FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in English: Structure and crystallography of solids
Main field of study (if applicable): Chemical and Process Engineering, Chemistry
Specialization (if applicable): Chemical Nano-Engineering, Medicinal Chemistry
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code: ICC025001
Group of courses: NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30	15			
Number of hours of total student workload (CNPS)	60	30			
Form of crediting	crediting with grade	crediting with grade			
For group of courses mark (X) final course					
Number of ECTS points	2	1			
including number of ECTS points for practical (P) classes		1			
including number of ECTS points for direct teacher-student contact (BK) classes	1	0,5			

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General knowledge of mathematics, physics and chemistry.

SUBJECT OBJECTIVES

C1 Knowledge of the structure, symmetry and diffraction of macro-, micro- and nanocrystals.
C2 Knowledge of directions of development of crystallography.
C3 Understanding data in crystallographic papers.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

A person who has completed the course:
PEK_W01 has knowledge of the structure and symmetry of crystals.
PEK_W02 understands the international symbols and graphical representation of space groups and the international symbols of crystal classes.
PEK_W03 knows the relationships between a diffraction pattern and crystal structure.
PEK_W04 has knowledge of directions of development of crystallography.

relating to skills:

A person who has completed the course:
PEK_U01 is able to study scientific literature on crystal structures and to evaluate crystal data.

related to social competences:

A person who has completed the course:
PEK_K01 is able to take part in discussions on crystallographic structural studies.
PEK_K01 understands the importance of crystallography in science and industry.

PROGRAMME CONTENT

Lectures		**Number of hours**
Lec 1	The historical and current definitions of crystals and crystallography. The internal structure of crystals. A crystal lattice, row lines, lattice planes, Miller symbols, a unit cell and cell types. The mosaic structure of real crystals, dislocations.	2
Lec 2, Lec 3	The internal symmetry of crystals. Symmetry elements and operations. Relationships between the internal and external symmetry of crystals. Crystal systems *vs* symmetry.	4
Lec 4	Crystal systems and cell parameters. The conventional choice of unit cells. The Bravais unit cells.	2
Lec 5	Space groups: international symbols and graphical representations. An asymmetric unit cell.	2
Lec 6	Relationships between the symbol of a space group and the symbol of a point group (crystal class). The types of point groups.	2
Lec 7	Examples of crystal structures. Crystallographic databases.	2
Lec 8	X-rays: properties and sources. Synchrotron radiation: sources of the first, second, third and fourth generations and properties. Synchrotron crystallographic studies.	2
Lec 9, Lec 10	The directions and intensities of diffracted beams. Factors influencing the directions and intensities. The phase problem. Diffraction pattern *vs* internal structure and symmetry of crystals.	4
Lec 11	Neutronography and electronography *vs* roentgenography. Crystallographic information files (cif).	2
Lec 12, Lec 13	Nanocrystals. The quantitative and qualitative definition. The internal structure of nanocrystals *vs* macrocrystals. Defects. External appearance. Diffraction in nanocrystals vs diffraction in microcrystalline materials. The broadening and shifting of peaks in powder diffraction patterns. Apparent lattice parameters: determination and influencing factors. Properties. Synchrotron crystallographic studies of nanocrystals.	4
Lec 14	Quasi crystals: 1D, 2D and 3D-dimensional. Internal and external structure. Diffraction. Properties.	2
Lec 15	Crystallographic data in scientific papers.	2
	Total hours	30
Classes		**Number of hours**
Proj 1	The preliminary classes.	1
Proj 2	Lattice points, row lines, lattice planes.	1
Proj 3, Proj 4, Proj 5	Symmetry elements: an inversion center, a mirror plane, rotation axes, rotoinversion axes. .	3
Proj 6, Proj 7	Screw axes and glide planes.	2
Proj 8	Bravais lattices.	1
Proj 9	Partial test I	1

Proj10, Proj 11	Systematic absences.	2
Proj12, Proj 13	Crystal classes: symbols and graphical representation	2
Proj 14	Physical properties of crystals.	1
Proj 15	Partial test II	1
	Total hours	15

TEACHING TOOLS USED

N1. A multimedia presentation
N2. Crystallographic models
N3. A blackboard

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1 (lectures)	PEK_W01, PEK_W02	partial test I
F2 (lectures)	PEK_W03, PEK_W04	partial test II
F3 (classes)	PEK_W01, PEK_W02	partial test I
F4 (classes)	PEK_W03, PEK_U01	partial test II

P1=(F1+F2)/2
P2=(F3+F4)/2

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] P. Luger, Modern X-Ray Analysis on Single Crystals, de Gruyter, Berlin, 2014.
[2] R. J. D. Tilley, Crystals and Crystal Structures, John Wiley & Sons Ltd, Chichester, 2006.

SECONDARY LITERATURE:

[1] C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti, Fundamentals of crystallography, C. Giacovazzo Ed., Oxford, 2011.
[2] International Tables for Crystallography, Volume A, Springer, 2005; Willey 2016.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Ilona Turowska-Tyrk, professor (ilona.turowska-tyrk@pwr.edu.pl)