

MATERIALS SCIENCE MA(S)TERS

developing a new master's degree

102

Syllabuses

Part 4



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PHYSICAL AND COLLOID CHEMISTRY FOR MATERIAL SCIENTISTS

Code: PCCMS

FIELD OF STUDY

Materials Science and Engineering

Level of study

Master Study

Year of study/semester

1

Language

English

Thematic block

Fundamental aspects of materials science

Form of tuition and number of hours*:

Lecture: 30h

Laboratory: 30h

ECTS

4

COURSE DESCRIPTION

A qualitative description of a process or phenomenon is only the first stage of scientific knowledge. The next higher level of research involves the analysis of causes and mechanisms of occurrence, as well as a quantitative description of the relevant relationships between various parameters of the process / phenomenon and external influence. This is the methodological cognitive role played by Physical Chemistry in the system of not only the chemical field of knowledge, but also material science.

The *Physical and Colloid Chemistry for Material Scientists* course is dedicated to the consideration of the fundamental foundations of this discipline, which providing students with knowledge for the further creation of new materials, physicochemical methods of studying their properties, etc.

The lectures will cover the basics of chemical thermodynamics, phase and chemical equilibrium, chemical kinetics and catalysis, chemistry of surface phenomena and physico-chemistry of dispersed systems. The laboratory practicum involves conducting research that will acquaint course participants with the most common methods of physico-chemical research, will enable a deeper understanding of the essence and regularities of physico-chemical processes and phenomena. In addition, students will gain practical skills in working with appropriate laboratory equipment, learn to work out experimental results and interpret them depending on the assigned tasks.

COURSE OBJECTIVES

After completing of *Physical and Colloidal Chemistry for Materials Scientists* course, the student should understand the physical meaning of basic physicochemical quantities and be able to apply basic physicochemical laws to characterize systems and processes considered in materials science. The course participant will be ready to use appropriate methods of physico-chemical research and correctly interpret the obtained experimental data.

PREREQUISITES FOR TAKING THE COURSE

To complete the course, it is recommended to implement learning outcomes related to the basics of physics, chemistry, mathematics, and materials science.



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LEARNING OUTCOMES OF THE MODULE

Code	Description
PCC_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials.
PCC_O_02	Has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.
PCC_O_03	Can use information from literature, databases and other available sources. He is able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems.
PCC_O_04	Can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.
PCC_O_05	Able to work individually and in a team as well as interact with others in teamwork.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: informative lecture (lectures with multimedia support); description; working with the program manual; working with another teaching tool	PCC_O_01 PCC_O_02 PCC_O_03
Meth_02	Laboratory practice: working with the program manual; working with another teaching tool; activating methods : flipped classroom; laboratory exercises / experiment; observation	PCC_O_03 PCC_O_04 PCC_O_05

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	30	exam	PCC_O_01 PCC_O_02	Meth_01
FT_02	laboratory practice	30	reports on the performance of laboratory tasks	PCC_O_03 PCC_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

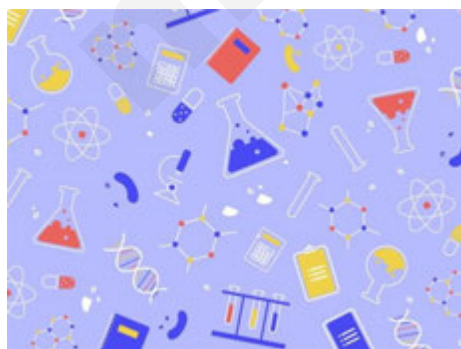
Student has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials. Also she/he has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.

COMMENTS

LECTURER

DO YOU KNOW

Historically, a large number of areas of research originated as components of Physical Chemistry, but evolved so much that today they are considered as separate chemical disciplines, such as Colloid Chemistry, Quantum Chemistry, Electrochemistry, Photochemistry, Chemistry of High Molecular Compounds, etc. In addition, such divisions of Physical Chemistry as Physical Organic Chemistry, Physical Inorganic Chemistry, Medical Chemistry, Biophysical Chemistry, Nanochemistry, Chemistry of Solid State etc., were formed at the border of two or more fields of knowledge.



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COURSE CONTENT - lecture

Topics 1

Physical Chemistry and Materials Science

During the lecture, the methodological role of Physical Chemistry as the theoretical foundation of the chemical field of knowledge, as well as its significance for Materials Science, will be discussed. Students will familiarize themselves with sections of Physical Chemistry and basic methods of physicochemical researches.

Topics 2

Basic concepts of Physical Chemistry

During the lecture, students will get acquainted with such concepts as the system, its state, types and parameters (properties), process and process path. In addition, the relationship between such concepts as energy, heat and work will be discussed.

Topics 3

Chemical thermodynamics. Thermodynamic functions

The lecture will be devoted to the thermodynamic approach to the analysis of systems and the thermodynamic principles (laws) underlying it. Thermodynamic functions that allow us to describe the state of the system and the processes in it will be considered, namely heat capacity, entropy, enthalpy, internal energy, Gibbs energy and Helmholtz energy, as well as the relationships between them.

Topics 4

Phase equilibrium

During the lecture, conditions of phase equilibrium in heterogeneous systems, as well as types of state diagrams of one-, two-, and three-component systems will be considered. The lecture also will familiarize students with phase transitions of the first and second order.

Topics 5

Chemical thermodynamics of solutions

The lecture will acquaint students with the classification and properties (in particular colligative) of liquid solutions. The application of the Lewis method for the description of non-ideal systems will also be analyzed.

Topics 6

Electrolyte solutions

The lecture will be devoted to the description of equilibrium in solutions of weak electrolytes, as well as the Debye-Hückel theory for strong electrolytes. The dependence of the electrical conductivity of electrolytes, transfer numbers and mobility of ions on concentration will be considered, as well as special cases of conductivity in the liquid and solid phase.

LEARNING OUTCOMES

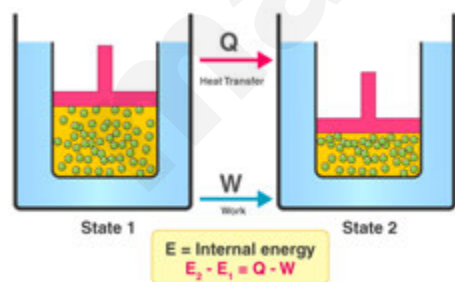
Students can use information from literature, databases and other available sources.

She/he also is able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems.

COMMENTS

DO YOU KNOW

Physical Chemistry is constantly developing. Its fundamental basis - Chemical Thermodynamics is based on three postulates (Laws of Thermodynamics), finally formulated in the 19th century. However, already in 1931, the fourth, so-called Zeroth Law of Thermodynamics was added to them, and today the question of introducing two additional postulates is widely discussed.



byjus.com

Topics 7

Electrode potential and electrochemical cells

During the lecture, the equilibrium conditions at the metal electrode - electrolyte solution interface, the concepts of electrochemical and electrode potential will be considered. In addition, students will be introduced to the classification of electrodes and electrochemical cells.

Topics 8

Surface layer and surface phenomena. Adsorption

During the lecture, the state of equilibrium at the liquid-gas and solid-gas interfaces will be considered, as well as questions dedicated to surface wetting, surface excess, surface tension, and surface pressure. Types of adsorption interaction on a solid surface and isotherms of mono- and polymolecular adsorption will be analyzed separately.

Topics 9

Chemical equilibrium

During the lecture, the conditions of chemical equilibrium in homogeneous and heterogeneous systems, ways of expressing the equilibrium constant and its dependence on temperature will be considered.

Topics 10

Chemical kinetics and catalysis

During the lecture, the kinetic analysis of chemical systems, the basic concepts of chemical kinetics, as well as the influence of various factors on the rate of chemical transformations will be considered.

Topics 11

Basics of photochemistry

The construction of the transmission electron microscope, the formation of contrast, image formation, and methods of interpreting microscopic and diffraction images will be discussed during the lecture.

Topics 12

Disperse systems and their properties

During the lecture, classification, ways of synthesis, interconversion and destruction, as well as properties and areas of application of dispersed systems of various types will be considered.

LEARNING OUTCOMES

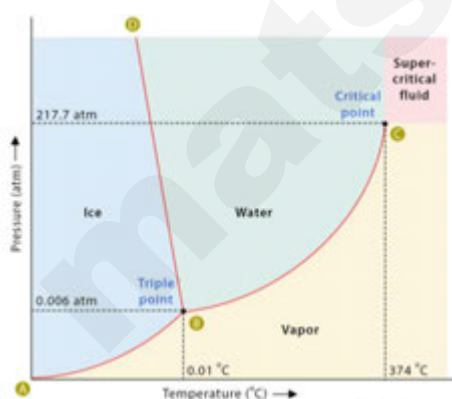
Students can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.

COMMENTS

INSTRUCTOR

DO YOU KNOW

There are 19 different crystalline modifications of ordinary water, not including water with metallic properties, which forms at pressures above 1TPa



www.chemistrylearner.com

COURSE CONTENT - laboratory classes

Topics 1

Determination of the thermal effect of a chemical reaction

Laboratory exercises are aimed at practical familiarizing the students with the features of the calorimetric method of researches. The practical part of the work involves determining the thermal effects of physical and chemical processes, in particular the enthalpy of the reaction of combustion of organic matter.

Topics 2

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

The subject of study during laboratory classes is the mutual solubility of three liquids and the principles of constructing phase diagrams of three-component systems

Topics 3

Thermal analysis of two-component systems

An essential element of technical materials is the phase changes occurring in them. During the laboratory sessions, the student will get acquainted with the principles of thermal analysis, types of the melting diagrams of binary systems, and will also learn to build them using the example of low-melting mixtures.

Topics 4 .

Cryoscopy

During laboratory work, the student will learn to use the cryoscopic research method to determine the molecular mass of a dissolved substance and the parameters of the intermolecular interaction of the components of liquid solutions.

Topics 5

Thermodynamics of a galvanic cell

Using the acquired knowledge, the student will acquire practical skills in measuring the electromotive force of a galvanic element, as well as calculating the thermodynamic parameters of the potential-determining reaction.

Topics 6

Electrical conductivity of electrolyte solutions

The experimentally obtained concentration dependences of the electrical conductivity of the solutions will be used by the student to calculate the thermodynamic constants of electrolytes and the activity coefficients of the corresponding ions.

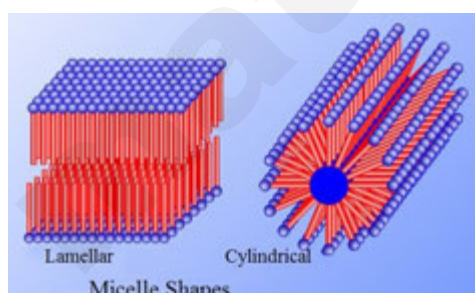
LEARNING OUTCOMES

Students able to work individually and in a team as well as interact with others in teamwork.

COMMENTS

DO YOU KNOW

A dispersed system is a heterogeneous system that contains two or more phases and is characterized by a strongly developed interface between them. Examples of dispersed systems are the well-known smoke, fog, milk, paints, foams, gels, sols, etc.



www.biochempeg.com

Topics 7

Study of the rate of sucrose inversion

Using the example of the inversion reaction of sucrose in an acidic environment, the student will get acquainted with the principles of kinetic research methods and acid-specific catalysis in aqueous solutions.

Topics 8

Sedimentation analysis of dispersed systems

During the laboratory session, the student will familiarize himself with and gain practical skills in determining the size distribution of colloidal particles according to their sedimentation rate in a liquid dispersed medium.

Topics 9

Adsorption of surfactants on solid adsorbents

Laboratory classes are aimed at students' practical familiarization with the phenomenon of sorption on a solid surface and with calculations of adsorption characteristics of adsorbents depending on the nature of the adsorbate and external conditions.

Topics 10

Study of the wetting phenomenon. Edge angle of wetting

The purpose of the laboratory session is to acquaint the student with the phenomenon of wetting the surface of a solid body, the wetting angle as a criterion of surface wettability, as well as to acquire the skills of measuring the wetting angle of surfaces of various nature.

Topics 11

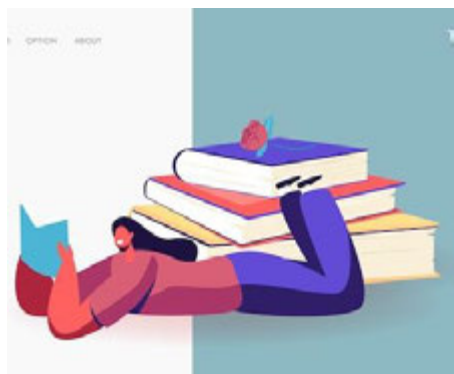
Determination of surface tension of aqueous surfactant solutions

The laboratory session will familiarize the student with surface-active substances and the concept of surface activity. The practical part of the lesson will enable the student to master the methods of measuring surface tension and determining the surface activity of surfactants by various methods.

Topics 12

Preparation and study of coagulation of sol with electrolytes

The laboratory session is devoted to the methods of obtaining, structure of particles, and the study of the aggregative stability of ultradispersed colloidal systems. In particular, it is expected that the student will practically determine the coagulation threshold of sol in the presence of an electrolytes of different nature.



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TEXTBOOK / READINGS

The mandatory reading for completing *Physical and Colloidal Chemistry for Materials Scientists*:

1. Peter Atkins, Julio de Paula, James Keeler, *Atkins' Physical Chemistry : Eleventh edition*, Oxford University Press 2019.
2. Paul C. Hiemenz, Raj Rajagopalan, *Principles of Colloid and Surface Chemistry : Third edition*, Marcel Dekker, Inc. 1997.
3. Georgios M. Kontogeorgis, Søren Kiil, *Introduction to Applied Colloid and Surface Chemistry*, John Wiley & Sons, Ltd. 2016.

For extending and supplementing knowledge recommended are:

1. Ira N. Levine, *Physical Chemistry : Sixth edition*, McGraw-Hill Higher Education 2009.
2. Duncan J. Shaw, *Introduction to Colloid and Surface Chemistry : Fourth edition*, Butterworth-Heinemann 2003.

ASSESSMENT

Exam:

The oral exam tests general theoretical knowledge in the field of physical and colloidal chemistry, principles and methods of physical and chemical research of materials and systems of various types.

Report:

Reports are the result of students' work during laboratory work; they relate to in-depth theoretical and practical knowledge of the tasks performed. They consist of a description of the purpose of the work, a theoretical introduction and an experimental part (methodology of the conducted research, experimental results and the calculation part). The reports end with a discussion of the obtained results and conclusions.

GRADING POLICY

The final evaluation is made based on the student achievement scoring system. The grade results from the sum of points obtained by the student during the semester from the laboratories and points received during the exam.

The exam is conducted in oral form and includes an initial test task (20 questions) and 3 oral knowledge questions containing theoretical and practical aspects of the studied educational material. For each correct answer to the test task, the student will receive 1 point. For the answer to each oral question, the student can receive a maximum of 10 points (for the most complete reasoned answer). The maximum number of points that can be obtained on the exam is 50.

During the assessment of laboratory works, the following are taken into account: the initial individual admission to the task, the work on its implementation and the quality of the prepared report, namely:

- admission to the performance of the task in the form of a control survey regarding the theoretical foundations and methods of the performed laboratory work (max. 1.5 points);
- content included in the theoretical introduction (max. 0.5 points);
- correctness of obtaining results (max. 1 points);
- correctness of calculations, illustrative materials (figures), interpretations and conclusions (max. 1.5 points);
- aesthetic design of the report (max. 0.5 points), for which the student receives a total of 5 points.

The student is obliged to perform the 10 laboratory tasks, which gives in maximum 50 points.

The final grade is defined as the sum of the points obtained in the exam and during the performance of laboratory work, which is illustrated in the table on the left.

ASSIGNMENT WEIGHTS AND POINTS

Exam	50 points
Laboratory	50 points

FINAL SCORE

Total	100 points
-------	------------

90 – 100 points = A
85 - 89 points = B+
81 – 84 points = B
75 – 79 points = C+
71 - 74 points = C
65 - 69 points = D+
61 - 64 points = D
55 - 59 points = E+
51 - 54 points = E
21 - 50 points = FX
0 - 20 points = F



COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

SMART CONJUGATED POLYMERS

Code: **SCP AEM-POLY003**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

3

Language

English

Thematic block

Applied Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 24h

ECTS

3

COURSE DESCRIPTION

The subject concerns smart conjugated polymers; methods of production, characterization, and use of conducting polymer materials for specific applications in organic electronics and material engineering.

The *Smart Conjugated Polymers* course, dedicated to the *AIEMPS - Advances in Innovative Engineering Materials and Processes for Sustainability* path, broadens knowledge about theoretical foundations in the field of production innovative electroactive materials based on organic polymers with a system of conjugated bonds. Students pursuing the *AIEMPS* path will improve practical skills for production conducting polymers, master the methods of researching properties, and deepen their knowledge of various aspects of application.

Lectures are aimed at providing information on conducting polymers, methods of their production, properties, and applications. Laboratory exercises are intended for individual and group student works, performance of experiments and analysis leading to individual elaboration of the obtained results in the form of a report along with relevant studies and conclusions.

COURSE OBJECTIVES

By the end of the *Smart Conjugated Polymers* course, students will gain an understanding of the theoretical models for describing the conductivity of π -conjugated polymers. Students will be able to provide methods of production conducting polymers and their application; establish the composition–structure–properties connection for a purposeful change in the conductivity of polymers during synthesis.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject *Smart Conjugated Polymers*, students should have a general knowledge of *Organic Chemistry*, *Physical Chemistry* and *Chemistry of High Molecular Weight Compounds*.



Printable polymer display

LEARNING OUTCOMES OF THE MODULE

Code module	Description
CP_O_01	He has extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and surface modification of engineering materials based on conjugated polymers, as well as development trends and the latest achievements.
CP_O_02	Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to the production and use of conjugated polymers.
CP_O_03	He can plan and carry out experiments, interpret the results and draw conclusions regarding the applications of conjugated polymers.
CP_O_04	Can prepare a scientific paper and present a presentation on the implementation of a research task, including critical analysis, synthesis and conclusions. Able to work individually and in a team and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	CP_O_01 CP_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate.	CP_O_03 CP_O_04
Meth_03	Team project: critical analysis, synthesis and conclusions; individual and team work, communicate on specialist topics, leading a debate.	CP_O_03 CP_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	Exam	CP_O_01 CP_O_02	Meth_01
FT_02	laboratory	24	course work	CP_O_03 CP_O_04	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

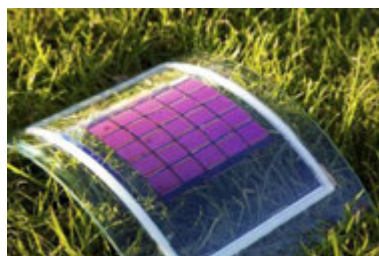
By the end of the *Smart Conjugated Polymers* course, students will gain an understanding of the theoretical models for describing the conductivity of π -conjugated polymers. Students will be able to provide methods of production conducting polymers and their application; establish the composition–structure–properties connection for a purposeful change in the conductivity of polymers during synthesis.

COMMENTS

LECTURER

DO YOU KNOW

Our most promising visions of a clean-powered future typically positions cheap, abundant solar energy as an important cornerstone. And solar panels would be a lot cheaper and abundant if they were made from plastic instead of silicon—that way, they could be 'printed' in a flexible material and easily applied to walls, windows, you name it. Plastic solar cells might speed the arrival of thin, bendable energy strips.



Plastic solar cells
<https://eandt.theiet.org>

COURSE CONTENT - LECTURE

Topics 1

During the lecture, as an introduction to the subject *Smart Conjugated Polymers*, the current state of organic electronics and the historical aspect of the development of the ideas about conducting polymers will be presented. Students will learn the chemical and electronic structure of conjugated polymers and types of polymers with alternating multiple bonds (2 hours)

Topics 2

The lecture will present the methods of conjugated polymers synthesis; Chemical synthesis of polyacetylene, polypyrrole, polythiophene, polyparaphenylene, and polyaniline; Mechanism of electrochemical synthesis of conjugated polymers; Anodic (oxidative) and cathodic (reductive) polymerization; Photopolymerization; Thermolysis of precursors (2 hours)

Topics 3

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 (2 hours)

Topics 4

The lecture will present types of charge carriers and the conductivity mechanism of conjugated polymers; Zone theory; Variable-range hopping model; Su–Schrieffer–Heeger (SSH) model; Kivelson's model; Domain theory of conductivity (2 hours)

Topics 5

The lecture will present features of the structure of the conjugated polymers in a thin layer; Methods of structure research: IR, UV, EPR, NMR spectroscopy, and X-ray phase analysis; Electronic properties of conjugated polymers (2 hours)

Topics 6

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 (2 hours)

Topics 7

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; Nanotechnological approaches to improve the characteristics of optoelectronic devices (2 hours)

LEARNING OUTCOMES

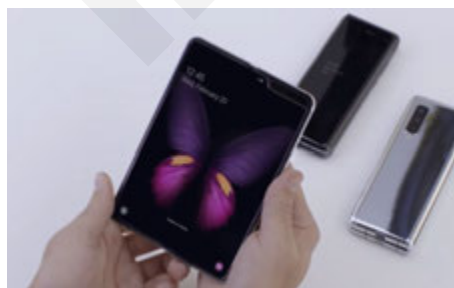
Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

DO YOU KNOW

The smart polymer coating can change color in response to external influences - color indication and sensitivity, for example, to pressure. The main components of the system are several layers of microstructured polysilane, which work as a pressure sensor, and a layer of electrochromic polymer changing color under voltage.



Samsung introduced the first flexible smartphone with electronic polymers
<https://youtu.be/aBYsTg5iT-A>

Topics 8

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(2 hours)

COURSE CONTENT –LABORATORY CLASSES

Topics 1

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. The completed experiment will be the basis for developing a report on the exercises(4 hours)

Topics 2

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. The completed experiment will be the basis for developing a report on the exercises(4 hours)

Topics 3

Students will perform electrochemical doping of conjugated polymers during laboratory classes and determine the charge transfer parameters in obtained thin films. The completed experiment will be the basis for developing a report on the exercises(4 hours)

Topics 4

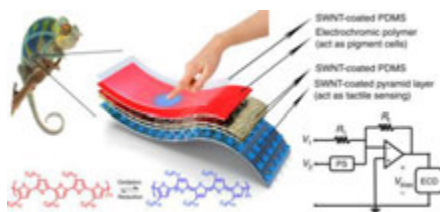
The topics of the laboratory classes are related to the temperature dependence of the conductivity of conjugated polymers. Students will determine the conductivity activation parameters. The completed experiment will be the basis for developing a report on the exercises(4 hours)

Topics 5

During the classes, 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. The completed experiment will be the basis for developing a report on the exercises(4 hours)

Topics 6

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. The completed experiment will be the basis for developing a report on the exercises(4 hours)



Electronic "chameleon skin"
<https://doi.org/10.1038/ncomms9011>



TEXTBOOK/READINGS

The mandatory reading for completing the subject *Smart Conjugated Polymers*:

1. *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>.
2. *Semiconducting and metallic polymers: the fourth generation of polymeric materials*. Heeger A. J., Synth. Met., 2001, Vol. 125, 23–42. <https://doi.org/10.1021/jp011611w>
3. *Handbook of Conducting Polymers*. Skotheim T. A., Reynolds J. CRC Press: New York, 2007. <https://doi.org/10.1201/b12346>

To deepen the course topics, optional recommended texts include articles in journals: *Progress in Materials Science*, *Nature Materials*, *Advanced Materials*, *Progress in Polymer Science*, *Nanoscale Research Letters*, *Journal of Alloys and Compounds*, *Materials Today*, *Applied Electronic Materials*, *Molecular Crystals and Liquid Crystals*, *Sensors and Actuators B: Chemical*, *Acta Physica Polonica A*

ASSESSMENT

Reports:

The reports relate to experimental laboratory exercises; contribute to deepening theoretical and practical knowledge in the field of conducting polymers. The reports contain theoretical background, description of performed experiments and analyses, together with discussion and conclusions.

Team project (during the semester):

Team project verifying knowledge of issues in the field of conducting polymers and ability to team work.

Exam (after the semester):

The oral exam verifying overall knowledge in the field of smart conducting polymers.

GRADING POLICY

The *Smart Conjugated Polymers* course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 5 points, i.e. 6 reports x 5 points = 30 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50. Student grades will be assessed as follows in the box on the left.

Assignment Weights	PERCENT
6 Reports	30%
Team project	10%
Debata	10%
Exam	50%
Total	100%

6 reports (max. 5 points each) – max. 30 points
 Team project – max. 10 points
 Debata – 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
 0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

matsci.us.edu.pl

ENVIRONMENTAL PROBLEMS OF MATERIALS SCIENCE

Code: **EPMS**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

3

Language

English

Thematic block

Applied Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 16h

ECTS

3

COURSE DESCRIPTION

The course is designed in such a way to highlight the causes of the global environmental crisis in the conditions of the growing use of various materials, the crisis of the "man-nature" relationship, which threatens the continued existence of life on Earth, as well as to establish possible ways out of this situation due to the use of eco-technologies in production and disposal of modern materials.

The course examines the environmental problems of modern materials science, which are related to the acquisition, use and disposal of structural materials of Acquaintance with modern global eco-technologies of prevention of generation, reuse and recycling of waste, purification of water, soil and air is expected.

COURSE OBJECTIVES

The discipline "Environmental problems of materials science" should provide both general education and professional development of students (masters) - materials scientists, form their competencies in the field of understanding problems related to environmental pollution, mechanisms of regulation of ecosystem processes and optimization of the state of ecosystems in the desired direction .

The course focuses on gaining awareness and developing skills in the field of production of environmentally friendly materials and provision of ecological technologies, in terms of combining and integrating knowledge from natural, social and economic relations.

As a result of studying the discipline, students must master the material provided by the program, which means know: basic laws of ecology; causes of global environmental crisis; modern approaches to the interpretation of the main environmental problems of materials science; basic physical and chemical methods of water, air, and soil purification; the place and role of chemistry and materials science in solving environmental problems.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject, the student should have general knowledge about different types of materials, their structure, properties and applications.



LEARNING OUTCOMES OF THE MODULE

Code module	Description
EP_O_01	Has the knowledge necessary to understand the ethical, economic and ecological aspects of the design of new engineering materials and their production technology and the impact of the development of materials engineering on the sustainable development and progress of civilization. Knows and understands the basic concepts and principles of intellectual and industrial property protection as well as copyright and patent law.
EP_O_02	Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to the production and use of sustainable nanomaterials.
EP_O_03	He can plan and carry out experiments, interpret the results and draw conclusions regarding the applications of sustainable engineering nanotechnology.
EP_O_04	Can prepare a scientific paper and present a presentation on the possibilities of sustainable nanotechnology, including critical analysis, synthesis and conclusions. Able to work individually and in a team, and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	EP_O_01 EP_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate	EP_O_03 EP_O_04
Meth_03	Team project: critical analysis, synthesis and conclusions; individual and team work, communicate on specialist topics, leading a debate.	EP_O_03 EP_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	exam	EP_O_01 EP_O_02	Meth_01
FT_02	laboratory	16	course work	EP_O_03 EP_O_04	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Finding materials and preparing presentations for participation in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

By the end of the "Environmental problems of materials science" course students must master the material provided by the program, which means know: basic laws of ecology; causes of global environmental crisis; modern approaches to the interpretation of the main environmental problems of materials science; basic physical and chemical methods of water, air, and soil purification; the place and role of chemistry and materials science in solving environmental problems.

COMMENTS

LECTURER

COURSE CONTENT - LECTURE

Topics 1

Scientific and technical progress and current tasks of nature protection.

Engineering-technical, socio-economic and moral-ethical aspects of environmental protection. The role of fundamental materials science in solving the problems of nature protection. (2 h)

Topics 2

Basics of teaching about the biosphere. The environment as an ecosystem. Biosphere, structure and composition of the biosphere. Natural environmental factors. Protective mechanisms of the environment, self-cleaning of the biosphere. Environmental monitoring. (2 h)

Topics 3

Anthropogenic environmental factors. The synthesis and use of materials of various nature are the most important factors of anthropogenic impact on natural objects. Concept of environmental pollutant. Priority pollutants of air, water and land. Production of materials of different chemical composition and purpose as a significant factor in environmental pollution. (2 h)

Topics 4

Hydrosphere. Protection and rational use of water. Anthropogenic impact on the hydrosphere. Sources and extent of pollution of surface and underground water due to production and use of various materials. Organization of rational water supply of industrial facilities and residential areas. (2 h)

Topics 5

Protection of the atmosphere. Environmental consequences of atmospheric air pollution. The Earth's atmosphere, structure, composition and properties, its connection with the functioning of the biosphere. The main sources and scales of atmospheric pollution as a result of the production and use of materials of different composition. (2 h)

Topics 6

Engineering and technological aspects of environmental protection. Interrelationship of problems of ecology and safety of chemical production. Economic, environmental and energy requirements for chemical technology. The relationship between energy and raw material costs and environmental pollution. The problem of choosing energy carriers and raw materials in the chemical industry. (4 h)

Topics 7

Radioecology. Impact of ionizing radiation on living organisms. Irradiation doses and radiological effect. Methods of assessment and diagnosis of the degree of radiation pollution of the surrounding environment. Classification of radioactive waste, methods of their processing and disposal. Possible ecological consequences for humanity of large-scale man-made nuclear accidents and the use of nuclear weapons. (2 h)

LEARNING OUTCOMES

Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

COURSE CONTENT – LABORATORY CLASSES

Topics 1

Analysis and purification of water from production areas and production of various materials. (4 h)

Topics 2

Evaluation of microhardness and elemental composition of materials of different composition and purpose (4 h)

Topics 3

Determination of changes in the degree of swelling and the degree of crosslinking of polymers of different composition (4 h)

Topics 4

Determination of the tensile strength of materials of different nature and purpose (4 h)



TEXTBOOK/READINGS

The mandatory reading for completing the subject "Environmental problems of materials science"



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. *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>

To deepen the course topics, optional recommended texts include:

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>
2. 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>

ASSESSMENT

Reports:

Reports refer to experimental laboratory work. Contribute deepening of theoretical and practical knowledge of environmental problems in materials science. The reports contain theoretical foundations, a detailed description of the conducted experiments, their analysis, discussion and conclusions.

Team project (during the semester):

A team project that tests knowledge of environmental issues in materials science and the ability to work in a team.

Exam (after the semester):

An oral exam that tests general knowledge in the field of environmental problems in materials science.

GRADING POLICY

The "Environmental problems of materials science" course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 10 points, i.e. 4 reports x 10 points = 40 points are assessed) and Team project (1 x 10 pts = 10 pts). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50. Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
4 Reports	40%
Team project	10%
Exam	50%
Total	100%

4 reports (max. 10 points each) – max. 40 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

0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic Tema	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

TESTING OF METALLIC AND CONVERSION CORROSION PROTECTION LAYERS

Code: TMCCPL

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

2

Language

English

Thematic block

Materials Testing Methods and Failure Analysis

Form of tuition and number of hours*:

Lecture: 16 h

Laboratory: 32 h

ECTS

4

COURSE DESCRIPTION

The course "*Testing of metallic and conversion corrosion protection layers*" is dedicated to the AIEMPS path - Advances in innovative engineering materials and processes for sustainable development. It is aimed at understanding the importance of corrosion processes in modern technologies, explaining the nature and character of corrosion destruction (damage), corrosion of metals and alloys, the role and significance of oxide and other films on the surface of metals, methods of research and assessment of corrosion resistance of metals and alloys, properties of metal and conversion anti-corrosion layers, methods of application and research of their anti-corrosion properties in relation to steel and aluminum surfaces. The subject also examines modern progressive technologies for the formation of metal and conversion protective coatings to increase the corrosion resistance of metals and alloys.

Teaching is divided into lectures and laboratory exercises. At the lectures, students will learn to understand the theoretical foundations of the course of corrosion processes and the influence of the state of metal surfaces on them. During laboratory exercises, students get to know and perform tasks on the preparation of samples of metals and alloys and the formation of protective anti-corrosion coatings on them, as well as learn to use various methods of analyzing the condition and effectiveness of anti-corrosion coatings.

COURSE OBJECTIVES

After completing the "*Testing of metallic and conversion corrosion protection layers*" course, the student will be able to distinguish the main types of corrosion and the nature of corrosion damage to metals and alloys; to be able to choose metals and alloys for use in various operating conditions; prevent corrosive destruction of structures by choosing appropriate interventions; propose and perform appropriate surface preparation and treatment; evaluate corrosion resistance using various test methods and research.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject "*Testing of metallic and conversion corrosion protection layers*", the student must have basic knowledge of physics, inorganic, analytical, and physical chemistry, as well as general knowledge of various types, properties, structure and application of various metals as structural materials.



LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	He has extensive knowledge in the field of determining the nature of corrosion damage, the application of modern physico-chemical methods for the study of surface films of various nature on metals and metal alloys, the selection of methods of forming protective anti-corrosion layers on metals for operation in various environments, methods of creating protective anti-corrosion layers of various nature.
MS_O_02	Can use information from the literature and other available sources in the field of general chemistry, analytical and physical chemistry, interpret and critically evaluate them.
MS_O_03	Can plan and conduct experiments, interpret results and draw conclusions about the corrosion properties of materials and their surface treatment to prevent corrosion.
MS_O_04	Can prepare and present results of corrosion resistance tests, including critical analysis, synthesis and conclusions. Able to work individually and in a team, and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	MS_O_01 MS_O_02
Meth_02	Laboratory classes: experiment demonstration; laboratory work; observation; problem teaching	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
TML_01	Lecture	16	exam	MS_O_01 MS_O_02	Meth_01
TML_02	Laboratory	32	course work	MS_O_03 MS_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

After studying the discipline "Testing of metallic and conversion corrosion protection layers", the student will be able to distinguish between the main types of corrosion and corrosion damage, evaluate the suitability of different types of metals and their alloys for use in different environments, prevent corrosion and degradation of materials through appropriate interventions in the design, to propose and carry out appropriate treatment of their surface and evaluate corrosion resistance by means of tests and studies under conditions close to operational ones.

COMMENTS

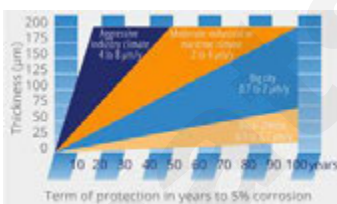
LECTURER

Have you seen this?



And do you know what it is?

Can you imagine the cost materials and restoration and replacement works damage caused by corrosion?



COURSE CONTENT - FORM OF TUITION (lecture)

Topics 1

Testing of metallic and conversion corrosion protection layers: Introduction (2 hours).

Topics 2

Corrosion of metals and alloys. Types of corrosion and their dependence on operating conditions (2 hours).

Topics 3

Protective anti-corrosion coatings based on nickel (2 hours).

Topics 4

Protective anti-corrosion coatings based on zinc (2 hours).

Topics 5

Tinning of the steel surface as an effective method of anti-corrosion protection (2 hours).

Topics 6

Oxide protective layers on the aluminum surface (2 hours).

Topics 7

Chemical and electrochemical oxidation of steel (2 hours).

Topics 8

Phosphate films on the surface of steel (2 hours).

LEARNING OUTCOMES

After studying the discipline "Testing of metallic and conversion corrosion protection layers", the student will be able to distinguish the main types of corrosion effects, determine the nature of corrosion damage/destruction of various metals, choose methods of anti-corrosion protection to prevent corrosion degradation of metals and alloys through appropriate interventions in the structure, propose and perform appropriate treatment metal surfaces and evaluate the corrosion resistance of coatings using modern test methods.

COMMENTS

INSTRUCTOR

COURSE CONTENT - FORM OF TUITION (laboratory classes)

Topics 1

Introduction to the laboratory workshop from the course.
Methods of testing protection layers of various nature (4 hours).

Topics 2

Investigation of the nature of corrosion destruction of metals and alloys (4 hours).

Topics 3

Electrochemical nickel plating of steel (4 hours).

Topics 4

Protective anti-corrosion coatings based on zinc and the study of their anti-corrosion properties (4 hours).

Topics 5

Electrolytic tinning of the steel surface as an effective method of anti-corrosion protection and the study of their anti-corrosion properties (4 hours).

Topics 6

The formation of oxide protective layers on the surface of aluminum and the study of their physico-chemical and anti-corrosion properties (4 hours).

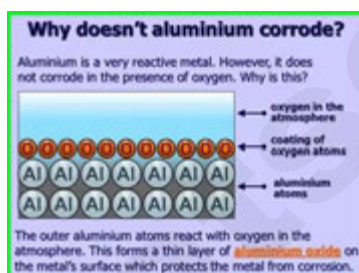
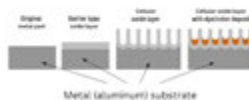
Topics 7

Electrochemical oxidation of steel, research and comparison of the properties of the obtained surfaces (4 hours).

Topics 8

Chemical phosphating of the steel surface and research on the properties of the phosphated surface (4 hours).

Anodizing



TEXTBOOK/READINGS

DO YOU KNOW

Corrosion can be avoided if you follow the path of the developers of this car.



What kind of car is this?

The mandatory reading for completing *Testing of metal and conversion protection layers* course.

POPOV, B.N.: Corrosion Engineering Principles and Solved Problems. Elsevier 2015, 774 s., ISBN 978-0-444-62722-3.

SCHWEITZER, P.A.: Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods. CRC Press, York 2009, 416 s. ISBN 978-1-4200-6770-5

ELAYAPERUMAL, K.: RAJA, V.S: Corrosion Failures: Theory, Case Studies, and Solutions. John Wiley & Sons 2015, 256 p. ISBN: 978-1-119-04327-0

BATCHELOR, A.W.: LOH, N.L.: CHANDRASEKARAN, M.: Characterization of surface coatings. Chapter 8. // Materials Degradation and Its Control by Surface Engineering. 2011, 287-333. doi:10.1142/9781848165021_0008

ASSESSMENT

Reports: Reports concern experimental laboratory exercises; contribute to the deepening of theoretical and practical knowledge in the field of metal protection with film metal and conversion coatings. The reports contain theoretical foundations, a description of the conducted experiments and analyses, together with a discussion and conclusions.

Team project (test during the semester): Team project verifying knowledge of issues in the field of testing of metallic and conversion corrosion protection layers and ability to team work.

Exam (after the semester): The oral exam verifying overall knowledge in the field of "Testing of metallic and conversion corrosion protection layers".

GRADING POLICY

The "*Testing of metallic and conversion corrosion protection layers*" course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 5 points, i.e. 6 reports x 5 points = 30 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50.

Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
10 Reports	30%
Team project	10%
Debata	10%
Examination	50%
Total	100%

10 reports (max. 2 points each) – max. 30 points
 Team project – max. 10 points
 Debata – max. 10 points
 Final exam – max. 60 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
 0 - 60 points = F

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

MODERN PHYSICOCHEMICAL METHODS OF SURFACE ANALYSIS

Code: MPhChMSA

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Advanced Methods for Materials Characterisation

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

4

COURSE DESCRIPTION

The course "Modern physicochemical methods of surface analysis" is devoted to modern methods of research of phase interfaces, mainly solid - gas and liquid - gas. Processes at the interphase boundary (in the interphase) are important for such fields of knowledge as chemical kinetics and catalysis, solid state chemistry and physics, materials science, nanotechnology, electrochemistry, organic electronics, etc.

The course is aimed to provide students with knowledge of the physico-chemical foundations of a certain method of surface research and the ability to choose the optimal method for obtaining the necessary experimental characteristics of investigated objects, as well as the skills of interpretation, generalization of the obtained results, and the use of modern experimental equipment.

The knowledge and skills acquired while studying this course will be useful to students for both academic and industrial research and development.

COURSE OBJECTIVES

The aim and task of the educational discipline "Modern physicochemical methods of surface analysis" is the formation of the necessary knowledge regarding the theoretical foundations, limits of application and practical significance of modern physico-chemical methods of analysis, as well as practical skills regarding their selection depending on the purpose of the research, preparation of samples, features of conducting experiment and interpretation of the obtained results.

The main goals of this course are:

- to acquaint students with a wide range of analytical methods used to characterize the surface of materials;
- to acquaint students with the principles underlying the methods of researching the characteristics of material surfaces;
- familiarize students with the specifics of each method, compare the information they allow you to obtain or cannot obtain;
- discuss the areas of application of these methods for surface analysis;
- to provide an understanding of these methods so that students can easily choose and justify the appropriate method(s) for investigating the selected material surface characteristics;
- familiarize students with the sample preparation procedure(s) for each of these methods,



- to acquaint students with limitations in the use of each method of analysis;
- show students how to process and interpret data obtained using these methods;
- also show the possibilities of applying analytical methods in the context of surface treatment.

The course covers popular methods of surface analysis: microscopic, spectroscopic and X-ray methods, etc.

PREREQUISITES FOR TAKING THE COURSE

This course requires basic knowledge of classical physics, general and physical chemistry, crystallography, and basic knowledge of physical and chemical materials science.

LEARNING OUTCOMES OF THE MODULE

Code module	Description
MPhChMSA _O_01	<p>The student studies the theoretical foundations of physicochemical methods of surface analysis, understands their complex use in practice.</p> <p>He studies the mechanism of interaction of incident radiation with matter in the methods used (characteristics of the phenomena on which the analytical signal is based), therefore, can assess their impact on the material under study and correctly choose the method of analysis.</p> <p>Learns the advantages and disadvantages of methods, understands which method is better to choose for surface research and what characteristics can be obtained, therefore, he is able to make informed decisions regarding the choice of analysis for obtaining the selected surface characteristics.</p> <p>Student studies and knows the principles and procedures used in surface research.</p> <p>He studies, knows and is able to describe different methods of sample preparation for each method in particular.</p> <p>He studies and knows the factors affecting the surface of the studied materials and the stages of the experiment.</p> <p>The student becomes familiar with and possesses the latest advances in surface preparation of samples for surface research and advances in surface analysis methods.</p>
MPhChMSA _O_02	<p>The student learns and knows to prepare the surface of a sample for a particular chosen method of surface analysis.</p> <p>The student knows how to conduct surface research and can independently plan and conduct experiments, interpret the obtained results and draw conclusions about the correctness of the method used and evaluate the obtained results.</p>
MPhChMSA _O_03	<p>Able to work with educational and scientific literature (find, analyze, critically evaluate and use the information obtained) to solve problems related to the choice of method and conducting research for different types of surfaces.</p> <p>Able to learn independently and gain new knowledge of the basics of materials science and methods of surface analysis.</p>
MPhChMSA _O_04	<p>The student can prepare, format and present the obtained results of the performed research. Able to work not only individually, but also in a team, able to communicate and use different means of communication.</p>

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures with multimedia support, interactive lectures with discussion	K01, K03, K04, K06, S03
Meth_02	Laboratory exercises; experiment demonstrations; observation; problem solving	S02, S03, S04
Meth_03	Team project: critical analysis, individual and team work, communication and presentation of information, debate	S01, S02, S03

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	Exam	MPhChMSA_O_01, MS_O_02	Meth_01
FT_02	Laboratory work	32	report	MPhChMSA_O_01 MPhChMSA_O_02 MPhChMSA_O_03 MPhChMSA_O_04	Meth_02, Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Preparation for exercises - finding the necessary information to participate in classes.	NO
a_02	Preparation for classes	Preparation, processing reports	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation if it necessary.	YES

LEARNING OUTCOMES

Students who successfully pass this course gain the following knowledge, skills and competency:

- the physical principle of surface research methods;
- advantages and disadvantages of the surface research methods;
- the choose of the optimal research method to obtain the necessary characteristics of surface;
- peculiarities of preparing samples for surface research.
- interpret the obtained results.

DO YOU KNOW

that in 1986 the Nobel Prize in Physics was awarded to:

1. Ernst Ruska "for his fundamental work in electron optics and for the development of the first electron microscope", and also
2. Gerd Binnig and Heinrich Rohrer "for their development of the scanning tunneling microscope"

<https://www.nobelprize.org/prizes/physics/1986/summary/>

COURSE CONTENT - LECTURE

Topics 1: Introduction to course. Electron microscopy (I): Scanning electron microscopy (SEM)

Description and definition of the concept of "surface"; surface types, morphology and structure. A brief description of physicochemical methods of surface research. Interaction of radiation (electrons, X-rays, ions etc.) with surface. **Electron microscopy**: physical principle. **Scanning electron microscope (SEM)**, principle of operation: components, characteristics. Interaction beam-sample, signals. Secondary electron and backscattered-electron images. Generation of X-rays, energy dispersive X-ray spectroscopy (EDS). Application of SEM. (2 hours)

Topics 2: Electron microscopy (II): Transmission electron microscopy

Transmission electron microscope. Electron scattering in TEM by atoms. Interaction beam of electrons - sample surface, image formation in TEM. High resolution TEM, bright field, dark field. Electron diffraction, diffraction contrast, phase contrast, pattern interpretation in TEM. Requirements for sample preparation for TEM. Application of TEM. (2 hours)

Topics 3: Scanning probe microscopy. Scanning tunneling microscopy (STM). Atomic force microscopy (AFM), electric force microscopy (EFM) and magnetic force microscopy (MFM))

Introduction to scanning probe microscopy. Instrumentation: probes, feedback system, data collection.

Scanning tunneling microscopy (STM): physical principles. Structure of microscope and principle of operation. STM operating modes, tunneling spectroscopy. Tip preparation. Sample preparation. Practical application.

Atomic force microscope (AFM): its structure, basic principles and modes of operation. Sample preparation. Application and opportunities. **Electric force microscope (EFM)**: principles and modes of operation, application. **Magnetic force microscopy (MFM)**: basic principles, modes. Opportunities and application. (2 hours)

Topic 4. Auger electron spectroscopy.

Auger electron spectroscopy: physical principles, advantages, limitation. Auger process. Auger spectrometer - structure and principles of operation. Registration of Auger electrons. Application of Auger Spectroscopy.(2 hours)

Topic 5. X-ray photoelectron spectroscopy. Ultraviolet photoelectron spectroscopy

Physical principles of **X-ray photoelectron spectroscopy (XPS)**. Structure and principles of operation of the spectrometer. Application of XPS: to measure the elemental composition, chemical state, and electronic state of the elements in an investigated compound. **Ultraviolet photoelectron spectroscopy (UPS)**: physical principles, practical aspects. Applications of UPS in chemistry and materials science. (2 hours)

Topic 6. Fourier Transform Infrared Spectroscopy (FT-IR)

FT-IR spectroscopy: principle of analysis, instrumentation. FTIR for surface material characterization: identification of polymers, identification of contaminants on surfaces, identification of organic films, particles, powders and liquids. Interpretation of IR-spectra. (2 hours)

[Kliknij tutaj, aby dodać podpis]

LEARNING OUTCOMES

Students who successfully pass this course gain the following knowledge, skills and competency:

- the physical principle of surface research methods;
- advantages and disadvantages of the surface research methods;
- the choice of the optimal research method to obtain the necessary characteristics of surface;
- peculiarities of preparing samples for surface research.
- interpret the obtained results.

DO YOU KNOW

that in 1986 the Nobel Prize in Physics was awarded to:

1. Ernst Ruska "for his fundamental work in electron optics and for the development of the first electron microscope", and also
2. Gerd Binnig and Heinrich Rohrer "for their development of the scanning tunneling microscope"

<https://www.nobelprize.org/prizes/physics/1986/summary/>

Topic 7. Mass spectrometry. Surface plasmon resonance spectroscopy.

Theoretical foundations of mass spectrometry methods, apparatus. Molecular ions and adducts. Fragmentation patterns. Qualitative and quantitative analysis. **Secondary ion mass spectrometry (SIMS)**: fundamental principles, instrumentation and applications. Interpretation of mass spectra. **Matrix-assisted laser desorption ionization (MALDI)**: principle, application. MALDI imaging. **Surface plasmon resonance spectroscopy**: principle, methodology, analytical implementations, applications of SPRS. (2 hours)

Topic 8. X-ray methods of analysis (X-ray diffraction, X-ray absorption spectroscopy, X-ray fluorescence spectroscopy, X-ray microanalysis)

X-ray sources. Interaction of X-rays with matter. **X-ray diffraction (XRD)**, principles, Bragg's Law. Study of the structure of polycrystalline materials by the Debye-Scherrer method. Study of the structure of single crystal materials by the Laue method. Debyeograms. **Small angle X-ray scattering (SAXS)**: theories and applications, instrumentation, sample preparation. **Wide-angle X-Ray scattering (WAXS)**: basic principles and applications. Difference between WAXS and SAXS. **X-ray absorption spectroscopy (XAS/XANES/EXAFS)**: principles, techniques of instrumentation, X-ray detectors, applications, sample preparation. **X-ray fluorescence spectroscopy (XRF)**: principles, advantages, EDX, WDX. **X-ray microanalysis**: principles, EDS, WDS, measurements, applications. (2 hours)

[Kliknij tutaj, aby dodać podpis]

LEARNING OUTCOMES

Students who successfully complete this course acquire the following knowledge, skills and competencies:

- work with equipment;
- be able to prepare samples for surface research;
- to be able to analyze and interpret the obtained results;
- compare research results obtained by different methods.

Analysis of the surface of materials is very important in various fields of science and technology (in particular, when creating new materials, coatings, and when monitoring the quality of products in industry). Therefore, the acquired knowledge about methods of surface research and maintenance of the corresponding equipment will be important not only in the laboratory.

DID YOU KNOW that the invention and creation of portable instruments (in particular the Portable X-ray Diffractometer with X-ray Fluorescence Analyzer) have greatly facilitated the study of art objects, forensic specimens, automotive parts, pipelines, archaeology, etc.



<https://www.photonicsonline.com/doc/portable-xrd-xrf-for-cultural-heritage-using-deep-cooled-ccd-camera-0001>

<https://www.shutterstock.com/image-photo/xray-fluorescence-analyzer-field-1565036563>

COURSE CONTENT - LABORATORY CLASSES

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) (4 hours)

Topic 2. Study of morphology, determination of the size and shape of particles by scanning electron microscopy (4 hours)

Topic 3. FTIR studies of polymers (films deposited on substrate, bulk material) (4 hours)

Topic 4. X-ray fluorescence analysis of inorganic materials (4 hours)

Topic 5. Qualitative analysis by X-ray fluorescence spectrometry (4 hours)

Topic 6. Quantitative analysis by X-ray fluorescence spectrometry (4 hours)

Topic 7. Phase analysis of materials, estimation of crystallite sizes of selected materials by X-ray phase analysis (using Scherrer's formula) (4 hours)

Topic 8. Atomic force microscopy analysis of surface (4 hours)

TEXTBOOK/READINGS

1. J. M. Walls (Ed.), *Methods of Surface Analysis*, Cambridge University Press, Cambridge, U.K., 1989. – 342 p.
2. J. C. VICKERMAN, I.S. GILMORE (Eds.), *Surface Analysis – The Principal Techniques* (2nd Ed.), John Wiley & Sons, Ltd., 2009. – 680p.
3. J. C. Riviere, S. Myhra (Eds.), *Handbook of surface and interface analysis - methods for problem solving* (2nd Ed.), 2009. – 671 p.
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.
5. Scanning Electron Microscope A To Z
<https://admin.jeol.com.cn/admin/static/uploadfiles/20170419/680fb98a-edd2-4e2b-80a9-8dcaecbb3dde.pdf>
6. Roberts, N.K., *Fourier Transform Infrared Spectroscopy of Surfaces*. In: 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 https://doi.org/10.1007/978-3-662-02767-7_8
7. Sabu Thomas Raju Thomas Ajesh K. Zachariah Raghvendra Kumar Mishra, *Spectroscopic Methods for Nanomaterials Characterization*. Vol. 2., Elsevier, 2017. - 444 p.
8. 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](https://doi.org/10.1016/0033-0655(85)80001-7)
9. Edmond de Hoffmann, Vincent Stroobant (Eds), *Mass Spectrometry. Principles and Applications* (3d Ed.), John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, England, 2007. - 502p.
10. J. Throck Watson, O. David Sparkman, *Introduction to mass spectrometry. Instrumentation, Applications and Strategies for Data Interpretation*, John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, England, 2007. – 854 p.
11. B.D. Cullity S.R. Stock, *Elements of X-Ray Diffraction*, Pearson Education Limited, 2014. – 654p.

ASSESSMENT

- Reports: The report is a result of a student's work during each lab classes. All reports intended for experimental laboratory research should contain the theory, description of the performed research, obtained results and conclusions.
- Tests: Tests during the semester indicate the current student's success.
- Team project (during the semester): team project verify the knowledge of students in field of surface analysis methods.
- Examination (end of semester): an oral survey that confirms general knowledge in the field of surface research methods.

GRADING POLICY

The discipline "Modern physical and chemical methods of surface analysis" is evaluated by points.

The final grades are the sum of the points received by the student for the semester (laboratory classes, tests, team project) and the points received for the exam (3 questions).

During the laboratory classes, the following is evaluated: theoretical preparation (oral survey before the laboratory class on the research topic, maximum 3 points) and a grade is given for the prepared report (maximum 1 points), i.e. the maximum mark: 8 reports x (3 points +1 points) = 32 points.

Team project (1 x 10 pts = 10 pts).

Tests (2 x 4 pts = 8 pts).

The maximum points during semester are 50.

The final grade consists of the student's points for the semester (for laboratory work, tests, team project) and points for the exam (3 questions). The points obtained for laboratory work (up to 50), team project (up to 10), tests (up to 8) are added to the points in the exam (maximum 50), which affects the final grade.

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.)

Assignment Weights	Percent
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
 0 - 60 points = F

CHEMO- AND BIOSENSORS. MATERIALS AND APPLICATIONS.

Code: **CBS**

Field of study

Materials Science and Engineering

Level of study

master study

Year of study/semester

3

Language

English

Thematic block

Applied Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 24h

ECTS

3

COURSE DESCRIPTION

The subject concerns the physico-chemical foundations of the functioning of sensitive layers, their manufacture and application for the determination of analytes. In particular, the main components of the sensor device are considered: the transducer, the sensitive layer, the components of the active layer. Considerable attention is paid to methods of immobilization of chemical and biological components of the sensitive layer on the surface of the transducer. The principles of operation, structure, types, main characteristics and examples of chemo- and biosensor devices based on electrochemical, optical, gravimetric, thermometric transducers are considered. The course program also includes an analysis of the current state and prospects for the development of sensor devices, new materials for creating a sensitive layer, and the expansion of the scope of application of sensor analysis.

The *Chemo- and biosensors. Materials and applications*, dedicated to the *AIEMPS - Advances in Innovative Engineering Materials and Processes for Sustainability* path, broadens knowledge about theoretical foundations in the field of materials and methods of creating sensor devices, basics of operation of sensor devices, types, structure and properties of transducers and recognition elements, main characteristics of sensors, principles of their operation, examples and areas of application. Students pursuing the *AIEMPS* path will improve practical skills for acquisition of practical skills of modification of the electrode surface, formation of transducers and sensitive layers, determination of sensitivity and selectivity of sensors, working range of substrate concentrations, kinetic parameters of the enzymatic reaction.

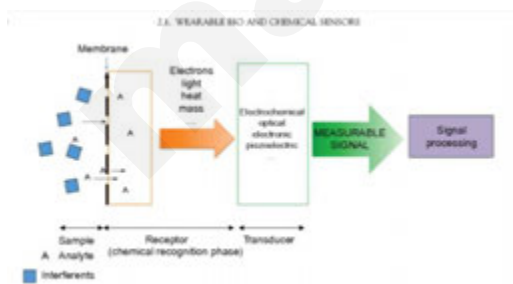
Lectures are aimed at providing information on chemo- and biosensors, basic laws of chemical and biological recognition of molecules, features of constructions, varieties and examples of electrochemical, optical, gravimetric, thermometric, etc. sensors; fields of application of chemo- and biosensors. Laboratory exercises are intended for individual and group student works, performance of experiments and analysis leading to individual elaboration of the obtained results in the form of a report along with relevant studies and conclusions.

COURSE OBJECTIVES

By the end of the *Chemo- and biosensors. Materials and applications.*, students will gain an understanding of the materials and methods of creating sensor devices, types, structure and properties of transducers and recognition elements. Students will be able to modify the electrode surface, form transducers and sensitive layers, immobilize biological components; design and research electrochemical, optical, gravimetric chemical and biosensors; experimentally determine the main characteristics of sensors.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject *Chemo- and biosensors. Materials and applications.*, students should have a general knowledge of *Physical chemistry, Analytical chemistry, Chemical technology, Physics, Inorganic chemistry, Organic chemistry.*



Chapter 2.1 - *Wearable Bio and Chemical Sensors*. Shirley Coyle, Vincenzo F. Curto, Fernando Benito-Lopez, Larisa Florea, Dermot Diamond. *Wearable Sensors. Fundamentals, Implementation and Applications*. 2014, P. 65-83.

<https://doi.org/10.1016/B978-0-12-418662-0.00002-7>

LEARNING OUTCOMES OF THE MODULE

Code module	Description
MP_O_01	He has extensive and in-depth substantive knowledge in the field of materials and methods of creating sensor devices, types, structure and properties of transducers and recognition elements, as well as basic laws of chemical and biological recognition of molecules, features of constructions, varieties and examples of sensors; fields of application of chemo- and biosensors.
MP_O_02	Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to the production and use of sensors and its components.
MP_O_03	He can plan and carry out experiments, interpret the results and draw conclusions regarding to the construction and applications of sensors and its components.
MP_O_04	Can prepare a scientific paper and present a presentation on the implementation of a research task, including critical analysis, synthesis and conclusions. Able to work individually and in a team and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	CP_O_01 CP_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate.	CP_O_03 CP_O_04
Meth_03	Team project: critical analysis, synthesis and conclusions; individual and teamwork, communicate on specialist topics, leading a debate.	CP_O_03 CP_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	Exam	CP_O_01 CP_O_02	Meth_01
FT_02	laboratory	24	course work	CP_O_03 CP_O_04	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

COURSE CONTENT – LECTURE

LEARNING OUTCOMES

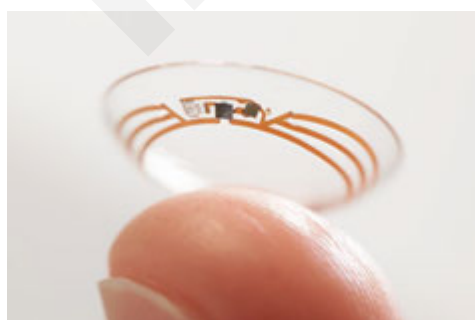
By the end of the Chemo- and biosensors. Materials and applications. course, students will gain an understanding of the types, structure and properties of transducers and recognition elements; physico-chemical basis of chemical and biological recognition of molecules, features of constructions, varieties and examples of electrochemical, optical, gravimetric, thermometric, etc. sensors; fields of application of chemo- and biosensors. Students will be able to explain the main physico-chemical laws, phenomena and processes on which the operation of sensor devices is based, as well as the types, structure and properties of transducers and recognition elements; modify the electrode surface, form transducers and sensitive layers, immobilize biological components; experimentally determine the main characteristics of sensors - selectivity, sensitivity, working range of substrate concentrations, linear range, detection limit, response time; calculate kinetic parameters of enzymatic reactions; design and research electrochemical, optical, piezoelectric chemical and biosensors.

COMMENTS

LECTURER

DO YOU KNOW

A Washington State University laboratory has created contact lenses that can measure the level of glucose in human tears and display the readings on a mobile phone screen.



Topics 1

During the lecture, as an introduction to the subject *Chemo- and biosensors. Materials and applications.*, 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. (2 hours)

Topics 2

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; π -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⁻, CPV/Br⁻ and CPV/I⁻ ions when it is exposed to aqueous solutions of KCl, KBr and KI. (2 hours)

Topics 3

During the lecture, students will learn 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. (2 hours)

Topics 4

The lecture will present 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. (2 hours)

Topics 5

The lecture will present 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 π -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; 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; Element with multiple broken total internal reflection Broken total internal reflection with fluorescence; Fluorescent light detection schemes; Surface plasmon resonance; Brewster's angle measurement; Generation of non-radiative plasmons in a Kretschmann prism; Optical sensors based on light scattering methods. (2 hours)

Topics 6

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. (2 hours)

Topics 7

The lecture will present general characteristics of biosensors: Factors affecting the characteristics of biosensors; Classification of 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; Electron transfer mediators and the scheme of functioning of the mediator enzyme sensor; The speed of the enzymatic reaction in the kinetic and diffusion regimes. (2 hours)

Topics 8

During the lecture, students will learn about the 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. (2 hours)

LEARNING OUTCOMES

Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

COURSE CONTENT – LABORATORY CLASSES

Topics 1

Students will perform 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 (4 hours)

Topics 2

Students will synthesize an electroactive polymer on a platinum electrode in potenti-, 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 (4 hours)

Topics 3

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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 4

Students will investigate the operation of 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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 5

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

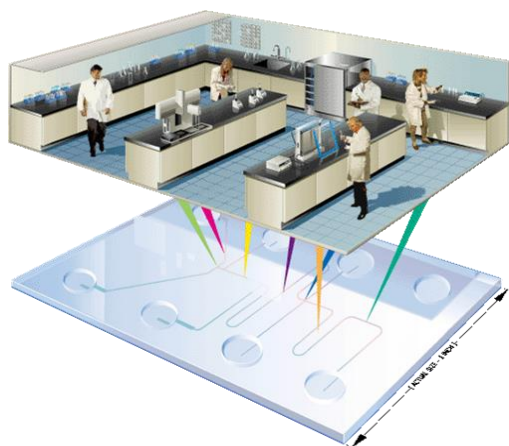
Biosensors of the future



constructed sensor. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 6

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. The completed experiment will be the basis for developing a report on the exercises (4 hours)



Lab-on-a-chip

<https://www.nanodtc.cam.ac.uk/category/current-projects/page/3/>

TEXTBOOK/READINGS

The mandatory reading for completing the subject *Chemo- and biosensors. Materials and applications*:

1. *Chemical Sensors and Biosensors*. Brian R. Eggins. Wiley; 1st edition. 2002. 300 p.
2. *Chemical Sensors and Biosensors: Fundamentals and Applications*. Florinel-Gabriel Bănică. 2012. John Wiley & Sons, Ltd. 576 p.
3. *Advanced microsystems for automotive applications*. Detlef Egbert Ricken, Wolfgang Gessner. Springer. 1999. 318 p.
4. *Chapter 7. Polyaniline in Chemo-and Biosensors: 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.

Actuators B: Chemical, Analytical chemistry, ECS Sensors Plus, Journal of Sensory Studies, Micro and Nano Technologies, Progress in Materials Science, Nature Materials, Advanced Materials, Progress in Polymer Science, Nanoscale Research Letters, Materials Today

To deepen the course topics, optional recommended texts include articles in journals: *Sensors, Sensors International, Sensors and*

ASSESSMENT

Reports:

The reports relate to experimental laboratory exercises; contribute to deepening theoretical and practical knowledge in the field of *Chemo- and biosensors. Materials and applications*. The reports contain theoretical background, description of performed experiments and analyses, together with discussion and conclusions.

Team project (during the semester):

Team project verifying knowledge of issues in the field of Chemo- and biosensors, and ability to team work.

Exam (after the semester):

The oral exam verifying overall knowledge in the field of Chemo- and biosensors.

GRADING POLICY

The *Chemo- and biosensors. Materials and applications*. course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 5 points, i.e. 6 reports x 5 points = 30 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam's 50. Student grades will be assessed as follows in the box on the right.

Assignment Weights	PERCENT
6 Reports	30%
Team project	10%
Debata	10%
Exam	50%
Total	100%

6 reports (max. 5 points each) – max. 30 points
 Team project – max. 10 points
 Debata – 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
 0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

MEMBRANE PROCESSES: MATERIALS, PROPERTIES AND APPLICATIONS

Code: **MPMPA**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

3

Language

English

Thematic block

Applied Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 24h

ECTS

3

COURSE DESCRIPTION

The subject concerns general patterns of mass transfer processes, the main methods and mechanisms of membrane separation, materials, structure, properties and methods of forming membranes.

The *Membrane Processes: Materials, Properties and Applications* course, dedicated to the *AIEMPS - Advances in Innovative Engineering Materials and Processes for Sustainability* path, broadens knowledge about theoretical foundations in the field of materials and methods of creating membranes, the physicochemical foundations of kinetics and thermodynamics of mass transfer processes, the structure and functioning of membrane apparatus assemblies. Students pursuing the *AIEMPS* path will improve practical skills for production membranes, master the methods of researching properties, membrane technologies, and deepen their knowledge of various aspects of membrane application.

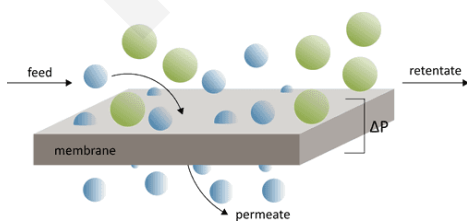
Lectures are aimed at providing information on membrane technologies, methods of membranes production, properties, and applications. Laboratory exercises are intended for individual and group student works, performance of experiments and analysis leading to individual elaboration of the obtained results in the form of a report along with relevant studies and conclusions.

COURSE OBJECTIVES

By the end of the *Membrane Processes: Materials, Properties and Applications* course, students will gain an understanding of the main characteristics of membrane separation processes, basics of mass transfer theory, types of membranes and their properties, basic principles of formation and modification of membranes, methods of membrane separation. Students will be able to provide determining the main parameters of membrane separation processes, pore size and specific surface area of membranes, receive, modify and research membranes.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject *Membrane Processes: Materials, Properties and Applications*, students should have a general knowledge of *Physical chemistry, Colloid chemistry, Chemical technology, Chemistry of high molecular compounds, Inorganic chemistry, Organic chemistry.*



The schematic of membrane separation

LEARNING OUTCOMES OF THE MODULE

Code module	Description
MP_O_01	He has extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and surface modification of membranes, as well as membrane separation processes.
MP_O_02	Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to the production and use of membranes.
MP_O_03	He can plan and carry out experiments, interpret the results and draw conclusions regarding the applications of membranes.
MP_O_04	Can prepare a scientific paper and present a presentation on the implementation of a research task, including critical analysis, synthesis and conclusions. Able to work individually and in a team and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	CP_O_01 CP_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate.	CP_O_03 CP_O_04
Meth_03	Team project: critical analysis, synthesis and conclusions; individual and team work, communicate on specialist topics, leading a debate.	CP_O_03 CP_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	Exam	CP_O_01 CP_O_02	Meth_01
FT_02	laboratory	24	course work	CP_O_03 CP_O_04	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

COURSE CONTENT – LECTURE

LEARNING OUTCOMES

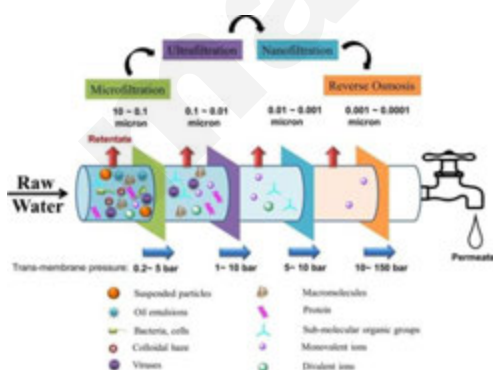
By the end of the Membrane Processes: Materials, Properties and Applications course, students will gain an understanding of the main characteristics of membrane separation processes, basics of mass transfer theory, types of membranes and their properties, basic principles of formation and modification of membranes, methods of membrane separation. Students will be able to provide determining the main parameters of membrane separation processes, pore size and specific surface area of membranes, receive, modify and research membranes.

COMMENTS

LECTURER

DO YOU KNOW

The first generation of polymeric membranes are Microfiltration, Ultrafiltration, Nanofiltration, and Reverse Osmosis.



https://nordicmembrane.com/membrane_technology

Topics 1

During the lecture, as an introduction to the subject *Membrane Processes: Materials, Properties and Applications*, the current state of membrane processes will be presented. Students will learn the 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 and temperature on the process of membrane separation. (2 hours)

Topics 2

The lecture will present the Basic laws of fluid flow in porous bodies; Determination of pore sizes by filtration method; Capillary impregnation; Mechanism of transfer of gases and components of solutions in porous bodies; Hydrodynamic mode of transfer of gases and components of solutions; Diffusion mode of substance transfer; Activated diffusion in micropores; Surface diffusion. (2 hours)

Topics 3

During the lecture, students will learn about the General characteristics, classification, production and properties of membranes; Classification of membranes according to their chemical structure - polymer membranes, rigid membranes, metal, ceramic, diffusion, dynamic, ion-exchange, symmetric and asymmetric, liquid membranes; Composite 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). (2 hours)

Topics 4

The lecture will present Structural Design of Membranes; Chemical Design of Membrane Materials; Physical Construction of Separation Membranes; Relation between Structure and Preparation Condition of Membrane; Structure of Liquid Membranes; Structure of Inorganic Membranes. (2 hours)

Topics 5

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. (2 hours)

Topics 6

During the lecture, students will learn about the Ultrafiltration and Microfiltration; Membranes for Ultrafiltration; Organic Membranes; Inorganic Membrane; Ultrafiltration Modes; Concentration Polarization and Fouling in Ultrafiltration; Ultrafiltration Technology and

LEARNING OUTCOMES

Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

Applications; Principle of Microfiltration; Membranes for Microfiltration; Membrane Materials; Microfiltration Technology. (2 hours)

Topics 7

The lecture will present the Ion Exchange Membrane Processes; Transport through Ion Exchange Membranes; Chemistry of Ion Exchange Membranes; Homogeneous Membranes; Heterogeneous Membranes; Electrodialysis; Concentration Polarization and Limiting Current Density; Current Efficiency and Power Consumption; System Design; Electrodialysis Applications; Bipolar Membranes; Fuel Cells. (2 hours)

Topics 8

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; 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. (2 hours)

COURSE CONTENT – LABORATORY CLASSES

Topics 1

Students will perform the suspension microfiltration 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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 2

Students will analyze of porous granular material, determine 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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 3

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. The completed experiment will be the basis for developing a report on the exercises (4 hours)



Membrane technology encompasses the related scientific and engineering approaches for the transport or rejection of components, species, or substances through or by the membranes.

From: Nanomaterial and Polymer Membranes, 2016

Topics 4

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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

Topics 5

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. The completed experiment will be the basis for developing a report on the exercises (4 hours)

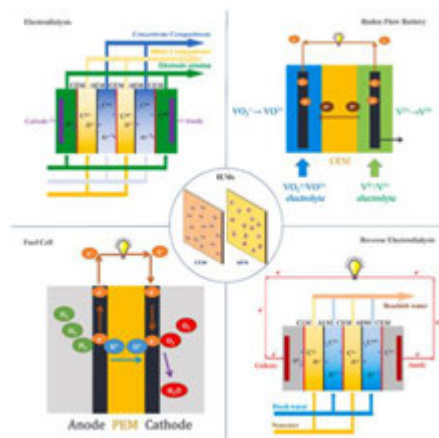
Topics 6

The topics of the laboratory classes are related to the basic principles of the electro dialysis method, anion- and cation-selective membranes. Students will study the scheme of the electro dialyzer, calculate of concentration distribution in the deionization section, manufacture of anion- and cation-selective membranes, determine of the ion-exchange capacity of a membrane. The completed experiment will be the basis for developing a report on the exercises (4 hours)

TEXTBOOK/READINGS

The mandatory reading for completing the subject *Membrane Processes: Materials, Properties and Applications*:

1. *Science and Technology of Separation Membranes*. Tadashi Uragami. Wiley. 2017. 848 p. ISBN: 978-1-118-93256-8
2. *Membrane Characterization*. Ahmad Fauzi Ismail, Darren Oatley-Radcliffe, Nidal Hilal, Takeshi Matsuura. Elsevier Science. 2017. 458 p. ISBN (Electronic) 9780444637918 ISBN (Print) 9780444637765
3. *Membrane Technology and Applications. Third Edition*. Richard W. Baker. John Wiley and Sons Ltd. 2012. 583 p. [https://www.eng.uc.edu/~beaucag/Classes/Properties/Books/Richard%20W.%20Baker\(auth.\)%20-%20Membrane%20Technology%20and%20Applications.%20Third%20Edition%20\(2012\).pdf](https://www.eng.uc.edu/~beaucag/Classes/Properties/Books/Richard%20W.%20Baker(auth.)%20-%20Membrane%20Technology%20and%20Applications.%20Third%20Edition%20(2012).pdf)



Applications of ion exchange A comprehensive review on the synthesis and applications of ion exchange membranes.
Shanxue Jiang, Haishu Sun, Huijiao Wang, Bradley P. Ladewig, Zhiliang Yao. *Chemosphere*. Vol. 282, 2021, 130817. <https://doi.org/10.1016/j.chemosphere.2021.130817>

To deepen the course topics, optional recommended texts include articles in journals: *Membranes, Membrane Technology, Journal of Membrane Science and Research, Journal of Membrane Science, Micro and Nano Technologies, Progress in Materials Science, Nature Materials, Advanced Materials, Progress in Polymer Science, Nanoscale Research Letters, Materials Today*

ASSESSMENT

Reports:

The reports relate to experimental laboratory exercises; contribute to deepening theoretical and practical knowledge in the field of membranes and membrane processes. The reports contain theoretical background, description of performed experiments and analyses, together with discussion and conclusions.

Team project (during the semester):

Team project verifying knowledge of issues in the field of membranes and membrane processes, and ability to team work.

Exam (after the semester):

The oral exam verifying overall knowledge in the field of smart conducting polymers.

GRADING POLICY

The *Membrane Processes: Materials, Properties and Applications* course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 5 points, i.e. 6 reports x 5 points = 30 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50. Student grades will be assessed as follows in the box on the left.

Assignment Weights	PERCENT
6 Reports	30%
Team project	10%
Debata	10%
Exam	50%
Total	100%

6 reports (max. 5 points each) – max. 30 points
Team project – max. 10 points
Debata – 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
0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

NANOMATERIALS AND NANOTECHNOLOGIES IN ECOLOGY

Code: NNE

COURSE DESCRIPTION

The course is designed in such a way to highlight the causes of environmental pollution in the context of the growing use of nanomaterials and nanotechnologies, which threatens the continued existence of life on Earth, as well as to establish possible ways out of this situation.

The course covers general issues of nanomaterials and nanotechnologies, as well as issues related to environmental pollution by nanoparticles. Acquaintance with modern global eco-technologies related to the use of nanomaterials and nanocomposites of various nature for water, soil and air purification.

COURSE OBJECTIVES

The discipline "Nanomaterials and nanotechnologies in ecology" should provide both general education and professional development of students (masters) - materials scientists, form their competence in the field of understanding problems related to the use of nanomaterials and nanotechnologies and environmental pollution, as well as ways to solve them.

The course focuses on acquiring knowledge and developing skills in the field of nanotechnology, providing environmental technologies, from the point of view of combining the valuable properties of nanomaterials and the impact on the environment.

As a result of studying the discipline, students must learn the material provided by the program, which means to know: basic concepts regarding nanomaterials and nanotechnologies, the causes of environmental problems associated with the use of nanomaterials and nanotechnologies; modern approaches to the use of nanomaterials and nanotechnologies in water, air, and soil purification.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject, the student should have general knowledge about different types of materials, in particular, nanomaterials of different nature, their structure, properties and applications.

Field of study

Materials Science and Engineering

Level of study

Master Study

Year of study/semester

3

Language

English

Thematic block

Applied Materials Science

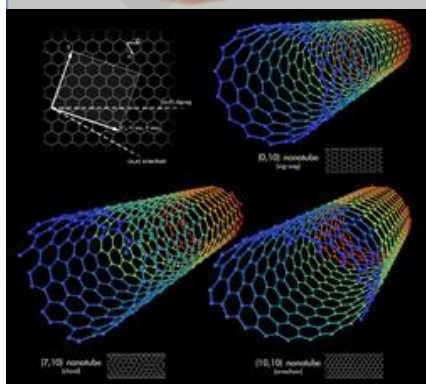
Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

4



LEARNING OUTCOMES OF THE MODULE

Code module	Description
EP_O_01	<p>Has the knowledge necessary to understand the ethical, economic and ecological aspects of the design of new engineering materials and their production technology and the impact of the development of materials engineering on the sustainable development and progress of civilization.</p> <p>Knows and understands the basic concepts and principles of intellectual and industrial property protection as well as copyright and patent law.</p>
EP_O_02	<p>Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions and formulate and solve problems related to the production and use of sustainable nanomaterials.</p>
EP_O_03	<p>He can plan and carry out experiments, interpret the results and draw conclusions regarding the applications of sustainable engineering nanotechnology.</p>
EP_O_04	<p>Can prepare a scientific paper and present a presentation on the possibilities of sustainable nanotechnology, including critical analysis, synthesis and conclusions. Able to work individually and in a team, and lead a debate.</p>
...	

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	<p>Lectures:</p> <p>lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support</p>	<p>EP_O_01</p> <p>EP_O_02</p>
Meth_02	<p>Laboratory exercises:</p> <p>experiment demonstrations; laboratory work; observation; problem learning; debate</p>	<p>EP_O_03</p> <p>EP_O_04</p>
Meth_03	<p>Team project:</p> <p>critical analysis, synthesis and conclusions; individual and team work, communicate on specialist topics, leading a debate.</p>	<p>EP_O_03</p> <p>EP_O_04</p>
...	
...		

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	exam	EP_O_01 EP_O_02	Meth_01
FT_02	laboratory	32	course work	EP_O_03 EP_O_04	Meth_02 Meth_03
...					
...					

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

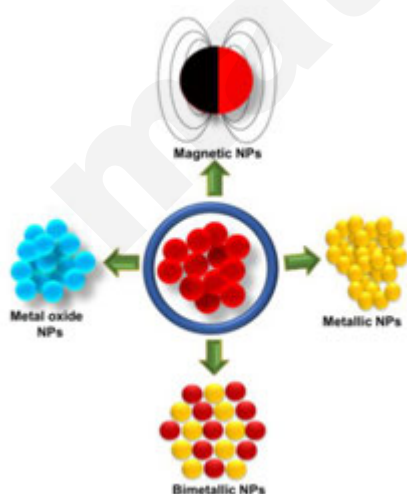
Code	Category	Name	Work with teacher
a_01	Reading literature	Finding materials and preparing presentations for participation in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

By the end of studying the course "Nanomaterials and nanotechnologies in ecology", students should master the material provided by the program, which means knowing: basic concepts related to nanomaterials and nanotechnologies; causes of environmental problems associated with the use of nanomaterials and nanotechnologies; modern approaches to the interpretation of the main environmental problems of materials science; modern methods of water, air, and soil purification using nanomaterials and nanotechnologies; the place and role of nanochemistry in solving environmental problems.

COMMENTS

LECTURER



COURSE CONTENT - LECTURE

Topics 1

Nanomaterials and nanotechnology. Nanotechnology as a key direction of technology development of the 21st century. Modern concepts of nanotechnology, nanoproduction and nanoscience. Nanoparticles. The main groups of nanomaterials: structure and practical use. The main types of carbon nanoparticles: modern methods of production and application. Carbon-based nanogels. Polymer nanoparticles. Polymeric nanosystems for therapeutic applications. Quantum dots and conjugated metal-organic frameworks for targeted drug delivery. Nanomagnetic materials for environmental improvement. Application of carbon dots as photocatalysts in cleaning processes. (2 h)

Topics 2

Nanomaterials based on metals and metal oxides. Methods of obtaining metal oxides. Use of metal oxides for environmental purposes. Nanocomposite materials, classification and application. Metal nanoparticles. Synthesis of nanomaterials using natural raw materials. (2 h)

Topics 3

The main areas of application of nanomaterials and nanotechnologies in ecology. Methods of obtaining and researching nanomaterials. Modern materials based on metal-organic frameworks for the adsorption of gases for the purpose of cleaning the environment. Layered double hydroxides: structure, properties, environmental applications for fluoride removal. The use of black titanium for the recovery of hazardous organic substances and the generation of hydrogen. Removal of carbon dioxide using sorbents from alkaline waste. Flexible polymer films modified with nanoparticles in self-cleaning processes. (2 h)

Topics 4

Use of nanotechnologies in soil restoration processes. Soil cleaning methods using nanomaterials. Advanced nanomaterials for removing arsenic from groundwater. The use of graphene nanocomposites in remediation of contaminated soils. (2 h)

Topics 5

Application of nanotechnologies to restore the state of natural waters. Wastewater treatment. Nanomaterials in water desalination. Preparation and use of nanoparticle-modified membranes for wastewater treatment. Membranes based on bentonite for micro-, ultra- and nanofiltration. Use of zeolites and composites based on them for purification from chromium compounds. Metal-organic frameworks as adsorbents of water pollutants. Dendritic polymers for restoration of water resources. Polymer nanocomposites for adsorption of azo dyes. (2 h)

Topics 6

Application of nanotechnologies and nanomaterials for cleaning polluted atmospheric air. Progressive technologies of using metal-organic frameworks as catalysts in pollutant oxidation processes. The use of ash in the treatment of liquid and gaseous phases. (2 h)

Topics 7

Problems of environmental pollution associated with the spread of nanoparticles. Sources and routes of entry of engineered nanoparticles into the environment. Accumulation and transformation of engineering nanoparticles in the atmosphere, water and soil. Physico-chemical and biological transformations of nanoparticles. Mechanisms of toxicity induced by nanoparticles. (2 h)

LEARNING OUTCOMES

Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR



Topics 8

Problems of environmental pollution associated with the use of nanotechnology and the creation of nanomaterials. Use of graphene and graphene oxide derivatives in environmental analysis. Nanoeffects and nanoobjects in nature. (2 h)

COURSE CONTENT – LABORATORY CLASSES

Evaluation of microhardness and elemental composition of initial and nanostructured amorphous alloys based on Fe, Co and Al (4 hours)

Study of the physical and chemical properties of modified polymers of different composition (4 hours)

Determination of the limit of strength of materials of different nature and purpose (4 hours)

Electrochemical studies of hydrogen release processes on nanostructured amorphous alloys. (4 hours)

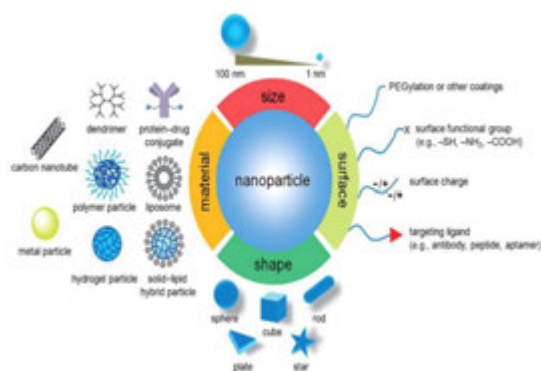
Wastewater treatment using nanostructured amorphous iron-based alloys. Obtaining EDH spectra and electronic maps of sample surfaces. (4 hours)

Electrochemical studies of initial and nanostructured amorphous alloys in alkaline and acidic solutions (4 hours)

Analysis and purification of wastewater using zeolite-based composites from chromium compounds (4 hours)

Analysis and purification of wastewater using polymer nanocomposites from azo dyes (4 hours)

TEXTBOOK/READINGS



mandatory reading for completing the subject "Environmental problems of materials science"

I. Cao, Synthesis, characterization, and applications of zero dimensional (0D) nanostructures, Synthesis and Applications of Inorganic Nanostructures, Chapter Wiley, 2017, pp. 21–146, <https://doi.org/10.1002/9783527698158>.

M. Nasrollahzadeh, Z. Issaabadi, M. Sajjadi, M. Sajadi, An Introduction to Green Nanotechnology, 1st, Elsevier, 2019.

<https://www.epa.gov/chemical-research/research-nanomaterials>

to deepen the course topics, optional recommended texts include:

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).

5. M.M. Sabzehmeidani, S. Mahnaee, M. Ghaedi, H. Heidari, V.A.L. Roy, Carbon based materials: a review of adsorbents for inorganic and organic compounds, Mater. Adv. 2 (2) (2021) 598–627.

ASSESSMENT

Reports:

Reports refer to research and laboratory works. Contribute to the deepening of theoretical and practical knowledge about nanomaterials and nanotechnologies and their impact on the environment. The reports contain theoretical foundations, a detailed description of the conducted experiments, their analysis, discussion and conclusions.

Team project (during the semester):

A team project that tests knowledge about nanomaterials and nanotechnologies in ecology and the ability to work in a team.

Exam (after the semester):

An oral exam that tests general knowledge in the field of nanomaterials and nanotechnologies, as well as their impact on the environment and applications in cleaning processes.

GRADING POLICY

The course "Nanomaterials and nanotechnologies in ecology" is evaluated by points. The grade is given by the sum of the points scored by the student during the semester (laboratory classes) and the points scored during the exam. During laboratory classes, the following are constantly evaluated: theoretical preparation (discussion at the beginning of laboratory classes as an introduction to conducting an experiment and preparation of a report), submitted reports (max. 5 points, i.e. 8 reports x 5 points). = evaluated 40 points) and team project (1 x 10 points = 10 points). The maximum number of points received for the performance of laboratory exercises is 50. The exam is conducted in oral form - 3 questions are selected from a previously set range of topics. The maximum number of points that can be obtained on the exam is 50. Students' marks will be evaluated as follows in the box on the left.

Assignment Weights	Percent
8 Reports	40%
Team project	10%
Exam	50%
Total	100%

8 reports (max. 5 points each) – max. 40 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

0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic Tema	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

TESTING OF POLYMER CORROSION PROTECTION LAYERS

Code: TPCPL

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

2

Language

English

Thematic block

Materials Testing Methods and Failure Analysis

Form of tuition and number of hours*:

Lecture: 16 h

Laboratory: 32 h

ECTS

4

COURSE DESCRIPTION

The course "Testing of polymer corrosion protection layers" is devoted to the path of AIEMPS - Advances in Innovative Engineering Materials and Processes for Sustainability. It is aimed at understanding the importance of protecting metals and alloys from corrosion processes with modern coatings formed by polymer films, films based on conductive polymers, composite polymer films based on smart-responsive and self-healing, as well as composite organic-inorganic coatings. The subject also considers modern methods of research and assessment of corrosion resistance of formed coatings of metals and alloys.

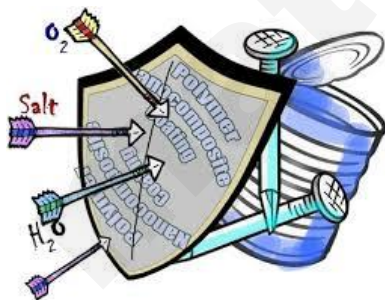
Education is divided into lectures and laboratory classes. At the lectures, students will learn to understand the theoretical foundations of corrosion processes of metals and alloys, the essence of corrosion protection methods using polymer coatings, as well as coatings based on conductive polymers and composites. In laboratory classes, students get to know and perform tasks related to the preparation of samples of metals and alloys and the formation of protective anti-corrosion coatings on them, as well as learn to use various methods of analyzing the condition and effectiveness of anti-corrosion coatings.

COURSE OBJECTIVES

After studying the course "Testing of polymer corrosion protection layers", the student will: be able to distinguish the main types of corrosion; to be able to choose anti-corrosion coatings based on polymers of different nature; form polymer coatings by electrochemical methods, as well as self-prepared composites based on conductive polymers by mechanical application on metals and alloys for use in various operating conditions; propose and perform appropriate surface preparation and treatment; evaluate corrosion resistance using various test methods and research.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject "Testing of polymer corrosion protection layers", the student must have basic knowledge of physic, inorganic, analytical, and physical chemistry, as well as general knowledge of various types, properties, structure and application of various metals as structural materials.



LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	He has extensive knowledge in the field of determining the nature of corrosion damage, the application of modern physico-chemical methods for the study of surface films of various nature on metals and metal alloys, the selection of methods of forming protective anti-corrosion layers on metals for operation in various environments, methods of creating protective corrosion layers of various polymers nature.
MS_O_02	Can use information from the literature and other available sources in the field of physic, general chemistry, analytical and physical chemistry, interpret and critically evaluate them.
MS_O_03	Can plan and conduct experiments, interpret results and draw conclusions about the corrosion properties of materials and their surface treatment to prevent corrosion.
MS_O_04	Can prepare and present results of corrosion resistance tests, including critical analysis, synthesis and conclusions. Able to work individually and in a team, and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	MS_O_01 MS_O_02
Meth_02	Laboratory classes: experiment demonstration; laboratory work; observation; problem teaching	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
TPL_01	Lecture	16	exam	MS_O_01 MS_O_02	Meth_01
TPL_02	Laboratory	32	course work	MS_O_03 MS_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

After studying the discipline "Testing of polymer corrosion protection layers", the student will be able to distinguish the main types of corrosion, modern research methods of protective corrosion coatings based on polymers, evaluate the suitability of various types of polymer coatings of metals and their alloys for use in various environments, prevent corrosion and degradation of materials through appropriate interventions in the project, propose and carry out appropriate treatment of their surface and evaluate corrosion resistance through tests and research in conditions close to operational ones.

COMMENTS

LECTURER

COURSE CONTENT - FORM OF TUITION (lecture)

Topics 1

Testing of polymer corrosion protection layers. Introduction (2 hours).

Topics 2

Corrosion of metals and alloys. Types of corrosion and their dependence on operating conditions (2 hours).

Topics 3

Characteristics of surface anticorrosion coatings by modern physical and analytical methods of researching the surface, composition and structure of protective coatings (2 hours).

Topics 4

Electrochemical application of protective polymer coatings on steel surfaces (2 hours).

Topics 5

Electrochemical application of protective conducting polymer coatings on steel surfaces (2 hours).

Topics 6

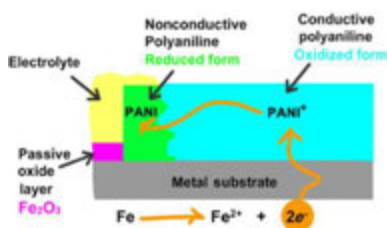
Protective conducting polymer coatings of aluminum surfaces (2 hours).

Topics 7

Polyaniline for smart-responsive and self-healing coatings for steel corrosion protection (2 hours).

Topics 8

Nanocomposite organic-inorganic coatings for corrosion protection of steel (2 hours).



LEARNING OUTCOMES

After studying the discipline “*Testing of polymer corrosion protection layers*”, the student will be able to: distinguish the main types of corrosion effects, determine the nature of corrosion damage/destruction of various polymer protective coatings of metals, choose methods of anti-corrosion protection to prevent corrosion degradation of metals and alloys through appropriate interventions in the structure, propose and implement appropriate treatment of metal surfaces with polymer coatings and to evaluate the corrosion resistance of coatings using modern test methods.

COMMENTS

INSTRUCTOR



COURSE CONTENT - FORM OF TUITION (laboratory classes)

Topics 1

Introduction to the laboratory workshop from the course (4 hours).

Topics 2

Study of the nature of damage to protective coatings of metals and alloys caused by metal corrosion (4 hours).

Topics 3

Methods of testing polymer protective coatings layers of various nature (4 hours).

Topics 4

Electrochemical application of protective polymer coatings on steel surfaces (4 hours).

Topics 5

Electrochemical application of protective polyaniline coatings on steel surfaces (4 hours).

Topics 6

Protective conducting polyaniline/polypyrrole coatings on aluminum surfaces (4 hours).

Topics 7

Polyaniline for smart-responsive and self-healing coatings for metals and their alloys corrosion protection (4 hours).

Topics 8

The formation of nanocomposite organic-inorganic coatings for corrosion protection of steel (4 hours).

TEXTBOOK/READINGS

DO YOU KNOW

Corrosion can be avoided if you follow the path of the developers of this car.



What kind of car is this?

The mandatory reading for completing *Testing of metal and conversion anti-corrosion layers* course.

POPOV, B.N.: Corrosion Engineering Principles and Solved Problems. Elsevier 2015, 774 s., ISBN 978-0-444-62722-3. doi:10.1016/C2012-0-03070-0

SCHWEITZER, P.A.: Fundamentals of Corrosion: Mechanisms, Causes, and Preventative Methods. CRC Press, York 2009, 416 s. ISBN 978-1-4200-6770-5

ELAYAPERUMAL, K.: RAJA, V.S: Corrosion Failures: Theory, Case Studies, and Solutions. John Wiley & Sons 2015, 256 p. ISBN: 978-1-119-04327-0

BATCHELOR, A.W.: LOH, N.L.: CHANDRASEKARAN, M.: Characterization of surface coatings. Chapter 8. // Materials Degradation and Its Control by Surface Engineering. 2011, 287-333. doi:10.1142/9781848165021_0008

ASSESSMENT

Reports: Reports concern experimental laboratory exercises; contribute to the deepening of theoretical and practical knowledge in the field of metal protection with film polymer corrosion protection layers. The reports contain theoretical foundations, a description of the conducted experiments and analyses, together with a discussion and conclusions.

Team project (test during the semester): Team project verifying knowledge of issues in the field of testing of of polymer corrosion protection layers and ability to team work.

Exam (after the semester): The oral exam verifying overall knowledge in the field of "Testing of polymer corrosion protection layers".

GRADING POLICY

The "*Testing of polymer corrosion protection layers*" course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 4 points, i.e. 8 reports x 4 points = 32 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 8 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50.

Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
8 Reports	32%
Team project	10%
Debata	8%
Examination	50%
Total	100%

8 reports (max. 4 points each) – max. 32 points
 Team project – max. 10 points
 Debata – max. 8 points
 Final exam – max. 60 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
 0 - 60 points = F

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

NEW ELECTROCHROMIC MATERIALS AND DEVICES

Code: EMD

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

3

Language

English

Thematic block

Applied Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 24h

ECTS

3

COURSE DESCRIPTION

The subject concerns new electrochromic materials, production methods, characterization, and use of electrochromic materials for optoelectronic devices designed for actual gadgets and constructions.

The *New Electrochromic Materials and Devices* course, dedicated to the *AIEMPS - Advances in Innovative Engineering Materials and Processes for Sustainability* path, broadens knowledge about theoretical foundations in the field of production innovative electrooptical materials based on organic and inorganic compounds able to color change under external voltage. Students pursuing the *AIEMPS* path will improve practical skills for production electrochromic materials, master the methods of researching properties, and deepen their knowledge of various aspects of application.

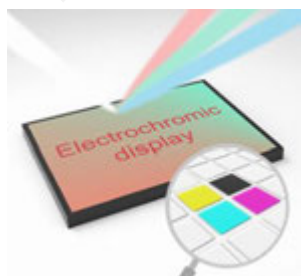
Lectures are aimed at providing information on electrochromic materials, production methods, properties, and applications. Laboratory exercises are intended for individual and group student work, performance of experiments, and analysis, leading to individual elaboration of the obtained results in the form of a report along with relevant studies and conclusions.

COURSE OBJECTIVES

By the end of the *New Electrochromic Materials and Devices* course, students will gain an understanding of the theoretical basis for the electro-optical transformation in electrochromic materials. Students will be able to provide methods of production of thin films and model devices with electrochromic layers and their application for flexible displays, smart windows, car mirrors, etc., establish the voltage–optical spectrum–color connection for a purposeful change in the optical transition and material color in model electrochromic devices under external electric field action.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of the subject *New Electrochromic Materials and Devices*, students should have a general knowledge of *Organic and Inorganic Chemistry*, *Physical Chemistry*, *Electroengineering*, and *Chemistry of Macromolecular Compounds*.



<https://doi.org/10.1021/acs.chemrev.1c01055>

LEARNING OUTCOMES OF THE MODULE

Code module	Description
MS_O_01	He has extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and modification of functional materials based on electrochromic substances, as well as development trends and the latest achievements in this area.
MS_O_02	Can use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to the production and use of electrochromic materials.
MS_O_03	He can plan and carry out experiments, interpret the results and draw conclusions regarding the applications of electrochromic materials.
MS_O_04	Can prepare a scientific paper and present a presentation on the implementation of a research task, including critical analysis, synthesis and conclusions. Able to work individually and in a team and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	MS_O_01 MS_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate.	MS_O_03 MS_O_04
Meth_03	Team project: critical analysis, synthesis and conclusions; individual and teamwork, communicate on specialist topics, leading a debate.	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of Hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory	24	course work	MS_O_03 MS_O_04	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

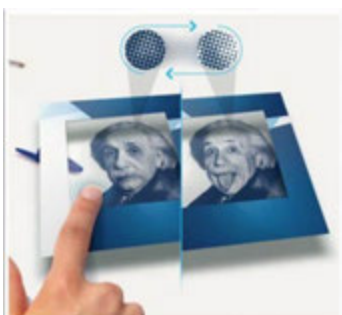
By the end of the *New Electrochromic Materials and Devices* course, students will gain an understanding of the theoretical basis for the electro-optical transformation in electrochromic materials. Students will be able to provide methods of production of thin films and model devices with electrochromic layers and their application for flexible displays, smart windows, car mirrors, etc., establish the voltage–optical spectrum–color connection for a purposeful change in the optical transition and material color in model electrochromic devices under external electric field action.

COMMENTS

LECTURER

DO YOU KNOW

Our most promising visions of a clean-powered future typically position cheap, abundant solar energy as an important cornerstone. Solar panels would be a lot cheaper and abundant if they were made from plastic instead of silicon – that way, they could be 'printed' in a flexible material and easily applied to walls, windows, you name it.



COURSE CONTENT - LECTURE

Topics 1

Introduction. Actual state of organic electronics

During the lecture, as an introduction to the subject *New Electrochromic Materials and Devices*, the current state and the historical development of the ideas about electrochromic materials and devices will be presented. Electrochromic phenomena as changes in the optical properties of a substance under an applied electric field. Works of Deb, Plath, Effects of Stark, Kerr, Faraday. (2 hours)

Topics 2

Methods of synthesis and production of electrochromic materials

The lecture will present the types of electrochromic materials, and their chemical and electronic structure; Methods of electrochromic materials synthesis and production and the methods for the formation of thin electrochromic layers on the conductive transparent surfaces: electrochemical polymerization, spin coating, dip coating, layer-by-layer assembling, Langmuir-Blodgett films, magnetron sputtering, thermo-vacuum deposition, 3D printing. (2 hours)

Topics 3

Optical properties and doping of electrochromic materials

During the lecture, students will learn about the optical properties of electrochromic materials; Classification of optical phenomena; Doping mechanism of electrochromic materials and its connection with color change; Donor and acceptor doping using chemical factors; Proton doping; Electrochemical doping; Effect of doping on the optical spectra of electrochromic films (2 hours)

Topics 4

Characterization of electrochromic systems and devices

The lecture will present main properties and characteristics of electrochromic systems; Architecture of electrochromic devices with light transmission, light absorption; light reflection and dual devices, microencapsulated electrophoretic displays; Determination of electrochromic efficiency, contrast ratio, time of quick action, switching voltage, parameters of charge transport, diffusion coefficient, carrier transition time in the electrochromic film. (2 hours)

Topics 5

Main classes of electrochromic materials

The lecture will present features of the main classes of electrochromic materials; Inorganic and organic electrochromes; Polypyridine complexes of transition metals; Viologens; Metal coordination complexes and metal phthalocyanines; Redox dyes; Liquid crystals Conductive conjugated polymers; Polymer electrolytes. (2 hours)

LEARNING OUTCOMES

Student will be able to prepare a report containing a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

DO YOU KNOW

The smart polymer coating can change color in response to external influences - color indication and sensitivity, for example, to pressure. The main components of the system are several layers of microstructured polysilane, which works as a pressure sensor, and a layer of electrochromic polymer changing color under voltage.



Electrochromic displays- RISE printer electronics
<https://www.bing.com/images/search?q=electrochromic+display&id>

Topics 6

Investigation of the structure and properties of electrochromic materials

The lecture will present the methods of investigation of the structure and properties of the electrochromic materials in a thin layer; Methods of structure research: IR, UV, NMR spectroscopy, transmissive and scanning electron microscopy, atom force microscopy, X-ray phase analysis; and electrochemical research -cyclic voltammetry, spectroelectrochemical experiments, impedance spectroscopy, connection between structure, electronic and optical properties of electrochromic materials. (2 hours)

Topics 7

Applications of electrochromic materials and devices

The lecture will present the applications of electrochromic materials; Structure and types of electrochromic cells; Non-radiation displays; Smart windows; Mirrors with controlled reflection; Light energy converters; Electronic books; children toys, articles in supermarkets, boards, flexible screens, mobile phone displays, adaptive camouflage. Color diagram and specification of color. (2 hours)

Topics 8

Nanotechnologies for improving electrochromic materials and devices

During the lecture, students will learn about nanotechnological approaches to improve the characteristics of optoelectronic devices; Basic principles of nanotechnologies; Nanofabrication of hybrid electrochromic layers, formation of composites of electrochromic compounds in flexible polymer matrices; Copolymerization; Doping of electrochromic materials by metallocomplex, carbon and oxide nanoclusters; Prospects for the development of the electrochromic materials and devices. (2 hours)

COURSE CONTENT – LABORATORY CLASSES

Topics 1

Electrochemical synthesis of conjugated polymers

Students will perform electrochemical synthesis of electrochromic materials based on 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. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

Topics 2

Formation of electrochromic “layer by layer” assembling technique

Students will perform the fabrication of electrochromic layers from PEDOT-PSS dispersion on the transparent conductive surface by self-assembling “layer by layer”, determine the thickness and morphology of the obtained films, measure the optical spectrum of the film in

LEARNING OUTCOMES

Student will be able to plan and carry out experiments, interpret the results and draw conclusions regarding the application of electrochromic materials.

COMMENTS

INSTRUCTOR

transmission and absorption modes. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

Topics 3

Electrochemical doping of electrochromic layers

Students will perform electrochemical doping of electrochromic layer based of conjugated polymers and determine the charge transfer parameters in obtained thin films – effective diffusion coefficient and speed of response. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

Topics 4

Spectroelectrochemical study of the electrochromic material

The topic of the laboratory classes is 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. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

Topics 5

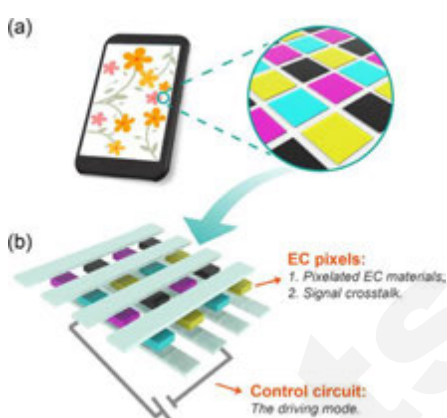
Optical properties of electrochromic polymers

During the classes, 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 build the calibration curves based on the changes in optical density and shifts in the position of the absorption maximum under applied voltage. The completed experiment will be the basis for developing a report on the exercises. (4 hours)

Topics 6

Design and characterization of electrochromic cell

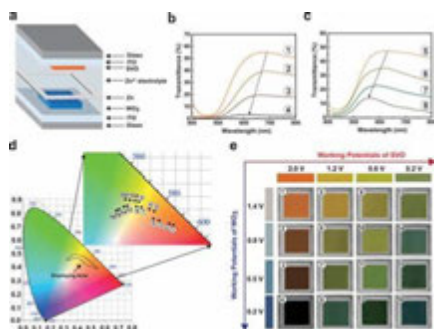
The topics of the laboratory classes are related to the design of electrochromic cells in two-electrode mode with conjugated polymer layer and gel electrolyte between transparent ITO plates. Students will study the effect of applied potential on color change in electrochromic cells and determine switching potential and coloration-discoloration conditions. The completed experiment will be the basis for developing a report on the exercises (4 hours)



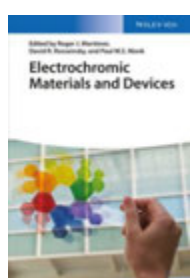
<https://doi.org/10.1021/acs.chemrev.1c01055>



<https://www.bing.com/images/search?q=Plasma+Display&form=R5FD2&first=1>



Electronic "chameleon skin"
<https://doi.org/10.1038/ncomms9011>



TEXTBOOK/READINGS

The mandatory reading for completing the subject *New Electrochromic Materials and Devices*:

1. *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>
2. *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>.
3. *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>

To deepen the course topics, optional recommended texts include articles in journals: *Progress in Materials Science*, *Nature Materials*, *Advanced Materials*, *Progress in Polymer Science*, *Nanoscale Research Letters*, *Materials Today*, *Applied Electronic Materials*, *Molecular Crystals and Liquid Crystals*, etc.

ASSESSMENT

Reports:

The reports relate to experimental laboratory exercises; contribute to deepening theoretical and practical knowledge in the field of electrochromic materials. The reports contain theoretical background, description of performed experiments and analyses, together with discussion and conclusions.

Team project (during the semester):

Team project verifying knowledge of issues in the field of electrochromic materials and ability to team work.

Exam (after the semester):

The oral exam verifying overall knowledge in the field of electrochromic materials and devices.

GRADING POLICY

The *New Electrochromic Materials and Devices* course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted reports (max. 5 points, i.e. 6 reports x 5 points = 30 points are assessed), Team project (1 x 10 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be

Assignment Weights	Percent
6 Reports	30%
Team project	10%
Debata	10%
Exam	50%
Total	100%

6 reports (max. 5 points each) – max. 30 points
 Team project – max. 10 points
 Debata – 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
0 - 60 points	= F

obtained in the exam is 50. Student grades will be assessed as follows in the box on the left.

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

CREATING A STARTUP

Code: **CS RD2-003**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

3

Language

English

Thematic block

*Research & Development in
Material Science and Engineering
part 2*

Form of tuition and number of hours*:

Lectures: 16h

Practical classes: 16h

ECTS

4

Lecturer:

Grygoriy Dmytriv, DSc, Prof.

COURSE DESCRIPTION

During the course students will have lectures with next practical lessons which cover step by step all aspects of creating of startups. First, we will learn to analyze startup idea for success, the next what we will learn is how to find target audience for product of startup and target market (elements of marketing). The next big block will focus on sources of financing startups: friends&family, venture capital, business angels, business incubators, grant funding, bank loans, crowdfunding and how universities can help with it on the example of the Scientific Park. Also, we will analyze types of business models to find a way to creating own business model and its layout. After creation of business model, the most important to manage startup and we will focus on the creating of a team and leadership skills. Finally, we will learn how to present a startup for investors. During course will be invited professional practitioners from the world of startups and persons who have experience in creating own startups.

COURSE OBJECTIVES

At the end of course students will be able to participate in start-up team, or in case of enough knowledge and leadership skills and to create own start-up. Also, students will be known how to present start-up to the public and raise a funding.

PREREQUISITES FOR TAKING THE COURSE

Basic knowledge from economic disciplines (previous bachelor educational program) and material science.



Lviv Startup Fest

LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	Students will have knowledge necessary to understand the ethical, economic and ecological aspects of the design of new engineering materials and their production technology and the impact of the development of materials engineering on the sustainable development and progress of civilization and will know and understand the basic concepts and principles of intellectual and industrial property protection as well as copyright and patent law.
MS_O_02	Students will have extensive knowledge of the basics of entrepreneurship and management, including intellectual property resource management and engineering materials quality management and will know the basic processes occurring in the life cycle of devices, facilities and technical systems used in materials engineering
MS_O_03	Students will use information from literature, databases and other available sources, will be able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems and will can solve practical engineering tasks that require the use of engineering standards and norms.
MS_O_04	Students will aware and know the possibilities of further training and improving professional, personal and social competences and understand the need for an interdisciplinary approach to solving problems and the need for a comprehensive, scientific analysis of problems in the field of materials engineering.
MS_O_05	Students will aware of the responsibility for his own work and taking responsibility for the tasks carried out in the team and able to lead a team and follow the rules of teamwork.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	A collection of knowledge assimilation / teaching methods	informative lecture
Meth_02	A set of practical methods	practice

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	course work	MS_O_01-05	Meth_01
FT_02	practical classes	16	project	MS_O_01-05	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Preparation for classes	Query of materials and review of activities necessary to participate in classes	NO

LEARNING OUTCOMES

By the end of the course "Creating a startup" students:

- will be able to generate an idea for their own startup and test it for viability using various methods;
- will be able to determine the target audience for a startup, create its portrait, and segment it using various methods;
- will 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;
- 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

DO YOU KNOW

Some startups become big, and they become unicorns, i.e. privately held startup companies valued at over US\$1 billion. The term was coined in 2013 by venture capitalist Aileen Lee, choosing the mythical animal to represent the statistical rarity of such successful ventures. According to TechCrunch, there were 452 unicorns as of May 2019, and most of the unicorns are in the US, followed by China. The largest unicorns included Ant Financial, ByteDance, DiDi, Uber, Xiaomi, and Airbnb.



Startup Lviv Hydrogene – winner of Lviv Startup Fest 2023 (spring edition)

COURSE CONTENT - LECTURES

Topics 1

First step to startups is an idea.

During the lecture, students should understand that in order to start a successful search for an idea for a startup, a combination of two components is necessary: internal motivation and research of market needs and market environment.

Topics 2

Target audience of startup

At the lecture, we will determine the main value of the target audience, namely, that the representatives of the selected group will probably want to buy a certain product created by the startup.

Topics 3

Startup marketing

During the lecture, the main tasks of startup marketing will be considered: researching the opinion of a potential client, creating a better value proposition and bringing the product to the market.

Topics 4

Startup and social networks

During the lecture, the general concept of digital marketing (the use of all possible forms of digital channels for brand promotion) will first be considered, and the main focus will be on social networks.

Topics 5

Startup funding

Various sources of funding will be considered: personal investment, F&F, venture capital, business angels, business incubators, grant funding, bank loans, crowdfunding.

Topics 6

Startup business model

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 works, makes money and how it intends to achieve its goals.

Topics 7

Startup leader and team

The lecture will show that a successful startup requires a strong leader who must put in a lot of effort to succeed, but it will also show that no matter what idea you have, the fate of your startup depends on your team.

Topics 8

Startup presentation

The lecture will cover recommendations for creating a successful startup presentation, as well as the secrets of pitch preparation.

LEARNING OUTCOMES

By the end of the course "Creating a startup" student:

- 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;
- 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;
- 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;
- 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.

DO YOU KNOW

The formal concept of business incubation began in the US in 1959 when Joseph L. Mancuso opened the Batavia Industrial Center in a Batavia, New York, warehouse. Incubation expanded in the U.S. in the 1980s and spread to the UK and Europe through various related forms (e.g. innovation centers, pépinières d'entreprises, technopoles/science parks). Ihub Science Park, Lviv University was founded in 2022.



Nazar Pavlyuk with start-up Lviv Hydrogen on the deep-tech business summit NORDEEP (Finland)

COURSE CONTENT - PRACTICAL CLASSES

Topics 1

Discussion of a startup idea.

During practical classes students will propose their own ideas for startups and discuss them in small groups to choose the most perspective and finally will be chosen the best from it according to market needs and market environment.

Topics 2

Search for the target audience of a startup.

During practical classes students will analyze which target audience is most appropriate for the startup which was chosen in the previous practical class and which main values of this audience.

Topics 3

Analysis of startup marketing

During practical classes students will analyze the target market for the startup which was chosen in the previous practical class define competitors and discuss steps of bringing the product to the market.

Topics 4

Creating of startup site in social networks

During practical classes students will create a site of their startup in the different social media (Facebook, Instagram, Twitter, Pinterest, LinkedIn, Snapchat).

Topics 5

Finding startup funding

During practical classes students will analyze different sources of their startup to choose a few of the most appropriate for it and propose ways for support by Science Park.

Topics 6

Creation of a startup business model

During practical classes students will create a business model of a startup by filling in all fields of canvas from <https://www.strategyzer.com/>

Topics 7

Creating of startup team and looking for a leader

During practical classes students will discuss about roles of all members of the startup team and their motivation for participation in it; finally, the leader of a startup will be chosen.

Topics 8

Startup presentation

During practical sessions, students will create a startup presentation and discuss all possible mistakes to avoid, as well as prepare a startup pitch.



Startup FESURFACE INNOVATION received 2nd price Lviv Startup Fest 2023 (winter edition)

TEXTBOOK/READINGS

1. Katernyak I, "Innovation Spring in Tech Startup: momentum to take off". Lviv: Publ. house of the Lviv University, 2021. – 172 p.
2. Mullins J. "The New Business Road Test". Pearson Education Ltd, 2010. – 337 p.
3. Katernyak, 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>

ASSESSMENT

During practical classes students had different tasks:

Task 1. Presentation of Startup idea: Students teams will present their own startup on the base 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 startup must be described.

Task 2. Presentation of results of Startup marketing investigation: Students teams will demonstrate by MS PowerPoint the results of the analysis of the target audience and target market for future startup and on the basis of received data predict steps of bringing the product to the market.

Task 3. Creating of startup site in social network: Students teams will create a startup site on one of the social media (for example Facebook, or any other) with advertising of the startup to cover the target audience and target established in the previous task.

Task 4. Presentation of financial sources of startup funding: Students teams will demonstrate by MS PowerPoint chart with an explanation of possibilities of involvement of all types of funding with comments on how each type of funding is appropriate to startup.

Task 5. Presentation of canvas of the business model of a startup: Students teams will demonstrate a business model of startup using a canvas template from <https://www.strategyzer.com>

Final Task. Startup presentation: Students teams will present their own startup in pitch format on the base of presentation in the format of MS PowerPoint which must be sent for assessment 3 days ahead of "pitching day".

GRADING POLICY

The *Creating a Startup* course is scored with points. All points will be collected during the semester after the completion of each of Tasks 1-5 and the Final Task. All completion will be expected during practical classes including Final Task at the end of the course. After completion of all Tasks 1-5 each student can receive max. 10 points per task. After completion of the Final task each student can receive max. 50 points (40 points for startup presentation in the format of MS PowerPoint and 10 points for pitching of startup).

Assignment Weights	Percent
Tasks 1-5	50%
Final task	50%
Total	100%

Tasks 1-5 – max 10 points
Final task – max 50 points
Total Points – max 100 points

Grading Scale

90% - 100% = A
81% - 89% = B
71% - 80% = C
61% - 70% = D
51% - 60% = E
0% - 50% = F

COURSE SCHEDULE?

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

ADVANCED FUNCTIONAL MATERIALS

Code: **AFM**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Advanced Engineering Materials

Form of tuition and number of hours*:

Lecture: 30h

Laboratory: 30h

ECTS

4

COURSE DESCRIPTION

The course is designed to explore characteristic properties of classical and modern functional materials to master's students based on theoretical concepts, to outline their areas and fields of applications and ways to optimize properties, to acquaint with recent methods of synthesis of organic and inorganic compounds with the purpose of their further application as functional materials.

The *Advanced Functional Materials* course, dedicated to the *AIEMPS – Advances in Innovative Engineering Materials and Processes for Sustainability* path, is designed to form a specialist who not only possesses a certain system of knowledge, abilities and skills, but also knows how to think independently, analyze, derive, qualitatively and quantitatively interpret the properties of composite, powder, superhard and magnetic materials, heat-resistant and amorphous alloys, compounds with various types of conductivity and nanomaterials, predict the influence of external factors on the properties of these materials, optimize methods of their synthesis.

Lectures are aimed at providing information on advanced functional materials, methods of their production, properties and applications. Laboratory exercises are intended for individual student work, independent performance of experiments and independent analysis leading to individual elaboration of the obtained results in the form of a report along with relevant studies and conclusions.

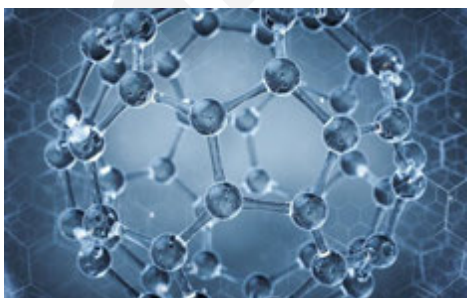
COURSE OBJECTIVES

The purpose of the *Advanced Functional Materials* course is the formation of ideas about functional materials based on inorganic and organic compounds that are used in various fields of industry, technology and everyday life and have prospects for use in the future.

Tasks of the *Advanced Functional Materials* course is the development of students' skills, mostly for understanding the principles of functioning of materials and the theoretical basis of their development.

PREREQUISITES FOR TAKING THE COURSE

Before starting the study of subject *Advanced Functional Materials*, a student should have a general knowledge of the various types of engineering materials, their structure, properties and applications.



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LEARNING OUTCOMES OF THE MODULE

Code module	Description
AF_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of advanced engineering materials.
AF_O_02	He has extensive and in-depth substantive knowledge in the field of methods, processes of production of advanced engineering materials
AF_O_03	Can use information from literature and other available sources, integrate the obtained information, interpret, and critically evaluate it, draw conclusions, and formulate and solve complex problems related to the production and use of advanced engineering materials.
AF_O_04	He is able to select the appropriate raw materials, technologies and techniques for the production, processing and testing of engineering materials. He can select and apply appropriate methods and tools, including advanced information and communication techniques.
AF_O_05	Can prepare a scientific paper and a presentation on the properties and use of advanced engineering materials, including critical analysis, synthesis, and conclusions. Able to work individually and in a team, and lead a debate.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	AF_O_01 AF_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; seminar; debate	AF_O_03 AF_O_04
Meth_03	Individual and Team projects: critical analysis, synthesis and conclusions; individual and team work, communicate on specialist topics, leading a debate, presentations	AF_O_03 AF_O_04 AF_O_05

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	30	exam	AF_O_01 AF_O_02	Meth_01
FT_02	laboratory	30	course work	AF_O_03 AF_O_04 AF_O_05	Meth_02 Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of presentations and reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

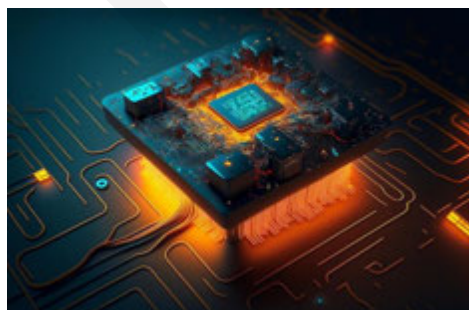
LEARNING OUTCOMES

By the end of the *Advanced Functional Materials* course, the student will be able to characterize different types of materials, provide methods of producing modern functional materials and their application; design new materials with the expected structure and properties for modern materials engineering.

COMMENTS

LECTURER

DO YOU KNOW



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COURSE CONTENT - LECTURE

Topics 1

Classification of inorganic compounds for practical use

During the lecture, as an introduction to the issue of advanced functional materials, the basic knowledge on the classification of inorganic compounds for practical use and basic definitions and types of composite materials will be presented. Metal and ceramic composite materials, cermets.

Topics 2

Constructive functional alloy-based materials

Heat-resistant alloys. Superalloys and intermetallics. Heat-resistant and highly resistant aluminum alloys. Constructive steels and alloys of increased reliability. Armored steel. Structural alloys for nuclear energy. Heat-resistant and corrosion-resistant alloys. Amorphous materials.

Topics 3

Powder ceramic materials. Superhard materials

Methods of synthesis and main characteristics of powder materials. Superhard materials based on diamond and boron nitride.

Topics 4

Conducting materials. Materials for electronics

Classification of conductors. Basic industrial conducting materials. Superconducting materials, their classification, main characteristics and areas of application. Characteristics of the superconducting state. HTSC. Synthesis of superconducting materials. Classic and modern semiconducting materials. Thin film materials. Solar energy materials. The main types of industrial insulators.

Topics 5

Magnetic materials

Magnetically hard and magnetically soft materials. Ferrites, garnets. Magnetostrictive materials.

Topics 6

Advanced nanocrystalline materials

Nanopowders – production and properties. Volumetric nanostructured materials. Nanofibers, nanowires and nanotubes. Fullerenes. Graphene.

LEARNING OUTCOMES

Student will be able to prepare a report and presentation with a critical analysis, synthesis and conclusions. He will be able to work individually and in a team as well as communicate on specialist topics, including leading a debate.

COMMENTS

INSTRUCTOR

DO YOU KNOW



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COURSE CONTENT –LABORATORY CLASSES

Topics 1

Composite materials

The topics of the laboratory classes are related to the main methods of fabrication of the metal and ceramic composite materials, their classification and application. Students working in groups will carry out a Team Projects.

Topics 2

Advanced alloy-based materials

The main topics of manufacturing and application of functional aluminum and copper-based alloy materials, frictional and antifrictional materials, intermetallic compounds, and amorphous alloys will be analyzed and discussed. During laboratory classes, students will analyse and choose the methods of synthesis of alloys, perform arc-melting and induction-melting synthesis. In order to carry out the phase and structural analyses of the synthesized alloys, the student will use energy dispersive X-ray spectroscopy and X-ray powder diffraction. The completed experiments will be the basis for developing of the reports.

Topics 3

Superhard materials and powder ceramic materials

The topics of the laboratory classes are related to the types and application of the advanced superhard materials, including engineering materials based on diamond and different polymorphs of boron nitride, methods of synthesis and main characteristics of powder ceramic materials. Students working in groups carry out an Individual and Team Projects.

Topics 4

Conductive, superconductive and semiconductor materials

The topics of the laboratory classes are related to the different types of the conducting materials, their fabrication and application in modern electronics and solar energy devices. Students working in groups will carry out an Individual Projects.

Topics 5

Advanced magnetic materials

The main topics of manufacturing and application of magnetically hard and magnetically soft materials, ferrites, garnets and magnetostrictive materials will be analyzed and discussed. Students carry out an Individual projects.

Topics 6

Application of nanomaterials

During laboratory classes, students will discuss the production methods and properties of nanopowders and volumetric nanostructured materials, nanofibers, nanowires, and nanotubes. During the classes, students will have the task of leading a debate on the topic “Nanostructuring as an instrument for the improvement of the required properties of advanced engineering materials”. Data from the lectures and self-prepared information with provided examples will be the substantive basis for conducting the debate.



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TEXTBOOK/READINGS

The mandatory reading for completing the subject *Advanced Functional Materials*:

1. A.R. West. *Solid State Chemistry and its Application*, 2nd Ed., Student Edition, Wiley, 2014.
2. *Intermetallic Compounds*. Eds. J.H. Westbrook, R.L. Fleischer, Vol. 1,2, Chichester: John Wiley & Sons, 1993. – 754 p.

To deepen the course topics, optional reading includes scientific journals:

1. *Advanced Materials*.
2. *Materials Letters*.
3. *Chemistry of Metals and Alloys*.
4. *Chemistry of Materials*.
5. *Journal of Material Chemistry*.
6. *Materials Research Letters*.

ASSESSMENT

Reports:

The reports relate to experimental laboratory exercises; contribute to deepening theoretical and practical knowledge in the field of advanced functional materials. The reports contain theoretical background, description of performed experiments and analyses, together with discussion and conclusions.

Individual projects:

Individual project is prepared in a form of presentation on a preset subject in the field of advanced functional materials.

Team projects:

Team project verifying knowledge of issues in the field of advanced functional materials and ability to team work.

Exam (after the semester):

The oral exam verifying overall knowledge in the field of advanced functional materials.

GRADING POLICY

The *Advanced Functional Materials* course is scored with points. The grade results from the sum of points obtained by the student during the semester (laboratory exercises) and points obtained during the exam. During laboratory exercises, the following are assessed on an ongoing basis: theoretical preparation (discussion at the beginning of laboratory exercises as an introduction to conducting the experiment and preparing the report), submitted and defended reports (max. 5 points, i.e. 3 reports x 5 points = 15 points are assessed), Individual projects (3 x 5 pts = 15 pts), Team project (2 x 5 pts = 10 pts) and Debate (1 x 10 points). The maximum number of points obtained in the laboratory exercises is 50. The exam is conducted in an oral form - 3 questions from the previously given range of topics are to be selected. The maximum number of points to be obtained in the exam is 50. Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
3 Reports	15%
Individual projects	15%
Team projects	10%
Debate	10%
Exam	50%
Total	100%

3 reports (max. 5 points each) – max. 15 points
 3 individual projects (max. 5 points each) – max. 15 points
 2 team projects (max. 5 points each) – max. 10 points
 Debate – 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
 0 - 60 points = F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

CRYSTAL CHEMISTRY (RELATIONSHIP COMPOSITION– STRUCTURE–PROPERTIES)

Code: CC(RCSP)

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Fundamental Aspects of Materials Science

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS 4

Lecturers:

Prof. Roman Gladyshevskii

Assoc. Prof. Svitlana Pukas

COURSE DESCRIPTION

The aim and task of the course *Crystal Chemistry (Relationship Composition–Structure–Properties)* in the master's study is to acquire practical skills for future specialists in the field of modern crystal chemistry – a science that plays a special role in the process of developing functional materials. In the content of the course *Crystal Chemistry (Relationship Composition–Structure–Properties)*, emphasis is placed on the directions of using solid inorganic compounds as materials for new techniques and technologies.

The lecture course consists of three main parts: ideal and real structures, modern methods of crystal structure research, and physical properties of certain classes of compounds. Precise determination of the crystal structure, calculation of the electronic structure and characteristics of the chemical bond, measurement of properties, and controlled change in the concentration of valence electrons are a prerequisite for synthesizing new phases that will be the basis of materials for practical use.

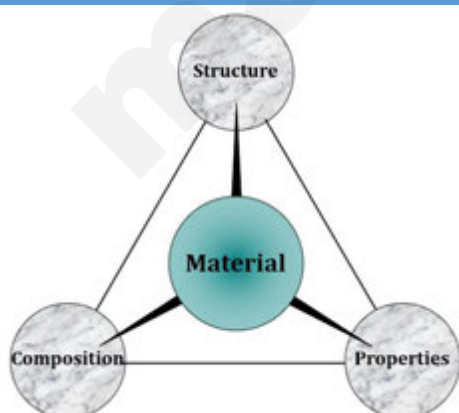
Laboratory classes are devoted to determining the structural and microstructural characteristics of compounds, construction of real modulated and hypothetical structures, analysis of diffraction data of polycrystalline samples using professional programs, establishment of structural affinity, the influence of crystal structure on the properties of compounds, composition-structure-properties relationship. The course is an important element in the formation of specialists not only in the field of chemistry but also in scientists in general.

COURSE OBJECTIVES

The course *Crystal Chemistry (Relationship Composition–Structure–Properties)* is designed in such a way as to provide students with the necessary knowledge and develop skills with the aim of revealing their own scientific potential. By the end of the course, students will gain an understanding of the real crystal structure, the causes of defects in crystals, X-ray diffraction methods on mono- and polycrystals, algorithms for the development of functional materials and will be able to determine structural and microstructural characteristics of compounds, derive magnetic symmetry groups, build hypothetical structures.

PREREQUISITES FOR TAKING THE COURSE

To complete the course, it is recommended that learning outcomes related to the basics of chemistry, physics, and materials science be implemented.



LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials.
MS_O_02	Has in-depth, theoretically based, and structured knowledge of modern techniques and research methods used in materials engineering.
MS_O_03	Can plan and carry out experiments, including measurements and computer simulations, interpret the results, and draw conclusions.
MS_O_04	Can prepare a scientific study and present a presentation on implementing a research task, containing a critical analysis, synthesis, and conclusions.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: interactive lectures with scientific discussion, lectures with multimedia support and the use of visual models of crystal polyhedra and structures, lectures with problem interpretation	MS_O_01 MS_O_02
Meth_02	Laboratory classes: laboratory work (individual and group tasks), experiment demonstrations, observation, problem learning, debate	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory	32	course work	MS_O_03 MS_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

Student has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials. Also she/he has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials science.

By the end of the Crystal Chemistry (Relationship Composition–Structure–Properties) course student will have extensive and in-depth knowledge about:

the real structure of a solid state,

the causes of defects in crystals,

the group-subgroup relationship between space groups,

modern trends in the development of structural analysis,

X-ray diffraction methods on mono- and polycrystals,

the relationship between the chemical composition, crystal structure and physical properties of compounds.

DO YOU KNOW

The physical properties of crystals are determined by their composition, the geometry of the crystal structure, and the type of chemical bond in them. The main properties of crystals are homogeneity, anisotropy, and the ability to self-edge.



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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, symmetry operations, Bravais lattices, and space groups, and get an idea of ideal, real, and average structures. The causes of structural defects will be discussed. Students will also learn about the liquids and amorphous substances. *2 hours.*

Topic 2

Defects in crystals

The lecture will discuss the influence of local changes on the formation of related ordered structures and the appearance of some defects in real crystals. In addition, students will be familiar with different kinds of defects: point defects, clusters of defects, antistructural defects, linear and planar defects. Students will be introduced to such concepts as nonstoichiometry, solid solutions, and superstructures. *2 hours.*

Topic 3

Group-subgroup relationships between space groups

The lecture will be devoted to phase transitions and the parameters that change during them. Students will be introduced to group-subgroup relationships between space groups and learn about a genealogical tree called Bärnighausen. Non-commensurate modulated and composite structures and quasicrystals will be shown. *2 hours.*

Topic 4

Modern trends in the development of structural analysis

This lecture will focus on determining defects and microstructure by diffraction methods. Analysis of the profile of diffraction peaks will be performed. Modern methods of X-ray diffraction on mono- and polycrystals and research at extreme temperatures and pressures will be discussed. *2 hours.*

Topic 5

X-ray, neutron, and electron diffraction analysis

Synchrotron diffraction, possibilities of neutron and electron diffraction, and methods of studying thin films will be discussed during the lecture. *2 hours.*

Topic 6

Material creation algorithm

The lecture will discuss the relationship between chemical composition, crystal structure and physical properties of compounds as a basis for materials development. During the lecture, students will be familiarized with Neumann principle and magnetic symmetry. *2 hours.*

LEARNING OUTCOMES

Students can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions. Also, she/he can prepare a scientific study and present a presentation on the implementation of a research task, containing a critical analysis, synthesis and conclusions.

By the end of the Crystal Chemistry (Relationship Composition–Structure–Properties) course student will be able to:

determine structural and microstructural characteristics of compounds using modern crystallographic computer programs,

carry out the description of the crystal structure,

establish the relationship between the structures,

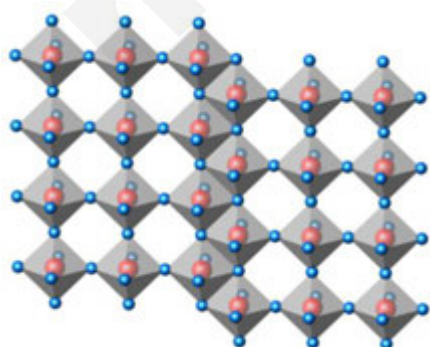
find homoatomic structural fragments based on the calculation of valence electron concentration,

derive magnetic symmetry groups,

build hypothetical structures.

DO YOU KNOW

In 2016 David J. Thouless, F. Duncan M. Haldane, and J. Michael Kosterlitz won the Nobel Prize in Physics for using topological concepts in theoretical condensed matter physics. They pioneered a new understanding of phase transitions through research on topological insulators, superconductors, and other materials.



Crystallographic shift in the structure of WO_3

Topic 7

Semiconductors and superconductors

The lecture will be devoted to semiconductors and their characteristics, particularly the band gap and the concentration of valence electrons. Students will also learn about superconductivity, the Meissner effect, and classical and high-temperature superconductors. *2 hours.*

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 such properties of substances as thermal expansion, elasticity, cleavage, pyroelectric effect, piezoelectric effect, refractive indices, and optical activity. Moreover, it will be shown that all these properties depend on the peculiarities of the crystal structure of the substance. *2 hours.*

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. *4 hours.*

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. *4 hours.*

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. *4 hours.*

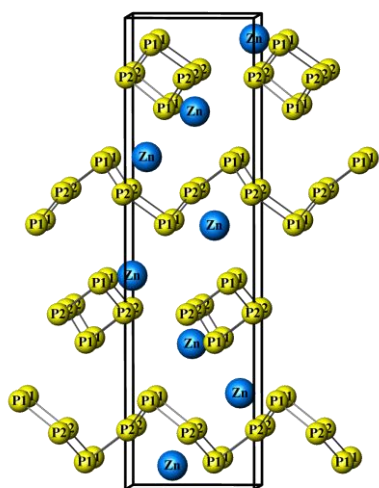
Topic 4

Modulated structures

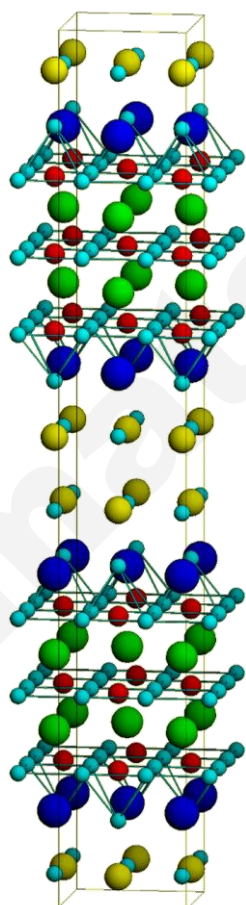
The laboratory aims to derive the crystal structure of the compound $\text{Er}_3\text{Si}_{5-x}$ using crystallographic transformations, calculate interatomic distances in it, plot the dependence of interatomic distances on superspace coordinate x_4 , and determine in which regions of x_4 Si atoms occupy the crystallographic sites. *4 hours.*

LEARNING OUTCOMES

Students can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions. Also, she/he can prepare a scientific study and present a presentation on the implementation of a research task, containing a critical analysis, synthesis, and conclusions.



ZnP_2 , $\text{VEC}_A = 6$, $n(\text{A-A}) = 2$



$\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$, $T_c = 110 \text{ K}$

Topic 5

Structure refinement

The laboratory aims to refine the crystal structure parameters of the intermetallic compounds: atomic coordinates, displacement parameters, and occupancies. *4 hours.*

Topic 6

Magnetic structure

The laboratory aims to derive magnetic symmetry groups, determine the change in the direction of the atom's spin when applying symmetry elements and the inversion operator, and, as a result, make a conclusion about the magnetic properties of the compound. *4 hours.*

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. *4 hours.*

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. *4 hours.*

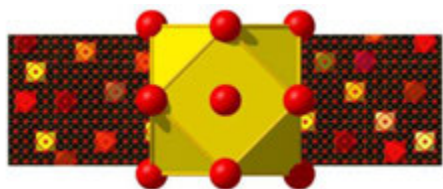
TEXTBOOK/READINGS

The mandatory reading for completing the course *Crystal Chemistry (Relationship Composition–Structure–Properties)*:

1. R.E. Gladyshevskii, S.Ya. Pukas, Applied Crystal Chemistry. Textbook, Publishing Center of Ivan Franko National University of Lviv, Lviv (2022) – 126 p.
2. R.E. Gladyshevskii, Methods to Determine Crystal Structures, Textbook, Publishing Center of Ivan Franko National University of Lviv, Lviv (2015) – 135 p.
3. A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons, Chichester, United Kingdom (1984) – 734 p.
4. P. Villars, K. Cenzual, R. Gladyshevskii, Handbook of Inorganic Substances 2017, Walter de Gruyter, Berlin (2017) – 1955 p.
5. V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.
6. R.L. Snyder, J. Fiala, H.J. Bunge, Eds., Defect and Microstructure Analysis by Diffraction, Oxford University Press, Oxford (1999) – 785 p.

Pearson's Crystal Data[®]

Crystal Structure Database for Inorganic Compounds



INFORMATION RESOURCES:

1. 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).
2. P. Villars, K. Cenzual, Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds, ASM International, Materials Park (OH) (2023).

ASSESSMENT

Reports:

The reports are the result of the student's work during the laboratories; they relate to in-depth theoretical and practical knowledge of the exercises performed. They consist of a theoretical introduction, a description of the purpose, the implementation of an experimental or calculation task, and conclude with a discussion of the obtained results and conclusions.

Tests:

During the semester, the tests reflect the student's current academic performance.

Debate:

During the debate, the ability to make logical arguments and explain their relevance to the topic, the ability to answer the questions of other participants, and the ability to actively listen and participate in the discussion with other participants of the debate will be evaluated.

Exam:

The exam verifies overall theoretical knowledge and practical skills in the field of crystal chemistry and materials science.

GRADING POLICY

The student is obliged to perform the 8 laboratories, 3 tests, and debate, which gives in a maximum of 100 points.

The exam is conducted in a written form – 2 questions from the knowledge contained theory and 4 questions of practical aspects. The maximum number of points to be obtained in the exam is 100.

The final evaluation is made based on the student achievement scoring system. The grade results from the sum of points obtained by the student during the semester by the evaluation of three types of work (laboratory work, test, debate) and points received during the exam. The final grade is determined by 50% of the points obtained in the exam and 50% of the points obtained in the laboratories. According to the table on the left, the sum of the percentages will result in the final grade.

Assignment Weights	Percent
Laboratories:	
8 Reports	40%
3 Tests	45%
Debate	15%
Total	100%
Reports - max. 40 points	
Tests – max. 45 points	
Debate – max. 15 points	
Total points – max. 100 points	
Exam	100%
max. 100 points	
Final grade:	
Laboratories	50%
Exam	50%
Total	100%
Grading Scale:	
90-100 points = A	
80-89 points = B	
70-79 points = C	
60-69 points = D	
51-59 points = E	
0-50 points = F	



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COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

matsci.us.edu.pl

PHASE DIAGRAMS OF MULTICOMPONENT SYSTEMS

Code: **PDMS**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

*Fundamental Aspects of
Materials Science*

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

4

Lecturers:

Oksana Zelinska, PhD, Assoc. Prof.

COURSE DESCRIPTION

The course *Phase Diagrams of Multicomponent Systems* explores the relationships between composition, temperature and pressure in various materials. Through a combination of theoretical concepts and practical applications, students will develop a deep understanding of phase equilibria and phase transitions in multicomponent systems providing a better understanding of the properties of materials.

The course begins by introducing the basis of thermodynamics, main concepts and definitions concerning phase diagrams. It acquaints students with different types of phase diagrams. Students will learn how to analyse and interpret unary, binary, ternary, and quaternary phase diagrams to determine the stability of different phases and understand phase transformations. They will gain insight into the effects of temperature, pressure, and composition on phase transitions and learn how to predict and interpret them. Students will comprehend the basic principles of constructing phase diagrams of multicomponent systems, and their isothermal and polythermal sections based on experimental data.

Practical applications of phase diagrams in materials science and engineering will be highlighted, including their role in the design and optimization of alloys, ceramics, etc. Additionally, the course will delve into case studies and real-world examples to demonstrate how phase diagrams can be used to control and manipulate material properties. Throughout the course, students will engage in hands-on activities, such as laboratory experiments, work with databases and special software, to reinforce their understanding of phase diagrams. Collaborative projects and discussions will also encourage critical thinking and problem-solving skills.

COURSE OBJECTIVES

After completing the course students will gain a comprehensive understanding of phase equilibria in multicomponent systems. They will be able to analyse and interpret phase diagrams to predict phase transformations and stability of phases, design and optimize materials by controlling phase compositions, and apply knowledge of phase diagrams to solve real-world materials science and engineering problems demonstrating critical thinking and problem-solving skills.

PREREQUISITES FOR TAKING THE COURSE

Prerequisites for taking the course include a basic knowledge of chemistry, physics and materials science. Understanding the correlation between the nature of chemical bonding, crystal structure, physical and chemical properties of solids may be helpful.

Select a proper graphic

LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of engineering materials.
MS_O_02	Has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.
MS_O_03	Can use information from literature, databases and other available sources. Able to integrate the obtained information, interpret and critically evaluate it, draw conclusions, and formulate and solve complex innovative problems.
MS_O_04	Can formulate and test hypotheses related to simple research and implementation problems. Can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.
MS_O_05	Able to select the appropriate raw materials, technologies and techniques for the production, processing and testing of engineering materials. Can select and apply appropriate methods and tools, including advanced information and communication techniques.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: multimedia lecture, interactive lecture, problem-based lecture	MS_O_01 MS_O_02
Meth_02	Laboratory exercises: laboratory work, demonstration, observation, problem learning, a case study, individual and team work, brainstorming, work with experimental data, databases, diagram models and computer programs	MS_O_03 MS_O_04 MS_O_05

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory classes	32	quizzes, reports, tests, debates	MS_O_03 MS_O_04 MS_O_05	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Review of the literature necessary for preparation for classes	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes	NO
a_03	Preparation of reports	Preparation and accomplishment of reports. Teaching consultation	YES

LEARNING OUTCOMES

By the end of the course students

- will know the basis of thermodynamics, main concepts and definitions concerning phase diagrams;
- will comprehend the classification of phase diagrams by the number of components and by variability;
- will analyse and interpret different types of phase diagrams;
- will build the cooling curves of the samples;
- will apply the lever rule and the rule of triangles to determine the phase compositions of the samples;
- will calculate the mass of the starting components and choose the conditions necessary for the synthesis of samples;
- will construct the phase diagrams of unary and binary systems, the isothermal and polythermal sections of ternary systems, perform triangulation of ternary and tetrahedration of quaternary systems;
- will apply thermodynamic principles and experimental methods to determine the phase equilibria in multicomponent systems;
- will be equipped with the skills to design and optimize materials, such as alloys, ceramics, and polymers, by controlling their phase compositions and properties;
- will analyse and critically evaluate the information from scientific journals and databases, draw conclusions, formulate and solve problems with consideration of phase diagrams;
- will develop the ability to prepare well-structured and clear reports that acquire skills in individual and teamwork, spatial imagination, critical thinking and analytical skills;
- will collaborate effectively to explore and discuss the practical applications of phase diagrams in materials science and engineering.

COMMENTS

INSTRUCTOR

COURSE CONTENT - LECTURE

Topics 1 Introduction to the phase diagrams.

The lecture introduces the fundamental theory applicable to all phase diagrams and some definitions (thermodynamic system, thermodynamic parameters, system components, phase, phase transition etc.). It acquaints students with Gibbs phase rule and condensed phase rule, other principles and rules (Le Chatelier, Van der Waals etc).

Topics 2 Unary phase diagrams.

The lecture acquaints students with single-component systems and their graphical representation in the form of p - T diagrams. The Gibbs phase rule for these systems is presented. The main types of unary phase diagrams such as water and sulphur are described in detail. Allotropy and allotropic modifications are outlined.

Topics 3 Binary phase diagrams.

The lecture acquaints students with binary condensed systems and their geometric representation in temperature-composition coordinates. General regularities of their construction are covered. The phase transformations that occur in these systems during heating and cooling are described.

Topics 4 Topology of binary phase diagrams.

The lecture introduces different types of binary phase diagrams and the relationships between them. The crystallization of alloys and the development of their microstructure are highlighted. The correlation between the type of phase diagram and the properties of alloys is demonstrated.

Topics 5 Ternary phase diagrams.

The lecture introduces students the main regularities and geometric bases of the construction of ternary phase diagrams. Students will get acquainted with the Roozeboom and Gibbs methods of determining the quantitative composition of the three-component samples.

Topics 6 Topology of ternary phase diagrams. Isothermal and polythermal sections.

The lecture presents the classification of ternary phase diagrams and their relationships. Students get acquainted with surfaces, curves and regions of the phase diagram, their projections on a concentration triangle, isothermal and polythermal sections of the phase diagrams and algorithm of their construction. Microstructural components of alloys and their crystallization are described.

Topics 7 Quaternary phase diagrams.

The lecture introduces the basics of constructions and characteristics of the phase diagrams of n -component systems. Students get acquainted with the classification of quaternary phase diagrams, the representation

of the quantitative composition of the samples and the main principles of the polyhydration of multicomponent systems.

Topics 8 Methods of the investigation of phase equilibria in multicomponent systems.

Gibbs phase rule and its application in the construction of phase diagrams of multicomponent systems is covered. Methods of the investigation of phase equilibria, identification of solid solutions and intermediate phases and construction of binary phase diagrams, isothermal and polythermal sections of ternary and quaternary systems are described. Experimental difficulties in studying phase equilibria and typical mistakes during the construction of isothermal and polythermal sections of the phase diagrams are pointed out.

COURSE CONTENT – LABORATORY CLASSES

Topics 1 Phase diagrams of unary systems: analysis and description.

During laboratory classes students will analyse and interpret p - T diagrams of metallic and non-metallic unary systems interesting from the point of view of their application (helium, carbon, iron, SiO_2 , TiO_2 , etc.), characterise phase regions, lines of monovariant equilibria and triple (invariant) points. They will also perform a reverse task - construct an unary phase diagram according to the description.

Topics 2 Binary isomorphous systems: interpretation of the phase diagrams, construction of sample cooling curves.

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 state (isomorphous), determine the phase composition of samples and build cooling curves. 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 solid state and the formation of ordered solid solutions will be carried out.

Topics 3 Phase diagrams of the binary systems with eutectic and peritectic nonvariant equilibria: analysis, description and construction of samples cooling curves.

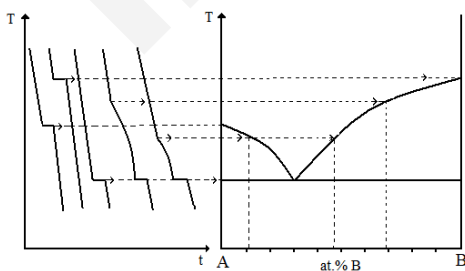
During laboratory classes students will analyse and describe binary phase diagrams with unlimited solubility of components in liquid state and without solubility or with limited solubility in solid state and the presence of eutectic or peritectic reactions. They will determine the phase composition of samples and build cooling curves. The phase diagrams which are interesting from the point of view of their practical use will be considered as an example.

Topics 4 Phase diagrams of binary systems with intermediate phases melting congruently and incongruently: analysis, interpretation and construction of samples cooling curves.

During laboratory classes students will consider and learn to interpret the phase diagrams of binary systems with intermediate phases melting congruently and incongruently with fixed compositions or with broad

DO YOU KNOW

Phase diagrams are powerful tool for understanding the behavior of substances under different pressure and temperature conditions. They provide valuable insights into the various phases of matter and the changes they undergo, helping better understand the physical and chemical properties of materials. They enable scientists to make informed decisions in various fields, including chemistry, materials science, and engineering, to create new materials with specific and functional properties.



Binary phase diagram from the results of thermal analysis

LEARNING OUTCOMES

By the end of the course students

- will know the basis of thermodynamics, main concepts and definitions concerning phase diagrams;
- will comprehend the classification of phase diagrams by the number of components and by variability;
- will analyse and interpret different types of phase diagrams;
- will build the cooling curves of the samples;
- will apply the lever rule and the rule of triangles to determine the phase compositions of the samples;
- will calculate the mass of the starting components and choose the conditions necessary for the synthesis of samples;
- will construct the phase diagrams of unary and binary systems, the isothermal and polythermal sections of ternary systems, perform triangulation of ternary and tetrahedration of quaternary systems;
- will apply thermodynamic principles and experimental methods to determine the phase equilibria in multicomponent systems;
- will be equipped with the skills to design and optimize materials, such as alloys, ceramics, and polymers, by controlling their phase compositions and properties;
- will analyse and critically evaluate the information from scientific journals and databases, draw conclusions, formulate and solve problems with consideration of phase diagrams;
- will develop the ability to prepare well-structured and clear reports that acquire skills in individual and teamwork, spatial imagination, critical thinking and analytical skills;
- will collaborate effectively to explore and discuss the practical applications of phase diagrams in materials science and engineering.

COMMENTS

INSTRUCTOR

homogeneity ranges. They will look at the phase diagrams with intermediate phases forming exclusively from the solid. Determining the phase composition of the samples and constructing their cooling curves will also be the task of the laboratory session.

Topics 5 Phase diagrams of binary systems with polymorphic transformation of intermediate phase: analysis, interpretation and construction of samples cooling curves.

During laboratory classes students will consolidate their knowledge of polymorphic transitions and consider the phase diagrams containing them. They will learn to interpret phase diagrams with polymorphic modifications of intermediate phases, determine the phase composition of samples and build cooling curves.

Topics 6 Phase diagrams of binary systems with allotropic modifications of the initial components: analysis, interpretation and construction of samples cooling curves.

During laboratory classes students will interpret phase diagrams with allotropic modifications of the initial components. They will learn to describe metatectic, eutectoid, peritectoid and monotectoid nonvariant equilibria, and build cooling curves of the samples.

Topics 7 Phase diagrams of binary systems with limited solubility of components in liquid state: analysis, interpretation and construction of sample cooling curves.

During laboratory classes students will analyse and describe phase diagrams with limited solubility of components in liquid state. They will learn to distinguish monotectic and syntectic nonvariant equilibria, determine the phase composition of samples and build their cooling curves.

Topics 8 Construction of the binary phase diagrams based on their description.

During laboratory classes students will learn to construct phase diagrams of the two-component systems based on their description applying the Gibbs phase rule and other thermodynamic principles.

Topics 9 Ternary systems. Exercises with Gibbs-Rooseboom triangle.

During laboratory classes students will determine the quantitative composition of samples in a ternary system by Rooseboom and Gibbs methods. They will calculate the mass of the starting components for the synthesis of three-component samples manually and with special software, e.g. Weight.

Topics 10 Ternary systems with unlimited solubility of components in liquid and solid state or without solubility in solid state.

During laboratory classes students will learn to interpret ternary systems with unlimited solubility of components in liquid and solid state or without solubility in solid state, analyse surfaces, curves and phase regions of the phase diagrams and project them on the concentration

triangles. They will construct isothermal and polythermal sections of the phase diagrams and cooling curves of samples.

Topics 11 Ternary systems with limited solid solutions.

During laboratory classes students will learn to analyse ternary systems with unlimited solubility of components in liquid state and with limited mutual solubility of components in the solid state, distinguish systems with four-phase equilibria of the first, second and third class, describe surfaces, curves and phase regions of the phase diagrams and project them on concentration triangles. They will build isothermal and polythermal sections of the phase diagrams and cooling curves of samples.

Topics 12 Ternary systems with intermediate phases.

During laboratory classes students will learn to interpret three-component systems with the formation of intermediate binary and ternary phases, analyse surfaces, curves and phase regions of the phase diagrams and project them on concentration triangles. They will build isothermal and polythermal sections of the phase diagrams and cooling curves of samples.

Topics 13 Interpretation of the isothermal sections of ternary systems.

During laboratory classes students will analyse the isothermal sections of ternary systems found in databases by describing the mutual solubility of components, the composition and homogeneity ranges of binary compounds and the solubility of the third component in them, characterizing the amount, composition and homogeneity ranges of ternary compounds, two-phase and three-phase equilibria in the systems.

Topics 14 Determination of the composition of samples in quaternary systems, calculation of the weight of components for sample production.

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 and calculating the weight of components for synthesis of the samples.

Topics 15 Polyhedration of quaternary systems.

During laboratory classes students will learn to describe quaternary systems and characterise phase regions and transitions. They will also acquire skills in performing singular tetrahedration of the quaternary system provided by the lecturer, determining its type, calling quasi-binary and quasi-ternary systems, and secondary four-component systems that appear in this case.

Topics 16 Construction of the phase diagrams based on experimental data.

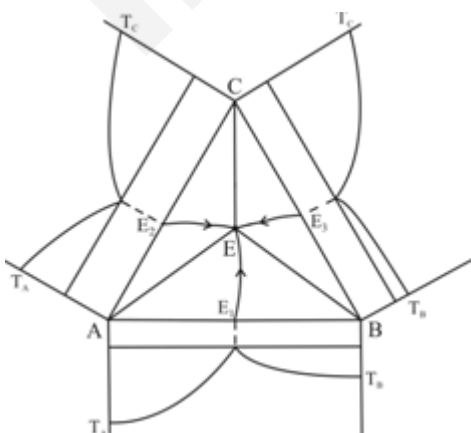
During laboratory classes students will gain an understanding of how experimental methods such as DTA, DSC, TG, XRD, EDX etc. help to investigate phase equilibria in multicomponent systems, identify and characterise intermediate phases. Students will also get acquainted with

DO YOU KNOW

The phase diagram is a graphical representation of substance behaviour under varying conditions of temperature and pressure. It allows to comprehend the transitions between different phases of matter, such as solid, liquid, and gas.

Phase diagrams can have different shapes, such as triangular, rectangular or more complex. The shape of a phase diagram is influenced by the characteristics of the substance and the phase transitions it undergoes.

Although phase diagrams may seem complex, delving into their intricacies can reveal a wealth of fascinating information.



Ternary eutectic phase diagram A-B-C

the methods of calculating and modelling phase equilibria. Based on experimental data students will try to construct a phase diagram of the binary system and an isothermal section of the ternary system.

TEXTBOOK/READINGS

The mandatory reading for completing the course *Phase Diagrams of Multicomponent Systems*:

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.

The optional reading:

1. Brent Fultz, Phase Transitions in Materials. Cambridge University Press, 2014. ISBN 9781108641449.
2. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformation. Their Thermodynamic Basis. Cambridge University Press, 2012. ISBN 9780511812781.

Handbooks and databases:

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.

ASSESSMENT

Quiz:

Students will take a short quiz on the lab topic at the beginning of each lab session to ensure that the relevant lecture and recommended literature have been read beforehand and that they are prepared for the lab.

Report:

At the end of each laboratory session, students should prepare a written report, which is the result of in-depth theoretical and practical knowledge obtained during performed exercises. The report should include a theoretical background, a description of the exercise's purpose and scope, a main part reporting the obtained results, their discussion and conclusions.

Test:

During the semester student will have tests that cover the main aspects of theory and practice related to the phase diagrams and reflect their current performance.

Debate:

The ability to make logical arguments and explain their relevance to the topic, answer the questions of other debaters, listen and participate in the discussion during the debate will be evaluated.

Exam:

Assignment Weights	Percent
Laboratories:	
8 Quizzes	16%
16 Reports	64%
2 Tests	10%
Debate	10%
Total	100%

Quizzes - max. 16 points
Reports - max. 64 points
Tests - max. 10 points
Debate - max. 10 points
Total points - max. 100 points

Exam	100% max. 100 points
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Final grade:	
Laboratories	50%
Exam	50%
Total	100%

Grading Scale:
90-100 points = A
80-89 points = B
70-79 points = C
60-69 points = D
51-59 points = E
0-50 points = F

The exam verifies theoretical knowledge and practical skills in the field of phase diagrams and materials science, the main principles of description and construction.

GRADING POLICY

The course *Phase Diagrams of Multicomponent Systems* is scored with points.

During the semester a student is expected to perform 8 laboratories and complete quizzes and reports related to them, pass 2 tests and take part in the debates giving a maximum of 100 points. The exam is conducted in written form and contains 2 theoretical and 4 practical questions. The maximum number of points that can be obtained on the exam is 100. The final grade is determined by 50% of the points obtained in the laboratories and 50% of the points obtained in the exam. Students will be graded according to the grading scale presented in a table to the left.

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

ASSEMBLING ELECTRICAL BATTERIES

Code: AEB MM-007

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

2

Language

English

Thematic block

Materials & Manufacturing

Form of tuition and number of hours*:

Lecture: 16 h

Laboratory: 32 h

ECTS

4

Lecturer:

Volodymyr Pavlyuk, DSc., Prof.

COURSE DESCRIPTION

The "Assembly of Electric Batteries" (AEB) course provides the student with the opportunity to acquire basic knowledge in the field of technology for manufacturing components for various types of batteries, especially metal-ion (such as) and metal hydride batteries, which occupy a significant place in energy production and storage systems. The content of the module contains the latest trends in the development of innovative electrode materials and electrolytes for modern batteries, which have significantly improved energy capacity and operational characteristics. The student will be able to familiarize himself with the main methods of synthesis and characterization of electrode and electrolyte materials for new high-efficiency batteries. Particular attention will be paid to the features of battery products depending on the size (disc, cylindrical, packet, etc.) and the energy range of use (household, starting, traction, etc.) Prospects for the practical use of batteries in various industries will be presented: household electrical appliances, local energy systems, electric transport, aircraft and space, and the military industry. The MHE module corresponds to the growing and promising consumption of electrical energy, the main assumptions and goals of which correspond to the national and European strategy in obtaining new energy-intensive, environmentally friendly, and cheaper sources of electrical energy.

COURSE OBJECTIVES

The main goal of the AEB course is the comprehensive preparation of students for work in energy related to the design and production of new high-energy batteries and their safe operation in various areas of use in energy-intensive equipment and technological processes. Students who complete the course will have the knowledge and skills necessary to manufacture and operate various types of batteries. According to the expected learning outcomes, they will be ready for professional work in the field of energy and various related fields.

PREREQUISITES FOR TAKING THE COURSE

Basic knowledge of the basics of materials science, inorganic chemistry and electrochemistry are the main prerequisites for completing the AEB course. Understanding the electrochemical processes involved in the generation of electrical energy during chemical reactions. Understanding engineering approaches to creating different types of batteries.



LEARNING OUTCOMES OF THE MODULE

Code module	Description
MS_O_01	Students will have extensive and in-depth knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of electrode materials.
MS_O_02	Students will have extensive and in-depth, theoretically based and structured knowledge of modern techniques and research methods used in battery electrode materials engineering.
MS_O_03	Students will have extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and processing of engineering materials, surface modification of engineering materials as well as development trends and the latest achievements.
MS_O_04	Students will use information from literature, databases and other available sources. Students will be able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems.
MS_O_05	Students will be able to select the appropriate raw materials, technologies and techniques for the production, processing and testing of electrode materials.

METHODS OF CONDUCTING CLASSES

Code	Description	Code module
Meth_01	Lectures: lectures with problem interpretation, interactive lectures with discussion, lectures with multimedia support	KO_01 KO_03 KO_04
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate	SO_01 SO_03

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Code module	Methods of conducting classes
FT_01	lecture	10	course work	KO_01 KO_03 KO_04	Meth_01
FT_02	laboratory	30	course work	SO_01 SO_03	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

By the end of the Assembly of Electric Batteries course student:

- will have extensive and in-depth knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of electrode materials.
- will be have extensive and in-depth, theoretically based and structured knowledge of modern techniques and research methods used in battery electrodes materials engineering.
- will have to extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and processing of engineering materials, surface modification of engineering materials as well as development trends and the latest achievements.
- will be use information from literature, databases and other available sources. He is able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems.
- will be able to select the appropriate raw materials, technologies and techniques for the production, processing and testing of electrode materials

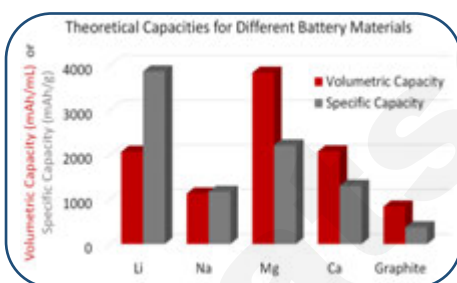
DO YOU KNOW

Lithium: The total remaining lithium supply on earth is only 80 million tons.

Price - €235.00 / 100 g (Merck).

Magnesium: The reserve of magnesium minerals amounts to 12 billion tons.

Price - €21.20 / 100 g (Merck)



Liu F, Wang T, Liu X, et al. *Adv Energy Mater.* 2020, 11, 2000787

COURSE CONTENT - LECTURE

Topics 1

Fundamental aspects of electrochemical energy sources. Mechanism of generation of electrical energy in batteries

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.

Topics 2

Components of cells and batteries.

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.

By the end of the Assembly of Electric Batteries course student:

- will have extensive and in-depth knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of electrode materials.
- will have extensive and in-depth, theoretically based and structured knowledge of modern techniques and research methods used in battery electrodes materials engineering.
- will have to extensive and in-depth substantive knowledge in the field of methods, processes of manufacturing and processing of engineering materials, surface modification of engineering materials as well as development trends and the latest achievements.
- will be use information from literature, databases and other available sources. He is able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems.
- will be able to select the appropriate raw materials, technologies and techniques for the production, processing and testing of electrode materials

COURSE CONTENT - LECTURE

Topics 3

The most important characteristics of batteries

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.

Topics 4

Primary Batteries

The lecture explains the fundamentals and principles of the main types of primary batteries: Alkaline batteries (Zinc/alkaline/Manganese Dioxide), Zinc-carbon batteries, Zinc-chloride batteries, Silver-oxide batteries, and Zinc-air batteries. Lithium based primary cells, which are batteries that have metallic lithium as an anode, will be also discussed. 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.

By the end of the Materials for Hydrogen Energy course student:

- will have extensive and in-depth knowledge about the construction and operation of various types of fuel cells. They will be able to experimentally determine the operating parameters of the fuel cell and select materials for the construction of the fuel cell, and design a laboratory model of the fuel cell.
- will be able to use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to materials for hydrogen energy with consideration of sustainable development principles.
- will be equipped with the skills to plan and conduct experiments to evaluate the impact of water electrolysis parameters on the corrosion resistance of electrode materials. In addition, they will have developed the ability to select appropriate testing methods, analyze the results, and optimize electrodeposition parameters in order to achieve the desired material properties.
- will be able to identify problems and challenges related to the safe use of hydrogen in the energy sector and prepare guidelines and issues relevant to the certification process for specialized entities. They will distinguish the issue of admitting a technology or product on special terms for the pilot or demonstration phase, as opposed to commercial solutions.
- will develop the ability to prepare scientific reports and presentations, including critical analysis, synthesis, and drawing conclusions. They will acquire skills in both individual and team-based work, as well as leading discussions on materials for hydrogen energy.

COURSE CONTENT - LECTURE

Topics 5

Secondary Batteries. Li-ion batteries

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 LiC₆/LiCoO₂ 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.

Topics 6

Secondary Batteries. Na-ion batteries

This lecture presents the current state of development of Na-ion batteries. Operating principle and electrode materials. Hard carbon's anodes and their ability to absorb sodium. Carbon arsenide (AsC₅) mono/bilayer as an anode material. Metals and semi-metals (Pb, P, Sn, Ge, etc.) electrodes for Na-ion batteries. The layered structure MoS₂ 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.

By the end of the Materials for Hydrogen Energy course student:

- will have extensive and in-depth knowledge about the construction and operation of various types of fuel cells. They will be able to experimentally determine the operating parameters of the fuel cell and select materials for the construction of the fuel cell, and design a laboratory model of the fuel cell.
- will be able to use information from literature and other available sources, interpret and critically evaluate them, draw conclusions, and formulate and solve problems related to materials for hydrogen energy with consideration of sustainable development principles.
- will be equipped with the skills to plan and conduct experiments to evaluate the impact of water electrolysis parameters on the corrosion resistance of electrode materials. In addition, they will have developed the ability to select appropriate testing methods, analyze the results, and optimize electrodeposition parameters in order to achieve the desired material properties.
- will be able to identify problems and challenges related to the safe use of hydrogen in the energy sector and prepare guidelines and issues relevant to the certification process for specialized entities. They will distinguish the issue of admitting a technology or product on special terms for the pilot or demonstration phase, as opposed to commercial solutions.
- will develop the ability to prepare scientific reports and presentations, including critical analysis, synthesis, and drawing conclusions. They will acquire skills in both individual and team-based work, as well as leading discussions on materials for hydrogen energy.

Topics 7

Metal hydride batteries and fuel cells

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).

Topics 8

Battery manufacturing

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.

Students will be able to:

- Synthesis of electrode materials
- Conduct phase analysis of the samples
- Investigation of the crystal structures of compounds
- Construct and test electrochemical properties of a batteries
- Study of electrochemical properties of electrode materials
- Construct of the laboratory battery prototype

COURSE CONTENT - LABORATORY

Topics 1

Synthesis of electrode materials

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.

Topics 2

Phase analysis of the samples

The aim of the laboratory is to determinate 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.

Topics 3

Investigation of the crystal structures of compounds

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.

Topics 4

Electrochemical properties of electrode materials.

The aim of the laboratory is the determination of electrochemical properties of electrode materials by electrochemical methods: Cyclic voltammetry (CVA), Chronopotentiometry (CP), Chronocoulometry (CC), and Electrochemical Impedance Spectroscopy (EIS).

Topics 5

Battery prototype manufacturing

The aim of the laboratory is the creation of a 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.

TEXTBOOK/READINGS

The mandatory reading for completing the subject *Assembly of Electric Batteries*:

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.

To deepen the course topics, optional recommended texts include:

1. Korthauer, Reiner, ed. Lithium-ion Batteries: Basics and Applications. Springer, 2018.
2. Dudney, Nancy J., William C. West, and Jagjit Nanda, eds. Handbook of Solid State Batteries. Vol. 6. World Scientific, 2015.

ASSESSMENT

Quiz:

At the start of each laboratory, a brief quiz will be given regarding the lab's subject matter that will be performed that day. This is done to ensure that the necessary literature recommended for the laboratory (and the concepts presented during the lecture) have been read beforehand and that the students are ready to conduct the lab.

Reports:

Students will be grouped into teams and tasked with producing a written report on their experimental laboratory exercises. The report should include a theoretical background, a description of the experiments conducted, an analysis of the results, and a discussion and conclusions section. Through these reports, students will deepen their theoretical and practical knowledge in the field of materials for hydrogen energy.

Debate:

During the debate, the ability to present logical arguments and explain their relevance to the topic, the ability to respond to questions posed by other participants, and the ability to actively listen and participate in the discussion with other debate participants will be subject to evaluation.

GRADING POLICY

The *Assembly of Electric Batteries* course is scored with points. The grade results from the sum of points obtained by the student during the semester (quizzes, reports, debate). The maximum number of points obtained in the laboratory exercises is 100. Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
4 Reports	50%
4 Quizzes	40%
Debate	10%
Total	100%

Reports - max. 50 points
Quizzes – max. 40 points
Debate – max. 10 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
0 - 60 points	= F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

MAGNETISM AND MAGNETIC MATERIALS

Code: MMM

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Advanced Engineering Materials

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

4

Lecturer:

Khrystyna Miliyanchuk, PhD, Assoc. Prof.

COURSE DESCRIPTION

The course is designed to provide participants with the necessary theoretical knowledge and develop experimental skills in the study of the magnetism of intermetallic and related materials. Therefore, the course presents the main theories of the evolution of magnetic properties of inorganic materials and the methodology of their experimental research and interpretation, including mathematical processing, critical analysis and modeling. The course is an important element in the formation of specialists in the field of chemistry, physics, engineering, materials science, and builds a solid foundation for the formation of interdisciplinary connections.

The lectures, which provide the theoretical basis, are divided into the following main parts: 1) the origin of magnetism in solid state; 2) exchange interactions and magnetically ordered systems; 3) experimental method in magnetism; 4) the most important classes of magnetic materials. The laboratory works include the studies of the magnetic susceptibility of paramagnetic materials, the determination of Curie temperature applying Arrott plots, interpretation of the susceptibility and magnetization curves for explanation of magnetic properties of materials.

COURSE OBJECTIVES

The aim and objectives of the course are the following: to get familiar with modern magnetic materials, having potential for application in various fields of modern science and technology; to introduce the quantitative characteristics and areas of application of the main magnetic materials.

PREREQUISITES FOR TAKING THE COURSE

Bachelor's degree in chemistry, physics or material science. For successful completion of the course, it is desirable to take courses OM1-010 "Crystal chemistry (relationship composition–structure–properties)", OM1-011 "Phase diagrams of multicomponent systems"

LEARNING OUTCOMES OF THE MODULE

Code	Description
MAG_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of engineering materials.
MAG_O_02	Has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.
MAG_O_03	Can formulate and test hypotheses related to simple research and implementation problems. Can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.
MAG_O_04	Is able to communicate on specialist topics with diverse audiences, including leading a debate. Can prepare a scientific study and present a presentation on the implementation of a research task, containing a critical analysis, synthesis and conclusions, both in their native language and in foreign languages, at level B2+ of the Common European Framework of Reference for Languages, using specialized terminology..
MAG_O_05	Able to work individually and in a team as well as interact with others in teamwork.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: informative lectures, description, explanation/clarification support	MAG_O_01 MAG_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation; problem learning; debate	MAG_O_03 MAG_O_04 MAG_O_05

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	essay, homework, test	MAG_O_01 MAG_O_02	Meth_01
FT_02	laboratory	32	laboratory reports	MAG_O_03 MAG_O_04 MAG_O_05	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Preparation for classes	Query of materials and review of activities necessary to participate in classes	NO
a_02	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

The lecture course provides the knowledge on:

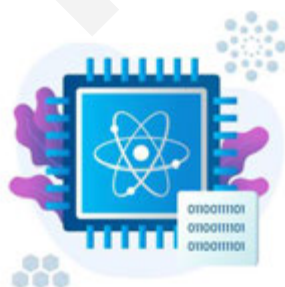
- how to explain the magnetic properties of modern intermetallic and related materials based on theoretical concepts
- how to outline the areas of application of individual classes of inorganic compounds
- ways to synthesize new compounds and to improve the magnetic properties of existing compounds in order to obtain the novel magnetic materials for various applications.

COMMENTS

LECTURER

DO YOU KNOW

The bottleneck for understanding magnetism by the beginning of 20th century was the calculation restrictions. "At this point it seems that the whole of chemistry and much of physics is understood in principle. The problem is that the equations are much difficult to solve...", wrote P. Dirac.



COURSE CONTENT – LECTURES

Topics 1

Classification of magnetic materials. Evolution of magnetic moments.

Diamagnetism, paramagnetism, magnetic order. Electronic structure. Aufbau principle and Hund's rules. Curie law: effective moments. Saturation magnetic moments. Paramagnetism in $3d$ and $4f$ metals.

Topics 2

Magnetically ordered systems

Ferromagnetism, antiferromagnetism, ferrimagnetism. Exchange interactions. Mean-field approach. Curie-Weiss law. Phase transitions. Hard magnets and soft magnets.

Topics 3

Magnetic structures. Magnetic phase diagrams.

Magnetic symmetry. Magnetic space groups. Magnetic structures of transition $3d$ metals. Magnetic anisotropy. Magnetic phase transitions and magnetic phase diagrams.

Topics 4

Magnetism in materials

Localized and band magnetism. Stoner criterium for band magnetism. De Gennes factor for lanthanide compounds. Magnets containing $4f$ and $3d$ elements. peculiarities of $5f$ magnetism.

Topics 5

Experimental methods in magnetism

Macroscopic and microscopic methods, direct and indirect methods. Force, induction, and SQUID magnetometers. Neutron diffraction. Mössbauer spectroscopy. Resistivity, dilatometry, specific heat of magnetic systems.

Topics 6

Magnetic materials

Permanent magnets. Hall effect and magnetoresistance. Giant and colossal magnetoresistance; magnetoresistance materials. Magnetocaloric effect; magnetic refrigerator.

Topics 7

Unconventional magnetism

Heavy fermion systems, Kondo lattice. Co-existence of magnetism and superconductivity. 1D- and 2D-systems. Thin layers. Quantum materials.

LEARNING OUTCOMES

The laboratory course will develop the skills of:

- planning the algorithm of studying the magnetic properties of intermetallic and related materials,
- calculating quantitative indicators characterizing magnetic properties
- interpreting the obtained results with respect to the chemical composition, electronic and crystal structure of compounds;
- critical assessment of educational and scientific literature and periodicals in the field of research on the magnetic properties of modern inorganic materials.

COMMENTS

INSTRUCTOR

DO YOU KNOW

That the application of magnets started thousands of years (compasses in China cca. 1000 BC) before the explanation of phenomena was proposed, what happened after the introduction of quantum and relativistic mechanics.

COURSE CONTENT – LABORATORY CLASSES

Topics 1

Introductory lesson. Safety techniques in laboratories

Calibration of the device for measuring the magnetic susceptibility of inorganic materials. Sample preparation.

Topics 2

Susceptibility of Curie-Weiss paramagnet

Determination of the temperature dependence of the magnetic susceptibility of a paramagnetic compound

Topics 3

Magnetically ordered systems

The determination of the type of magnetic order and the quantitative parameters (effective moment, saturation moment, spontaneous magnetization) of metallic system

Topics 4

Magnetic susceptibility of multi-phase alloys

Calculation of the effective Curie moment and paramagnetic temperature for a Curie-Weiss paramagnet in the presence of a ferromagnetic impurity

Topics 5

Arrott plots

Determination of the temperature of the ferromagnetic transition by the method of plotting the Arrott graph based on the Landau theory of II order phase transitions.



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TEXTBOOK/READINGS

Due to the evolving nature of additive manufacturing technologies, no single textbook currently covers all the topics that will be discussed in this course. The vast majority of course content will be freely available via course lecture notes, website content, and academic papers accessible through the University network.

For a deeper understanding of the course subject matter, optional recommended texts include:

1. N.W. Ashcroft, N.D. Mermin. Solid State Physics, Saunders, 1976.
2. S. Blundell. Magnetism in Condensed Matter, N.Y.: Oxford University Press, 2001.
3. Ch. Kittel. Introduction to Solid State Physics, 7th Ed., Wiley, 1996.
4. A.R. West. Basic Solid State Chemistry, 2nd Ed., John Wiley & Sons, Ltd, 1999.
5. Buschow KHJ, de Boer FR Physics of magnetism and magnetic materials. - NY: Kluwer Academic Publishers, 2004.

ASSESSMENT

Laboratory works: Students will prepare written reports on their experimental laboratory exercises. The report should include a theoretical background, a description of the experiments conducted, an analysis of the results, and a discussion and conclusions section. Through these reports, students will deepen their theoretical and practical knowledge in the field of magnetism.

Critical essay: A written essay on the chosen topic covering magnetic phenomena and magnetic materials from the suggested list (each year will be presented) is required. The critical analysis and original conclusions are expected.

Homework: Two assessments will be provided: 1) calculating theoretical values of magnetic moments; 2) description of magnetic properties of materials based on a set of experimental data.

Final test: The questions and problems cover the theory delivered on lectures.

GRADING POLICY

The control of studying the course "Magnetism and magnetic materials" is carried out based on the results of the final test, a critical essay, homework, as well as the results of carrying out and defense of laboratory works. The maximum number of points obtained during the course is 100. The assignment weight and grading scale are given in the box.

Assignment Weights	Percent
Laboratory works	40%
Critical Essay	15%
Homework	15%
Final test	30%
Total	100%

Grading Scale

91% - 100%	= A
81% - 80%	= B
71% - 70%	= C
61% - 60%	= D
51% - 50%	= D
0% - 50%	= F

COURSE SCHEDULE?

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

DATABASES FOR MACHINE LEARNING

Code: DBML

Field of study

Materials Science and Engineering

Level of study

Master study

Semester

2

Language

English

Thematic block

Computational methods and their applications in materials science

Form of tuition and number of hours*

Lecture: 16h

Laboratory: 32h

ECTS

3

Lecturers:

Roman Gladyshevskii, DSc, Prof.

Nataliya Muts, PhD, Assoc. Prof.

COURSE DESCRIPTION

The number of possibilities to combine chemical elements in different proportions under different conditions is astronomically high. However, a large amount of experimentally determined data have been published over the last 100 years, and tools for machine learning, including AI, open new possibilities to explore novel directions in the search for materials with desired properties. For a proper analysis and sensible output, it is necessary to critically evaluate and process the data.

The course "Databases for machine learning" is designed to make the student familiar with information retrieval using modern databases and tools and to develop critical thinking and analysis.

A holistic view on inorganic substances will be presented by taking into consideration crystal structures, phase diagrams, chemical and physical properties. The purpose of the course is to teach the students to collect data from various sources (databases, handbooks, journal sites), critically analyze the information, systematize it, search for regularities, and elaborate scientific hypotheses, in view of proposing new materials with particular physical properties.

Through the combination of lectures and laboratory classes the students will develop a holistic view on materials, interconnecting different groups of chemical and physical data.

COURSE OBJECTIVES

By the end of the course, the students will have acquired theoretical knowledge and practical skills in searching for information using modern databases, and learnt to critically analyze the obtained information about compounds and materials.

PREREQUISITES

Basic knowledge of chemistry, crystal chemistry, and solid-state chemistry and physics is necessary. Codes of courses, prior completion of which is recommended: AMTM-007, AEM-M007, AEM-M008, AEM-M009, AEM-CER003, OM1-010, OM1-011. Good knowledge of English is required.



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LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	He/She is able to - find and extract information from scientific literature, databases and other available sources, - summarize and standardize the obtained information, interpret and critically evaluate it, - draw conclusions, formulate hypotheses and solve simple problems.
MS_O_02	He/She is able to select chemical substances for the production, processing and testing of engineering materials.
MS_O_03	He/She is able to work individually and interact with others in teamwork.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: informative lectures, conversational lectures, discussion, multimedia support	MS_O_01 MS_O_02
Meth_02	Laboratory classes: data collection, conversion and standardization, materials design, discussion/debate (brainstorm), critical analysis, individual and team work, communication on specialist topics, work with computer	MS_O_01 MS_O_02 MS_O_03

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory	32	project	MS_O_01 MS_O_02 MS_O_03	Meth_02

THE STUDENTS' WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation of projects and presentation	Consultation. Preparation and development of projects and presentation.	YES

LEARNING OUTCOMES (Lectures)

The student will be able to:

- collect information on a specific topic in an efficient way;
- critically analyze information about phase equilibria, crystal structures, and basic physical properties of substances formed in binary and multinary systems

The PAULING FILE project was launched in 1993, and 30 years later this world-largest materials database contains over 500'000 database entries for inorganic crystalline solids, summarizing over 160'000 scientific publications



Pauling File Inorganic Materials Database and Design System

CONTENTS OF THE COURSE - Lectures

Topic 1

Scientific information retrieval systems

Overview of common information search systems: Scirus; BASE: Bielefeld Academic Search Engine; WorldWideScience; FindArticles; Science Research Portal; Chemical Abstracts Service (CAS); ScienceDirect; Scopus; Web of Science; Google Scholar.

Topic 2

Crystallographic databases

Overview of databases storing crystallographic data: 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.

Topic 3

Pauling File Inorganic Materials Database and Design System and ASM Alloy Phase Diagram Database. Phase diagrams of chemical systems

Analysis of experimentally determined and calculated phase diagrams. Search tools. The phase diagram as a basis for choosing conditions for synthesis.

Topic 4

Pauling File Inorganic Materials Database and Design System. Crystal structures and physical properties of binary compounds

Analysis of crystal structures (structure type, symmetry, cell parameters, atom coordinates, etc.) and physical properties (hardness, melting point, magnetization, ferroelectricity, enthalpy of formation, electrical resistivity, energy gap, thermopower, superconductivity) of binary compounds. Search tools.

Topic 5

Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds. Crystal chemistry of inorganic substances

Compound search tools: chemical composition, structure type, symmetry, Pearson symbol, cell parameters. Crystallographic characteristics of compounds. Analysis of interatomic distances, coordination polyhedra.

Topic 6

LEARNING OUTCOMES (Laboratory classes)

By the end of the course, the students will be able to:

- find and extract information from literature, databases and other available sources;
- summarize the obtained information, interpret and critically evaluate it;
- draw conclusions;
- solve simple innovative problems;
- plan and perform the synthesis of new materials;
- select appropriate substances for the production, processing and testing of engineering materials;
- work individually and interact with others in a teamwork.

Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds. Phase analysis of samples of inorganic compounds

Principles of phase analysis. Comparison of observed X-ray powder diffraction pattern with calculated pattern. Building theoretical patterns using different radiations. Search tools.

Topic 7

Holistic view on inorganic compounds

General approach/concepts to obtain a holistic view on materials: bottom-up approach (BUA) and the top-down approach (TDA).

Topic 8

Searching for materials with predefined properties

Relationships between phase diagrams, crystal structures, and physical properties as a basis for synthesizing materials with predefined properties.

COURSE CONTENT - Laboratory classes

Topic 1

Materials for heterogeneous catalysis

Literature search using databases and scientific articles on materials used in catalysis. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for potential catalysts (Project) (2 h).

Topic 2

Magnetic materials

Literature search using databases and scientific articles on magnetic materials. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

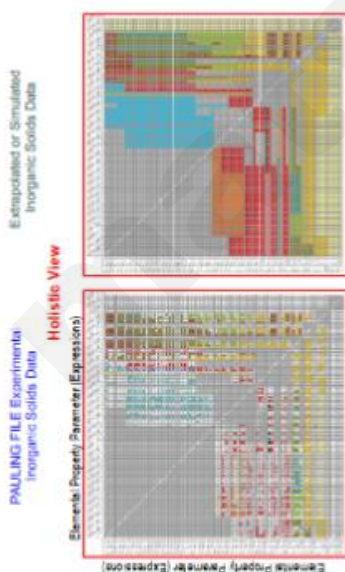
Proposals for potential magnetic materials (Project) (2 h).

Topic 3

High-density materials

Literature search using databases and scientific articles on materials with high density. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for potential high-density materials (Project) (2 h).



Topic 4

Superhard ceramic materials

Literature search using databases and scientific articles on superhard ceramic materials. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for superhard ceramic materials (Project) (2 h).

Topic 5

High-entropy alloys

Literature search using databases and scientific articles on high-entropy alloys. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for high-entropy alloys (Project) (2 h).

Topic 6

Semiconductors

Literature search using databases and scientific articles on semiconductors. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for semiconductors (Project) (2 h).

Topic 7

Intermetallic hydrides

Literature search using databases and scientific articles on intermetallic hydrides. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for intermetallic hydrides (Project) (2 h).

Topic 8

Superconductors

Literature search using databases and scientific articles on superconductors. Analysis of chemical composition, crystal structure, physical properties. Search for regularities (2 h).

Proposals for superconductors (Project) (2 h).



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TEXTBOOK/READINGS

1. P. Villars, K. Cenzual, R. Gladyshevskii. Handbook of Inorganic Substances 2017. Berlin: Walter de Gruyter. 2017. 1955 p.
2. P. Villars, K. Cenzual (Eds.). Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds, ASM International: Materials Park, Ohio, USA, Release 2023/24.
3. E. Parthé, L. Gelato, B. Chabot, M. Penzo, K. Cenzual, R. Gladyshevskii TYPIX - Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types. Vol. 1–4. Springer-Verlag : Heidelberg, 1993. 1596 p.
4. 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.
5. 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.

ASSESSMENT

Project:

During the course “Databases for Machine Learning”, the student is asked to prepare four projects. Each project should contain a review of literature data on the functional material, a description of the crystal structure, physical properties and synthesis conditions. The highest score is 25 points for each project.

GRADING POLICY

The course “Databases for Machine Learning” is evaluated out of 100 points. The total grade is determined by the sum of points scored by the student for the semester.

Assignment Weights	Percent
Project	100%
Total	100%

Grading Scale

90 – 100 points = A
 81 – 89 points = B
 71 – 80 points = C
 61 – 70 points = D
 51 – 60 points = E

Below:

21 – 50 points = FX
 0 – 20 points = F

COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				
6				
7				
8				

PEROVSKITE-BASED MATERIALS

Code: **PBM**

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Advanced Engineering Materials

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

3

Lecturer: *Oksana Zaremba, Assoc. Prof.*

COURSE DESCRIPTION

This course is designed to provide a comprehensive understanding of the synthesis conditions, crystal structure, physical characteristics and applications of perovskite-based materials. Perovskites form a huge family of ceramics derived from the structure of the CaTiO_3 compound. They possess numerous unique physical properties, among which colossal magnetoresistance, magnetic ordering, thermal, optical, dielectric, piezoelectric and ferroelectric properties, electronic conductivity, superconductivity, catalytic activity, etc. The perovskite phases have gained significant attention in recent years due to their exceptional properties, making them promising candidates for various applications such as energy storage, solar cells, light-emitting diodes, photodetectors, lasers, catalysis, and many others.

The course will cover the main aspects on the crystal structure of perovskites, their physical properties, as well as the methods for their synthesis and characterization. Students will gain insights into the latest research developments and technological advancements in the field of perovskite-based materials, and their potential impact on the renewable energy and electronics industries.

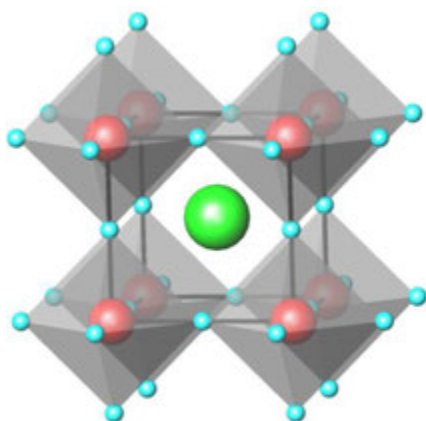
Through the combination of lectures and laboratory classes the students will have an opportunity to explore the practical aspects of working with perovskite-based materials, including the optimization of production and characterization by different methods. The course will also address the challenges and future prospects associated with the commercialization of perovskite-based technologies.

COURSE OBJECTIVES

By the end of the course, students will be equipped with the theoretical knowledge to critically evaluate the potential of perovskites in various applications and practical skills in manufacturing and testing of perovskite-based materials.

PREREQUISITES FOR TAKING THE COURSE

Basic knowledge of chemistry, crystal chemistry, and solid-state physics is necessary. Codes of courses which prior completion is recommended to complete this course: AMTM-011, AMTM-012, AMTM-013, AEM-M008, AEM-M009, OM1-010, OM1-011.



The crystal structure of CaTiO_3

(large spheres – the Ca atoms,
medium spheres – the Ti atoms,
small spheres – the O atoms).

LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of engineering materials.
MS_O_02	Has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.
MS_O_03	Can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.
MS_O_04	Able to work individually and in a team as well as interact with others in teamwork.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: informative lecture, monographic lecture, description, conversational lecture, presentation.	MS_O_01 MS_O_02
Meth_02	Laboratory classes: activating methods: peer learning, show/demonstration, work with computer, reconstruction/restoration, laboratory exercise/experiment, practice.	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory	32	report	MS_O_03 MS_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation of reports and presentation	Consultation. Preparation and development of reports and presentation.	YES

LEARNING OUTCOMES (Lectures)

The learning outcomes aim to provide:

- an extended and in-depth knowledge in the field of perovskite-based materials;
- a comprehensive understanding of the relationship between composition, synthesis conditions, crystal structure and physical properties of perovskites;
- proper orientation in the modern fields of their application, latest developments, the main advantages and limitations;
- an awareness of potential prospects and impact of such kind of materials on modern technology and industry.

DO YOU KNOW

Calcium titanate (CaTiO_3) – the first member of the perovskite family – was discovered in 1839 by the chemist Gustav Rose during an expedition in the Ural Mountains. He named the mineral “perovskite” in honor of the mineralogist Lev Perovski. Any materials with the same crystal structure that were subsequently found in nature or created synthetically, were classified as perovskite.



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COURSE CONTENT - Lectures

Topic 1

Review of the perovskite family. The crystal structure of perovskite and its derivatives.

The lecture will shed light on a class of compounds belonging to the perovskite family and their importance to modern materials science. Students will be presented with the history of discovery, classification, crystal structure peculiarities of perovskite and its derivatives, the concept of the tolerance factor and flexibility of unique perovskite structure (2 h).

Topic 2

Methods of synthesis of perovskites and their characteristics.

During the lecture, the audience will be introduced with a variety of methods for the synthesis of compounds with a perovskite structure and their brief characteristics, in particular, by the solid-state reaction, sol-gel method, obtaining them in the form of single crystals, thin films, etc. (2 h).

Topic 3

Application of perovskites as catalysts.

The lecture will reveal the importance of improving catalysts for chemical and electrochemical reactions that underlie many aspects of modern technology and industry, from energy storage and conversion to solving environmental problems with harmful emissions, etc. It will show the prospects of environmentally friendly, cost-effective and easy tunable catalysts based on perovskites as an alternative to the existing expensive catalysts containing noble metals (2 h).

Topic 4

Perovskite piezoelectrics and ferroelectrics.

The students will be familiarized with the applications of perovskite piezoelectrics and ferroelectrics, two cutting-edge materials with remarkable properties that have the potential to revolutionize various fields, including electronics, energy, and sensing technologies (actuators, memory devices, energy harvesting, sensors, etc.) (2 h).

Topic 5

Superconducting materials based on perovskites.

The lecture will explore the phenomenon of superconductivity, where materials exhibit zero electrical resistance and expel magnetic fields. The focus will be on the discovery of superconducting perovskites, which have attracted significant attention due to their potential for high-temperature superconductivity. The current challenges and opportunities in the field of perovskite-based superconductors will be discussed (2 h).

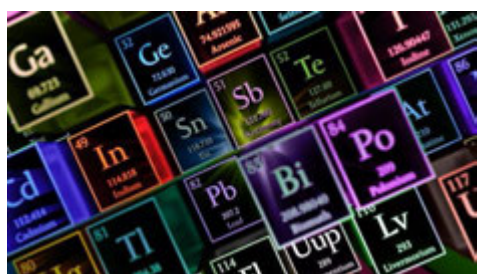
LEARNING OUTCOMES (Laboratory classes)

By the end of the course, students will be able to:

- plan and perform the synthesis of perovskite ceramics, select the suitable method of manufacturing, initial reagents, optimal conditions for the experiment based on the systematic analysis of literature data;
- carry out the characterization of the produced materials, in particular by scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray fluorescence spectroscopy.
- execute the X-ray phase, structural and crystal chemical analysis;
- measure the mechanical, electrochemical and magnetic properties of perovskites;
- acquire the skills to operate specialized software essential for the manipulation and examination of research data;
- interpret the received scientific results, make generalizations and conclusions, draw up a report,
- critically assess the quality of task performance.

DO YOU KNOW

The perovskite family of materials is extensive due to the significant flexibility in the ions that can be incorporated into the formula. More than 90% of the metals in the periodic table can be utilized, allowing perovskites to be finely adjusted for specific applications.



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Topic 6

Exploitation of perovskites in the solar cell development.

The lecture will provide an engaging and informative overview of this rapidly developing field, highlighting its potential to drive sustainable and efficient sources of energy production and storage based on perovskite and their advantages over traditional materials (2 h).

Topic 7

Testing of perovskites in lithium-ion batteries.

The participants will be presented with the most exemplary instances of perovskite material examination for the advancement of lithium-ion batteries, encompassing both electrodes and solid-state electrolyte components (2 h).

Topic 8

Perovskite-based magnetic materials.

The lecture will cover the main aspects of the magnetic properties of perovskite-based materials. First of all, this concerns the phenomenon of colossal magnetoresistance, which is characteristic, mainly, of manganites with a perovskite structure, where the electrical resistance of the material changes dramatically in the presence of an external magnetic field. This effect has potential applications in magnetic sensors, data storage, spintronic devices, etc (2 h).

COURSE CONTENT - Laboratory classes

Topic 1

Pre-experimental preparation – literature data analysis.

The aim of the laboratory class is to enhance proficiency in utilizing literature sources and databases for the facilitation of the selection and optimization of synthesis conditions for ceramics possessing a perovskite structure (4 h).

Topic 2

Producing of perovskite ceramics.

During the laboratory class, students will be trained on practice the solid-state reaction method for preparation of multicomponent perovskite-based materials (4 h).

Topic 3

Surface morphology and composition control.

The laboratory class is aimed at familiarization with scanning electron microscopy, X-ray energy-dispersive spectroscopy and X-ray fluorescent

spectroscopy to control the qualitative and quantitative composition of perovskite ceramics (4 h).

Topic 4

X-ray phase analysis.

During the laboratory class, students will be acquainted with the methodology and software for phase identifying within polycrystalline ceramic samples, encompassing multiphase materials. This analysis will be conducted using diffraction data that has been previously acquired on an automated diffractometer (4 h).

Topic 5

Crystal structure characterization.

The laboratory class will provide a comprehensive understanding of the fundamental concepts and principles in crystal structure solving, with a specific focus on perovskite structures. The 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 (4 h).

Topic 6

Examination of mechanical properties.

During the laboratory class, students will be acquainted with the basic principles of measuring mechanical properties, in particular, the Vickers microhardness testing method as applied to ceramic materials. This practical class aims to provide students with a comprehensive understanding of the techniques and equipment involved in assessing the mechanical properties of materials (4 h).

Topic 7

Electrochemical behavior study.

The task of the laboratory class is to familiarize the students with the algorithm for designing a lithium-ion energy storage system. During the tutorial, students will be able to investigate the electrochemical properties of a perovskite-based material, specifically in the context of evaluating its suitability as a battery electrode (4 h).

Topic 8

Magnetic properties measurements.

The laboratory session will focus on improving students' practical skills related to the measurement of magnetic properties in perovskite ceramics, as well as the interpretation of the data obtained from these experiments. This hands-on experience will provide students with a valuable opportunity to gain a deeper understanding of the theoretical concepts discussed in the classroom, and to develop proficiency in experimental techniques relevant to the field of materials science (4 h).



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TEXTBOOK/READINGS

The mandatory reading for completing *Perovskite-Based Materials*:

1. R. J. D. Tilley *Perovskites Structure–Property Relationships*, John Wiley & Sons, Ltd., UK, 2016, ISBN: 9781118935668.
2. S. Thomas, A. Thankappan. *Perovskite Photovoltaics. Basic to Advanced Concepts and Implementation*, Academic Press, Elsevier, 2018, ISBN: 9780128129159.
3. M. Borowski. *Perovskites: Structure, Properties and Uses*, Nova Science Publishers, 2011. ISBN: 978-1616685256

For extending and supplementing knowledge recommended are:

1. 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.

ASSESSMENT

Reports:

Based on the results of each laboratory work, the student is obliged to perform the report. It is necessary to assess the quality of the student's assimilation of theoretical material and the ability to apply it on practice. The report has a clearly defined structure and consists of a brief review of literary sources related to the topic of the laboratory work, a short overview of the research methods, equipment and starting reagents, a description of the experiment strategy, the obtained experimental data and results of their processing, scientific conclusions. In this particular category of work, the highest achievable score is 40 points.

Presentation:

During the course, the student is required to prepare a presentation on a self-selected topic related to the subject of the course, which is not included in the list of lecture materials. This type of work will be rated at a maximum of 10 points.

Exam:

The final part of evaluation is an exam that is proposed in oral form. The questions concern theoretical and experimental aspects of perovskite-based materials including manufacturing, structure characterization, physical property measurement, and fields of practical application. The maximum number of points to be obtained in the exam is 50.

GRADING POLICY

The total score, amounting to 100 points, comprises the assessment of the results of 8 laboratory classes, designed as reports ($8 \times 5 = 40$ points), an individual presentation ($1 \times 10 = 10$ points), and an oral examination ($1 \times 50 = 50$ points). Attainment of 51 points or higher is deemed a favorable outcome for the course.

Assignment Weights

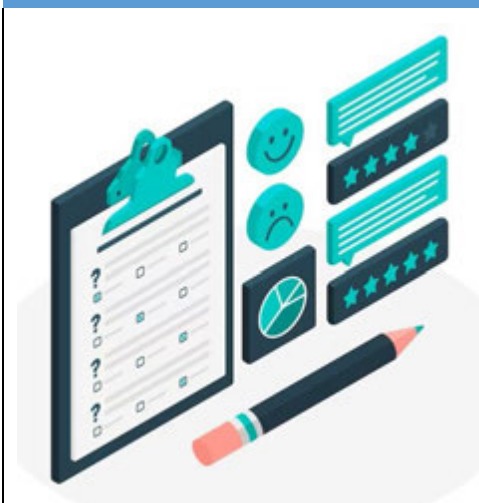
Assignment Weights	Percent
Reports	40%
Presentation	10%
Exam	50%
Total	100%

Grading Scale

90 – 100 points = A
81 – 89 points = B
71 – 80 points = C
61 – 70 points = D
51 – 60 points = E

Below:

21 – 50 points = FX
0 – 20 points = F



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COURSE SCHEDULE?

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

SCANNING ELECTRON MICROSCOPY AND ENERGY DISPERSIVE X-RAYS ANALYSIS FOR MATERIALS SCIENCE

Code: SEM

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

english

Thematic block

Advanced Methods for Materials Characterisation

Form of tuition and number of hours*:

Lecture: 16h

Laboratory: 32h

ECTS

4

Lecturer: *Vasyl Kordan, PhD,
Research Fellow*

COURSE DESCRIPTION

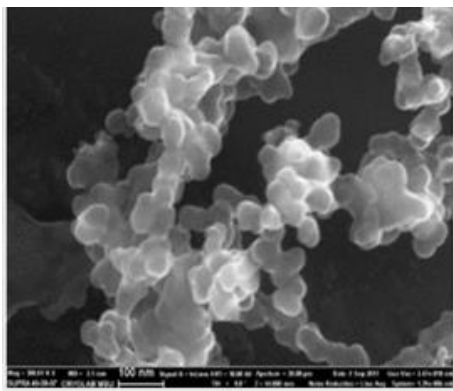
The Scanning electron microscopy and energy dispersive X-rays analysis for materials science course enables the student to acquire knowledge in the field of technological requirements for investigation, developers and control of the phase and chemical composition of the materials at the micro- and nano-levels. The course is devoted to the study of various types of chemical compounds (metals, salts, oxides, etc.), composites, and coatings (films, ceramics), in particular, they can be metal alloys, semiconductor single crystals, functional coatings or composites for batteries, electronics, sensors or constructive materials. Having theoretical training from previous Physics courses, students can easily understand the principles and regularities underlying effects and phenomena during research. Students are able to set a non-standard task and solve it by selecting a set of methods and conditions for research. SEM and EDX methods are essential for every stage of synthesis, development or processing of materials to produce high-quality products. The course consists of 8 lectures and 16 laboratory works, which are closely related for the positive effect from studying the course.

COURSE OBJECTIVES

The main objective of the course is to comprehensively prepare students for work in the material science sector related to the production, and use of different materials as well as the design and technological processes in which functional materials are used. Students have the knowledge and skills to solve material problems that occur in the field of responsibility of enterprises, institutions, or local government units and, in accordance with the assumed learning outcomes, are prepared to take up professional work in the field of the hard industry, metallurgy and microelectronics, as well as related fields.

PREREQUISITES FOR TAKING THE COURSE

Prerequisites for taking the course include a basic knowledge of engineering materials, especially understanding the correlation between the nature of chemical bonds, crystallographic structure, electronic structure, microstructure and surface morphology.



SEM-image of aerosol particles

LEARNING OUTCOMES OF THE MODULE

Code	Description
MS_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of designing, manufacturing, testing and application of engineering materials.
MS_O_02	Has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials engineering.
MS_O_03	Can use information from literature, databases and other available sources. Is able to integrate the obtained information, interpret and critically evaluate it, draw conclusions and formulate and solve complex innovative problems. Can solve practical engineering tasks that require the use of engineering standards and norms.
MS_O_04	Can formulate and test hypotheses related to simple research and implementation problems. He can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions.

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	lectures with problem interpretation, interactive lectures with discussion	MS_O_01 MS_O_02
Meth_02	Laboratory exercises: experiment demonstrations; laboratory work; observation	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01 Meth_02
FT_02	laboratory	32	report	MS_O_01	Meth_03
FT_03	practical classes	72	report	MS_O_01	Meth_03

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Preparation for classes	Query of materials and review of activities necessary to participate in classes	NO
a_02	Reading literature	Preparation and development of reports. Consultation.	YES

Students who attend the course Scanning electron microscopy and energy dispersive X-rays analysis for materials science will gain in-depth knowledge of the microstructure of various substances. They will also be able to find relationships between the received SEM image and the process of synthesis and processing of materials and characterize the phase composition of substances and their chemical composition

COURSE CONTENT - FORM OF TUITION (e.g. lecture)

Topics 1

Introduction to Microscopy. The theoretical principle of the method. Types of microscopes

The lecture will include the general theory of obtaining electron flows for surface analysis. Schematic diagram of different types of microscopes (light, atomic force, scanning and transmission) will be considered and analyzed in the lecture.

Topics 2

Types of cathodes and detectors for image acquisition in microscopy. Practical requirements and preparation of samples for analysis.

The lectures will consider methods of generating electron flows and main types of materials for thermal emission (W-cathode, LaB₆-cathode etc.). Also we will consider the main aspects for the preparation, installation and studying conditions of various type samples.

Topics 3

Energy dispersive X-ray spectrum. Overlapping lines of the energy spectrum

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).

Topics 4

Analysis of objects of metal systems (bulk, polycrystalline and films) synthesized methods of electric arc and induction fusion, powder metallurgy etc.)

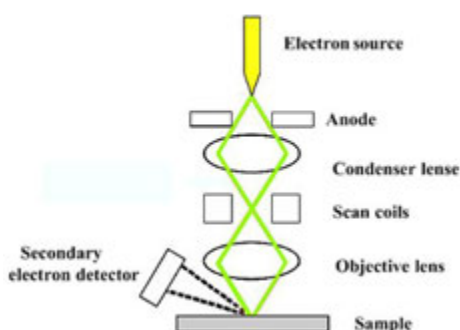
The lecture includes information about the conditions and peculiarities of researching metal objects that do not require sputtering of conductive applications. In the following, it will be shown how the method of synthesis of samples affect on the differs in size, shape of crystals and the presence of defects in the sample.

Topics 5

Quantitative analysis of objects with different chemical composition (oxides, chalcogenides, pnictides, borides etc.)

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.

Scanning Electron Microscope



SEM: The principle of method

Topics 6

Quantitative analysis of multiphase samples

The lecture will cover theoretical and applied aspects of the analysis (SEM and EDX) of multiphase samples (alloys, polycrystals, films, powders, bulk samples, and minerals).

Topics 7

Analysis of composite systems (catalysts, electrocatalysts, electrodes, functional surfaces)

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).

Topics 8

Nanoscale systems. Methods and technologies of formation and analysis of nanostructures.

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.

COURSE CONTENT - FORM OF TUITION (e.g. laboratory classes)

Topics 1

Preparation of metal samples for analysis (film and bulk sample). Image acquisition, interpretation of results.

Discussion, selection of conditions, objects for research and interpretation of results. SE- and BSE-mode scanning

Topics 2

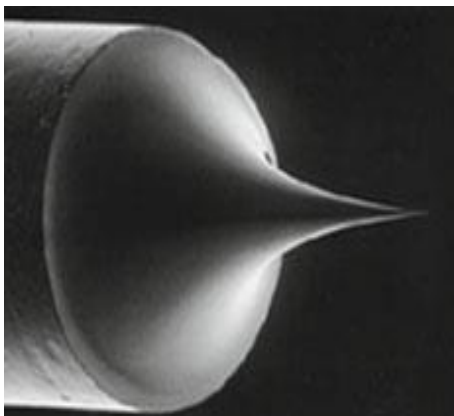
EDX and XRF analysis for general sample composition

Research of the general composition of individual samples by EDX (energy dispersive X-ray spectroscopy) and XRF (X-ray fluorescent spectroscopy) methods, analysis of spectra and interpretation of results

Topics 3

Examination of metal samples after thermal structuring, annealing or modification. Analysis of solid phase reactions and eutectics

Acquisition and comparison of SEM- images of metal samples obtained under various conditions: rapid crystallization, thermal structuring, annealing, epitaxy, etc.



Field emission gun electron

Topics 4

Research of non-conductive samples. Application of conductive surfaces (C- or Au-nanofilms)

Preparation for the study of non-conductive samples using the example of ceramics, applying conductive nano-films, obtaining an image and quantitative composition.

Topics 5

Analysis of single crystals and polycrystalline. Determination of amounts of impurities

Preparation of single crystals, polycrystalline for the analysis, analysis, interpretation of results, determination of the of impurity content, defects, and sample porosity

Topics 6

Analysis of electrodeposited surfaces and modified catalysts

Features of doping components electrodeposited on the cathode and anode surfaces. Obtaining a SEM-image, determining the dimensional characteristics of grains, films, calculating of the distribution diagrams and studying the composition and amounts of alloying additives

Topics 7

SEM in battery research. Morphology investigation of electrodes.

SEM –investigation of cathode and anode materials in the Li-ion, Ni-metal hydride batteries and electrodes for fuel cells

Topics 8

Analysis of multiphase samples

Obtaining an SEM-image, determination the chemical composition of the elemental distribution of each phase

Topics 9

Analysis of composites with polymers

Preparation for the investigation, image acquisition, and determination of the chemical composition of a composite sample containing polymers (polyethylene, polypropylene, polyaniline, etc.)

Topics 10

Investigation of the samples with concentration polymorphism.

Study of samples with concentration polymorphism, determination of phase composition. Statistical processing of results

Topics 11

Femtosecond laser-induced nano- and microstructuring

Study of functional surfaces obtained by laser processing. Analysis of the formed products

Topics 12

SEM-investigation of biological objects and composite biosensors

Peculiarities of application of samples, research of biocomposites and samples of biological origin, and biosensors

Topics 13

Morphology of superhard materials. Investigation of microhardness of the samples

SEM-research of superhard surfaces and coatings, analysis of the surface of materials after measuring the mechanical properties of the substance (micro-hardness, crack resistance)

Topics 14

Microstructure and phase analysis of MAX phases.

SEM investigation, RXF- and EDX-analysis of multicomponents MAX phases. Dimensional characteristics of 2D microstructures

Topics 15

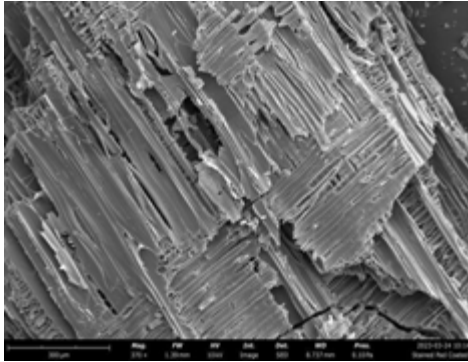
Microstructure and composition of high-entropy alloys

SEM investigation and EDX-analysis of multicomponents high-entropy alloys with mechanical, electrotransport and electrochemical properties

Topics 16

Microstructure and composition of the objects for micro- and nano-electronics

Investigation of the microstructure of various electronic parts to estimate the thickness of the deposited layers and control the composition of functional elements



SEM-image of C-containing sample

TEXTBOOK/READINGS

For a deeper understanding of the course subject matter, optional recommended texts include:

[1] 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.

[2] D. B. Williams and C. B. Carter, *Transmission Electron Microscopy*, Springer, 2009.

[3] Stokes, J. Debbie *Principles and Practice of Variable Pressure Environmental Scanning Electron Microscopy (VP-ESEM)*. Chichester: John Wiley & Sons, 2008.

[4] D. E. Chandler, R. W. Roberson. *Bioimaging: current concepts in light and electron microscopy*. Sudbury, Mass.: Jones and Bartlett Publishers, 2009.

ASSESSMENT

Exam:

The exam will include theoretical and practical tasks and an exercise to determine the dimensional characteristics of particles

Quiz:

A quiz will include theoretical information for carrying out laboratory research

Reports:

Students will be grouped into teams and tasked with producing a written report on their experimental laboratory exercises. The report should include a theoretical background, a description of the experiments conducted, an analysis of the results, and a discussion and conclusions section.

GRADING POLICY

The *Scanning electron microscopy and energy dispersive X-ray analysis for materials science* course is scored with points. The grade results from the sum of points obtained in Exam, Reports and Quiz. The maximum number of points obtained in the laboratory exercises is 100. Student grades will be assessed as follows in the box on the left.

Assignment Weights	Percent
Exam:	50%
8 Reports:	40%
Quiz:	10%
Total	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

COURSE SCHEDULE?

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

* In this field, provide information in what didactic form the course is implemented (e.g. lecture, seminar classes, laboratory, field activities, etc.). If the subject is implemented in several didactic forms (consists of e.g. lecture and laboratory, etc.), all forms of the subject implementation should be indicated. In this field, you should also specify the number of hours organized for a given form of classes (separately for lectures, separately for laboratory classes, etc.).

X-RAY DIFFRACTION: ATOMIC STRUCTURE AND MICROSTRUCTURE

Code: XRDASM

Field of study

Materials Science and Engineering

Level of study

Master Study

Semester

1

Language

English

Thematic block

Advanced Methods for Materials Characterisation

Form of tuition and number of hours*:

Lecture: 16 h

Laboratory: 16 h

ECTS 4

Lecturer:

*Pavlo Demchenko,
PhD, Leading Researcher*

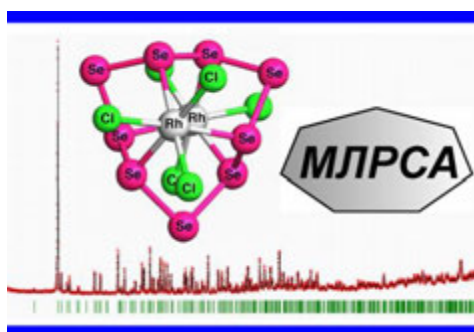
COURSE DESCRIPTION

The aim and task of the course *X-ray Diffraction: Atomic Structure and Microstructure* in the master's study is to acquire theoretical and practical skills for future specialists in the field of Materials Science and Engineering, especially in the methods for materials characterisation using X-ray diffraction. Research methods based on the phenomenon of X-ray diffraction on three-dimensional crystal lattices are today one of the most accurate and accessible for determining the crystal structure of a substance (establishing the number of atoms in the unit cell, its parameters, atomic coordinates, their coordination environment, microstructural parameters (size of coherently diffraction domains, microstrains, textures), etc.). Moreover, XRD is a suitable method for the characterisation of the structure of solids (amorphous glasses, polymers) at short- and medium range order (radial distribution function, first sharp diffraction peak, etc.). In order to master modern methods of X-ray research of both single-crystal and powder objects, it is necessary to have in-depth theoretical knowledge of the geometry, physics and chemistry of crystals, the theory of X-ray scattering, as well as to acquire practical skills in working with modern high-tech equipment, in particular automatic diffractometers, and professional software for X-ray phase and X-ray structural analysis.

The lecture course consists of two main parts: fundamentals of crystalline state and X-ray diffraction together with experimental techniques, crystal structure determination/refinement and microstructural analysis at short-medium- and long-range order. Laboratory classes are devoted to study the crystal structures, preparation of the samples, obtaining XRD raw data, analysis of diffraction data using professional programs, determining the structural and microstructural characteristics of compounds, the influence of crystal structure on the properties of compounds.

COURSE OBJECTIVES

The course *X-ray Diffraction: Atomic Structure and Microstructure* is designed in such a way as to provide students with the necessary knowledge and develop skills with the aim of revealing their own scientific potential. The skills acquired by students will become a valuable tool in their future professional activities as specialists in the field of material science and natural sciences in general. By the end of the course, students will gain an understanding and knowledge of elements of geometry, physics and chemistry of crystals, the theory of X-ray scattering; methods and equipment for investigation of mono- and polycrystalline materials in photographic and diffractometric versions, processing of experimental data using computer programs; and will be able to: determine an unit cell, derive symmetry space groups, describe crystal structures of compounds, analyze interatomic distances, coordination of atoms, build projections of crystal structures, record and index diffractograms, solve and refine crystal structures, perform X-ray phase analysis, specify refined parameters of an unit cell, atomic coordinates, displacement and occupancy parameters, determine microstructural and short-range order parameters.



PREREQUISITES FOR TAKING THE COURSE

To complete the course, it is recommended that learning outcomes related to the basics of chemistry, physics, and materials science be implemented.

LEARNING OUTCOMES OF THE MODULE

Code	Description	Learning outcomes of the programme
MS_O_01	Has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials.	K_01
MS_O_02	Has in-depth, theoretically based, and structured knowledge of modern techniques and research methods used in materials engineering.	K_03
MS_O_03	Can plan and carry out experiments, including measurements and computer simulations, interpret the results, and draw conclusions.	S02 S02_eng
MS_O_04	Can prepare a scientific study and present a presentation on implementing a research task, containing a critical analysis, synthesis, and conclusions.	S05

METHODS OF CONDUCTING CLASSES

Code	Description	Learning outcomes of the programme
Meth_01	Lectures: interactive lectures with scientific discussion, lectures with multimedia support and the use of visual models of crystal polyhedra and structures, laboratory equipment, lectures with problem interpretation	MS_O_01 MS_O_02
Meth_02	Laboratory classes: laboratory work (individual and group tasks), experiment demonstrations, observation, problem learning, debate	MS_O_03 MS_O_04

FORM OF TEACHING

Code	Name	Number of hours	Assessment of the learning outcomes of the module	Learning outcomes of the module	Methods of conducting classes
FT_01	lecture	16	exam	MS_O_01 MS_O_02	Meth_01
FT_02	laboratory	16	course work	MS_O_03 MS_O_04	Meth_02

THE STUDENT'S WORK, APART FROM PARTICIPATION IN CLASSES, INCLUDES IN PARTICULAR

Code	Category	Name	Work with teacher
a_01	Reading literature	Query of materials and review of activities necessary to participate in classes.	NO
a_02	Preparation for classes	Query of materials and review of activities necessary to participate in classes. Preparation and development of reports.	NO
a_03	Preparation of reports	Preparation and development of reports. Consultation.	YES

LEARNING OUTCOMES

Student has extended and in-depth knowledge in the field of general knowledge, which is the basis for understanding complex relationships in the processes of testing of engineering materials. Also, she/he has in-depth, theoretically based and structured knowledge of modern techniques and research methods used in materials science.

By the end of the X-ray Diffraction: Atomic Structure and Microstructure course student will have extensive and in-depth knowledge about:

the ideal and real structure of a solid state, phase transitions,

fundamentals of diffraction,

research equipment,

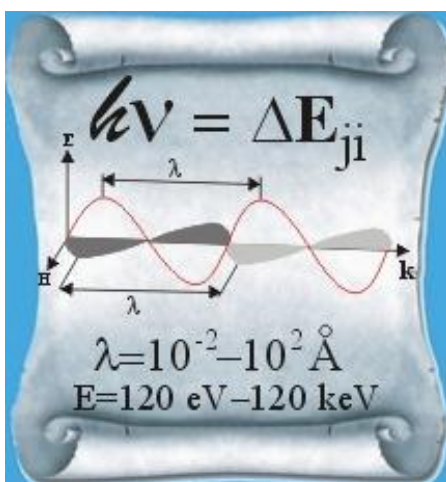
modern trends in the development of structural analysis,

X-ray diffraction methods on mono- and polycrystals,

selection of experimental conditions, stages of data recording and processing.

DO YOU KNOW

In 1901 W. C. Roentgen won the Nobel Prize in Physics for the discovery of X-rays (1895). The first crystal structure ever solved by X-ray diffraction was the one of zinc sulfide ZnS (W. H. Bragg 1912). The first crystal structure solution of LiF from powder was performed in 1916 by P. Debye and P. Scherrer.



COURSE CONTENT – lecture

Topic 1

Fundamentals of crystalline state: Part I

During the lecture, students will be familiarized with the concepts of crystalline state, symmetry operations, crystal systems, Bravais lattices, atomic coordinates, and space groups, and get an idea of ideal, real, and average structures. Students will also learn about the liquids and amorphous substances as examples of short- and medium-range order.

Topic 2

Fundamentals of crystalline state: Part II

The lecture will discuss the types of crystal structures, atomic radii, interatomic distances and angles, close-packed structures, atomic coordination and polyhedra. In addition, students will be familiar with ionic and covalent compounds, VEC, hydrogen bonding, different kinds of defects. Students will be introduced to such concepts as structure types 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.

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 the nature, properties and production of x-rays, x-ray spectra, classification of detectors, scattering factor.

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.

Topic 5

Crystal structure solution

Modern methods of crystal structure determination will be discussed during the lecture. 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.

LEARNING OUTCOMES

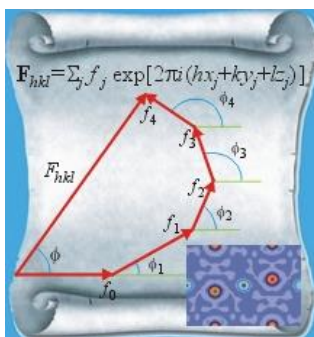
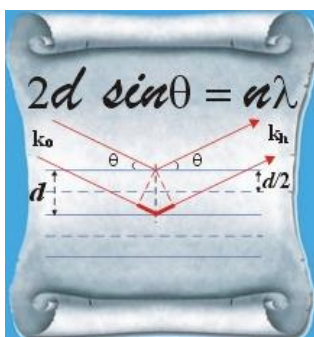
Students can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions. Also, she/he can prepare a scientific study and present a presentation on the implementation of a research task, containing a critical analysis, synthesis and conclusions.

By the end of the X-ray Diffraction: Atomic Structure and Microstructure course student will be able to:

- prepare samples for measurements,
- collect and preliminary proceed experimental XRD data,
- determine structural and microstructural characteristics of compounds using modern crystallographic computer programs,
- perform X-ray phase and structural analysis, together with solve and refine unknown crystal structures,
- carry out the description of the crystal structure.

DO YOU KNOW

In 1985 H. Hauptman and J. Karle won the Nobel Prize in Chemistry for direct methods to determine X-ray structures.



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.

Topic 7

Microstructural analysis

This lecture will focus 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.

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).

COURSE CONTENT – laboratory classes

Topic 1

Applied crystallography

The aim of the laboratory is to define the elements of symmetry, unit cells, planar systems. Establishing syngonies, Bravais lattice types, unit cell parameters, atomic coordinates.

Topic 2

Applied crystal chemistry

The aim of the laboratory is to draw the projections of crystal structures, visualize of crystal structures of compounds. Derivation of space symmetry groups. Coordination of atoms. Space filling factor. The densest packing. Calculation of interatomic distances. Crystal chemical analysis.

Topic 3

XRD data collection

The aim of the laboratory is to prepare the samples, record and obtain raw diffraction data.

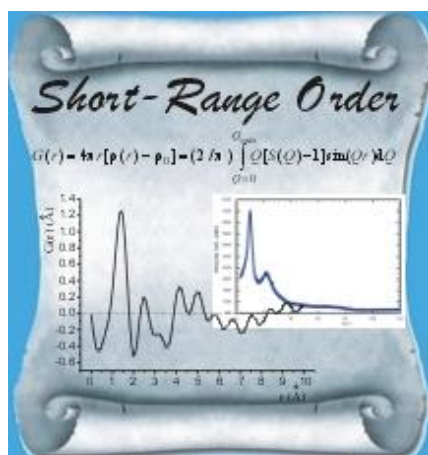
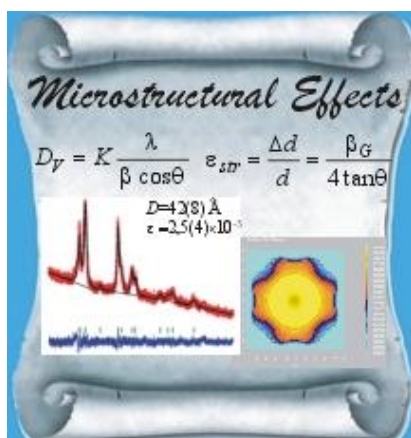
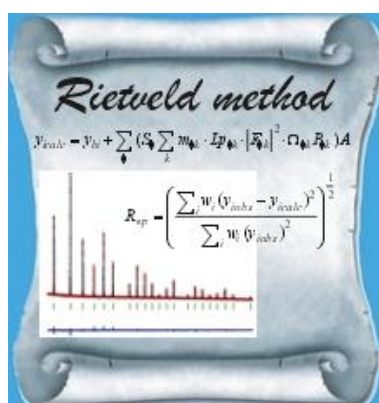
Topic 4

XRD data proceedings

The aim of the laboratory is to familiarize students with corrections of raw XRD data, indexing of diffractograms, unit cell search, phase identification.

LEARNING OUTCOMES

Students can plan and carry out experiments, including measurements and computer simulations, interpret the results and draw conclusions. Also, she/he can prepare a scientific study and present a presentation on the implementation of a research task, containing a critical analysis, synthesis, and conclusions.



Topic 5

Structure solution

The aim of the laboratory is to solve the crystal structure of selected compounds: determine atomic coordinates, displacement parameters, and occupancies, and perform the quality crystal chemical test.

Topic 6

Structure refinement

The aim of the laboratory is to refine the crystal structure parameters of the inorganic compounds: atomic coordinates, displacement parameters, and occupancies, perform the quality and quantitative X-ray phase analysis.

Topic 7

Microstructural analysis

The aim of the laboratory is to evaluate the preferred orientation (texture), calculate the microstructural parameters (size of coherently diffraction domains, microstrains).

Topic 8

Short-range order analysis

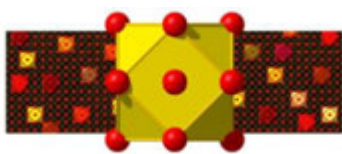
The aim of the laboratory is to obtain radial and pair distribution functions, evaluate other parameters for amorphous solids.

TEXTBOOK/READINGS

The mandatory reading for completing the course *X-ray Diffraction: Atomic Structure and Microstructure*:

1. International Tables for Crystallography (2006). Volume C, Mathematical, physical and chemical tables. <https://it.iucr.org/C/>
2. V.K. Pecharsky, P.Y. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer Science + Business Media, New York (2009) – 741 p.
3. A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons, Chichester, United Kingdom (1984) – 734 p.
4. E. A. Lord, A. L. Mackay, S. Ranganathan, New geometries for new materials, Cambridge University Press, Cambridge (2006) – 257 p.
5. R.A. Young (Ed.), The Rietveld Method, IUCr Monographs of Crystallography. N 5. International Union of Crystallography, Oxford University Press, 1993, 298 p.
6. R.E. Gladyshevskii, Methods to Determine Crystal Structures, Textbook, Publishing Center of Ivan Franko National University of Lviv, Lviv (2015) – 135 p.
7. R.L. Snyder, J. Fiala, H.J. Bunge, Eds., Defect and Microstructure Analysis by Diffraction, Oxford University Press, Oxford (1999) – 785 p.
8. T. Egami, S.J.I. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials, Elsevier, Pergamon Materials Series (2012) – 422 p.

Pearson's Crystal Data
Crystal Structure Database for Inorganic Compounds



INFORMATION RESOURCES:

1. 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).
2. P. Villars, K. Cenzual, Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds, ASM International, Materials Park (OH) (2023).
3. International Centre for Diffraction Data® (ICDD®) Home Page XRD Database. <https://www.icdd.com/>

ASSESSMENT

Reports:

The reports are the result of the student's work during the laboratories; they relate to in-depth theoretical and practical knowledge of the exercises performed. They consist of a theoretical introduction, a description of the purpose, the implementation of an experimental or calculation task, and conclude with a discussion of the obtained results and conclusions.

Tests:

During the semester, the tests reflect the student's current academic performance.

Debate:

During the debate, the ability to make logical arguments and explain their relevance to the topic, the ability to answer the questions of other participants, and the ability to actively listen and participate in the discussion with other participants of the debate will be evaluated.

Exam:

The exam verifies overall theoretical knowledge and practical skills in the field of crystal chemistry, X-ray diffraction and materials science.

GRADING POLICY

The student is obliged to perform the 8 laboratories, 3 tests, and debate, which gives in a maximum of 100 points.

The exam is conducted in a written form – 2 questions from the knowledge contained theory and 4 questions of practical aspects. The maximum number of points to be obtained in the exam is 100.

The final evaluation is made based on the student achievement scoring system. The grade results from the sum of points obtained by the student during the semester by the evaluation of three types of work (laboratory work, test, debate) and points received during the exam. The final grade is determined by 50% of the points obtained in the exam and 50% of the points obtained in the laboratories. According to the table on the left, the sum of the percentages will result in the final grade.

Assignment Weights	Percent
Laboratories:	
8 Reports	40%
3 Tests	45%
Debate	15%
Total	100%
Reports - max. 40 points	
Tests – max. 45 points	
Debate – max. 15 points	
Total points – max. 100 points	
Exam	100%
max. 100 points	
Final grade:	
Laboratories	50%
Exam	50%
Total	100%
Grading Scale:	
90-100 points = A	
80-89 points = B	
70-79 points = C	
60-69 points = D	
51-59 points = E	
0-50 points = F	



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COURSE SCHEDULE

Day	Date	Topic	Assignment	Due Today
1				
2				
3				
4				
5				

MATERIALS SCIENCE MA(S)TERS

developing a new master's degree

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).



Co-funded by
the European Union

This project has been funded with support from the European Commission. This publication reflects the views only of the author and the Commission cannot be held responsible for any use which may be made of the information contained therein.



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