

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in English: Advanced diffraction methods
 Main field of study (if applicable): Materials Engineering
 Specialization (if applicable): Advanced functional materials
 Profile: academic
 Level and form of studies: 2nd level, full-time
 Kind of subject: obligatory
 Subject code:
 Group of courses: NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30	15	15		
Number of hours of total student workload (CNPS)	90	30	60		
Form of crediting	Exam	Crediting with grade	Crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	3	1	2		
including number of ECTS points for practical (P) classes		1	2		
including number of ECTS points for direct teacher-student contact (BK) classes	1,3	0,7	0,7		

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General knowledge of mathematics, physics and chemistry.

SUBJECT OBJECTIVES

- C1 The enlargement of knowledge of structure of periodic crystals and quasi crystals. Knowledge of structure of nanocrystals.
 C2 Knowledge of diffraction methods for single crystals, micro- and nanocrystalline materials and macromolecular crystals.
 C3 Understanding the relationships between a diffraction pattern and internal crystal structure.
 C4 Knowledge of the most important crystallographic programs.
 C5 Understanding crystal data in scientific papers.

SUBJECT LEARNING OUTCOMES

related to knowledge:

A person who has completed the course:

- PEK_W01 – has knowledge of structure of macro-, micro- and nanocrystals, macromolecular crystals and quasi crystals.
 PEK_W02 – knows the diffraction methods for macro- micro and nanocrystals and macromolecular crystals.
 PEK_W03 – knows the relationships between a diffraction pattern and crystal internal structure.
 PEK_W04 – knows the most important crystallographic programs.
 PEK_W05 – understands crystallographic data in scientific papers

related to skills:

A person who has completed the course:

- PEK_U01 – is able to create graphical representations for space groups and point groups.
 PEK_U02 – is able to interpret symmetry of diffraction patterns.
 PEK_U03 – is able to determine an internal crystal structure at an atomic level.
 PEK_U04 – is able to analyze powder diffractograms.

PEK_U05 – is able to use the most important crystallographic programs. related to social competences: A person who has completed the course: PEK_K01 – is able to take part in discussions about crystallographic structural studies. PEK_K01 – understands the importance of crystallography in science and industry.		
PROGRAMME CONTENT		
Lectures		Number of hours
Lec 1	Periodic crystals. A crystal lattice: lattice points, row lines, lattice planes and their symbols. Mosaic structure.	2
Lec 2, Lec 3	Symmetry elements and operations. Crystal systems. Unit cells. An asymmetric unit cell. The international symbols and graphical representations of space groups.	4
Lec 4	The relationships between internal and external structures of crystals. A point group as a group. The types of point groups vs crystal properties.	2
Lec 5, Lec 6	Synchrotron radiation: sources, properties. Crystallographic synchrotron studies.	4
Lec 7	Factors influencing reflection intensities. Diffraction pattern symmetry vs crystal symmetry. The determination of a crystal system and a space group.	2
Lec 8	Polymorphism. Hirshfeld surfaces.	2
Lec 9, Lec 10	Nanocrystals: internal structure, external structure, diffraction, properties.	4
Lec 11, Lec 12	Macromolecular crystallography: crystallization, crystal symmetry, a phase problem and its solution, structure quality, examples.	4
Lec 13	High pressure crystallography. Photo-induced structural transformations. Examples.	2
Lec 14	Neutronography.	2
Lec 15	Aperiodic crystals: internal structure, symmetry, diffraction, properties, applications. The summary of the lectures.	2
	Total hours	30
Classes		Number of hours
Cl 1, Cl 2	Selected space groups: graphical representations, international symbols, symmetry codes.	6
Cl 3	Selected points groups: graphical representations, international symbols.	3
Cl 4	The analysis of diffraction patterns and selected diffraction groups.	3
Cl 5	The test concerning Proj1 - Proj4. Indexing powder diffractograms.	3
	Total hours	15
Laboratory		Number of hours

Lab 1	The graphical representations of crystal lattices by the <i>Mercury</i> program. Molecular geometry, intermolecular geometry, crystal data.	3
Lab 2	Powder diffractograms for pure components and mixtures.	3
Lab 3	Data collection: single crystal preparation, centering, cell parameters determination, data collection.	3
Lab 4	Phase problem solutions using <i>Shelxs</i> and data collection files. E map interpretation.	3
Lab 5	Refinement using <i>Shelxl</i> and the analysis of results. The presentation of a scientific crystallographic paper.	3
	Total hours	15
TEACHING TOOLS USED		
N1. A multimedia presentation N2. A blackboard N3. Solutions of crystallographic problems N4. A diffractometer N5. Crystallographic programs		
EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT		
Evaluation (F – forming (during semester), P – concluding (at semester end))	Educational effect number	Way of evaluating educational effect achievement
F1 (lecture)		Exam
F2 (classes)		Test
F3 – F7 (laboratory)		4 tests, 1 multimedia presentation, reports
P1=F1 P2=F2 P3=(F3+F4+F5+F6+F7)/5		
PRIMARY AND SECONDARY LITERATURE		
PRIMARY LITERATURE:		
[1] Z. Kosturkiewicz, <i>Metody krystalografii</i> , Wydaw. Naukowe UAM, 2000, 2004. [2] P. Luger, <i>Rentgenografia strukturalna monokryształów</i> , PWN, Warszawa, 1989. [3] Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, <i>Krystalografia</i> , PWN, Warszawa, 2007, 2008. [4] <i>Modern Diffraction Methods</i> , E. J. Mittemeijer and U. Welzel Eds., Wiley-VCH Verlag GmbH, Weinheim, 2013.		
SECONDARY LITERATURE:		
[1] C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti, <i>Fundamentals of crystallography</i> , C. Giacovazzo Ed., Oxford, 2002, 2011. [2] International Tables for Crystallography, Volume A, Kluwer Academic Publishers, 1996; Springer, 2005. [3] Instrukcje do ćwiczeń z krystalografii, pod redakcją Z. Ciunika, Wyd. Uniwersytetu Wrocławskiego, Wrocław 1995, 1999. [4] Internal instructions for the laboratories.		
SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)		
Prof. dr hab. Ilona Turowska-Tyrk, ilona.turowska-tyrk@pwr.edu.pl		