorphous solids.

### 3. Learning outcomes

Upon completion of this laboratory session, students will be able:

- to understand the general concept of X-ray atomic pair distribution function method for study short-range order.
- to perform the short-range order analysis.
- to understand the importance of the concept of the atomic pair distribution function for studying the structure of matter at nanoscale level.
- to discuss own choices and propositions.
- to draw up the obtained results and conclusions in the form of a report.

### 4. Necessary equipment, materials, etc

- Personal computers or laptops, with internet connections, databases, specialized software packages.
- X-ray diffraction data (previously recorded files).

### 5. Didactic methods used (description of student/teacher activities in the classroom/laboratory, taking into account didactic/teaching methods)

a. Laboratory classes are carried out with the use of specialist research equipment and specialized software.

b. Students will labor in a group, sharing tasks and working together to create a strategic plan, analyze and discuss the results and draw conclusions.

c. Besides, during laboratory class, students will receive an individual task and perform it independently.

d. At all stages of laboratory class, the teacher will advise, assist and monitor the work of students.

Such teaching methods as peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice will be engaged during laboratory class.

### 6. Recommended reading, pre-lesson preparation (required knowledge of students on the topics)

Students should prepare a theoretical introduction to the laboratory class. Literature is related to Lecture 8. Students should prepare a theoretical introduction to the laboratories.

### 7. Additional notes

The topic will be covered in 2 teaching hours.

Based on the results of laboratory work, the student is obliged to prepare a report.

The assessment of the results of laboratory class, designed as report, is a maximum 5 points.

### 8. Optional information

The necessary demonstration and working equipment, software and instructions for practical work will be available.



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Content preparation: Project Team of Materials Science Ma(s)ters, Ivan Franko National University of Lviv





# MATERIALS SCIENCE MA(S)TERS

## developing a new master's degree

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