GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Crystallochemistry, PG_00048984		
Field of study	Corrosion		
Date of commencement of studies	February 2023	Academic year of realisation of subject	2022/2023
Education level	second-cycle studies	Subject group	Optional subject group Subject group related to scientific research in the field of study
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	1	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Jarosław Chojnacki	
	Teachers	prof. dr hab. inż. Jarosław Chojnacki	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	30.0	0.0	0.0	45

E-learning hours included: 0.0

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	45	5.0	25.0	75

Subject objectives

Students know basics of crystallography and crystal chemistry

Learning outcomes

Course outcome	Subject outcome	Method of verification
K7_U01	uses Mercury program for deep analyses of crystal structures. Can gather information from Crystal Structure Database. Can interprete powder diffractograms. Understands meaning of space group symbols	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
K7_W01	knows meaning of basic terms in crystallography: unit cell, asymmetric unit, Miller indices of planes, symmetry in crystal. Knows basic types of inorganic structures. Knows relations between symmetry and physical properties of materials. Knows how to access quality of diffraction measurement, Can prepare description of a new crystal structure including analysis of intermolecular interactions in the solid state based on a given CIF file.	[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects

Subject contents	Lecture: 1. Fundamentals of crystallography: crystal, unit cell, crystallographic system, indexing of nodes, directions and planes. Changing coordinate systems. 2. Symmetry of finite objects. Point symmetry groups. 3. Symmetry of infinite objects. Space groups. 4. Symbols of space groups. Presentation of symetry in International Tables for Crystallography and Mercury program. 5. Practical significance of assigning space groups 6. Diffraction phenomenon. Reciprocal space. Ewald sphere. 7. Diffraction on monocrystals and powders. Analysis of diffractograms, identification of phases and size of crystals (Scherrer equation) 8. Systematic absencies. Overview of crystal structure determination. 9. Dense packing, coordination numbers. Description of typical structures of elements and chemical compounds 10 Polymorphism and isomorphism, solid solutions. 11.Theory of crystallization, Industrial and laboratory methods for crystal growing. 12. Typical description of crystal structures 13. Relation between physical properties and crystal symmetry 15. Cryocrystallography and high-pressure crystallography. Laboratory 1. Calculation of theoretical density. Stoichiometry of the elemental cell, transformations of coordinate systems 2. Indexing planes and directions in crystals. 3. Point groups. Assignment of symbols for given objects. 4. Exercises with space group symmetry international symbols. 5. Exercises in application of the Laue equation for the interpretation of diffraction patterns. 6. Analysis of powder diffractogams. 7. Presentation of real X-ray diffraction experiment 8. Phishing information in CSD database and analysis of results by available computer programs. Preparation of a structural report based on the supplied CIF file. 9. The influence of crystallization conditions on crystal growth. Principles of crystals morphology. 10. Growing crystals by sublimation or from melt. 11. Crystallization process, seeding and crystal growth rate. 12. Optical properties of crystals. Polarisation microscopy in crystallography.
Prerequisites and co-requisites	
Assessment methods and criteria	

Subject passing criteria	Passing threshold	Percentage of the final grade
Written exam	60.0%	49.0%
Midterm colloquium + reports	60.0%	51.0%

Recommended reading	Basic literature	1. Z. Kosturkiewicz: Metody krystalografii. Wydawnictwo Naukowe UAM, Poznań 2000. (ISBN 83-232-1040-3) 2. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, Krystalografia. Wydawnictwo Naukowe PWN, Warszawa 2007. (ISBN 978-83-01-14704-4) 3. Z. Trzaska Durski, H Trzaska Durska, Podstawy krystalografii strukturalnej i rentgenowskiej. Wydawnictwo Naukowe PWN, Warszawa 1994. (ISBN 83-01-11388-X).
	Supplementary literature	1. Muzeum Geologiczne Wydziału Nauk Geogr. Uniw. Łódzkiego, Kryształy w przyrodzie i technice, Wydawnictwo UŁ, Łódź 2005 (ISBN 83-7171-856-X). 2. P. Luger, Rentgenografia strukturalna monokryształów. PWN Warszawa 1989 (ISBN 83-01-08815-X)
	eResources addresses	
Example issues/ example questions/ tasks being completed	Based on space group symbol specify: crystal system, point symmetry of crystals and presence or absence of inversion center in structure for selected groups a) $P6_3/mmc$ and b) $I4_32_12$ Draw schematically structure of tungsten (A2 type) and perovskite $CaTiO_3$.	
Work placement	Not applicable	