GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Diffraction Methods for Structural Characterization of Materials, PG_00069345		
Field of study	Nanotechnology		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2026/2027
Education level	first-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	Polish
Semester of study	4	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Solid State Physics -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Tomasz Klimczuk	
	Teachers	prof. dr hab. inż. Tomasz Klimczuk	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	15.0	0.0	0.0	15

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	15	3.0	32.0	50

Subject objectives

The aim of the course is to train students with the various diffraction methods and computer tools for analysis xrd data and visualization of crystal structures.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U02] can analyze and solve simple scientific and technical problems based on possessed knowledge, applying analytical, numerical, simulation and experimental methods.	Students solve scientific problems based on their knowledge. In doing so, they apply the methods they have learned in other subjects.	[SU2] Assessment of ability to analyse information
[K6_W07] has systematic knowledge of the physical and chemical principles of nanotechnology (methods of obtaining nanostructures, types of nanostructures, their properties, basic research methods).	The student has knowledge of how various nanostructures are obtained, what their physical properties are, and how these properties can be studied.	[SW3] Assessment of knowledge contained in written work and projects
[K6_U04] can plan and conduct experiments, critically analyze their results, draw conclusions and formulate opinions. Has laboratory experience.	The student is ready for laboratory work. He plans and conducts experiments, analyzes the results very carefully, draws only accurate conclusions, and formulates only brilliant opinions.	[SU4] Assessment of ability to use methods and tools

Subject contents

Course content – laboratory

1. Introduction to the course. 2. Diffraction methods. 3. Introduction to Database ICSD / FindIt and CoD. Simulations using PowderCell. 4. Visualization of crystal structures using VESTA. 5. Introduction to the Rietveld method and LeBail. 6. Mathematical basis of the Rietveld method. .

Prerequisites and co-requisites

Basic knowledge in crystallography.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Practical test	60.0%	40.0%
Final test	60.0%	60.0%

Recommended reading	Basic literature	1. FullProf manual: https://www.psi.ch/sinq/dmc/ManualsEN/fullprof.pdf 2. L.B. McCusker, et al. *Rietveld refinement guidelines*, J. Appl. Cryst. (1999) vol. 32, 36-50 3. B. H. Toby, *R-factors: how good is good enough?*, Powder Diffraction (2006) vol. 21, 67-70 4. D. S. Sivia*, Elementary Scattering Theory For X-ray and Neutron Users,* Oxford University Press (2014) 5. H. M. Rietveld, A profile refinement method for nuclear and magnetic structures, Journal of Applied Crystallography (1969) vol. 2, 65-71 http://epswww.unm.edu/media/pdf/Rietveld-1969-ProfileRefinement.pdf
	Supplementary literature	1. G. Will, *Powder Diffraction: The Rietveld Method and the Two Stage Method to Determine and Refine Crystal Structures from Powder Diffraction Data*, Springer (2006) http://link.springer.com/book/10.1007/3-540-27986-5
	eResources addresses	
Example issues/ example questions/ tasks being completed	Using Vesta software draw and then discuss the details of the structure of Mg10Ir19B16 compound.	
Practical activites within the subject	Not applicable	

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