GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Diffraction methods of structural analysis, PG_00058968		
Field of study	Nanotechnology		
Date of commencement of studies	October 2022	Academic year of realisation of subject	2024/2025
Education level	first-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	3	Language of instruction	Polish
Semester of study	5	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Solid State Physics -> Faculty of Applied Physics and Mathematics		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Tomasz Klimczuk	
	Teachers	prof. dr hab. inż. Tomasz Klimczuk	

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	0.0	0.0	45

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_K05	The student critically evaluates his own performance, constructively evaluates the results of the work of others.	[SK2] Assessment of progress of work
K6_W07	The student is an expert in the physical and chemical basis of nanotechnology.	[SW2] Assessment of knowledge contained in presentation
K6_U06	The student accurately, clearly but not oversimplified, explains even the most intricate technological and scientific problems related to the manufacture and applications of nanostructures.	[SU2] Assessment of ability to analyse information

Subject contents

1. Introduction to the course. (2 hours)2. Diffraction methods. (4 hours)3. Introduction to Database ICSD / FindIt and CoD. Simulations using PowderCell. (2 hours)4. Visualization of crystal structures using VESTA. (4 hours)5. Introduction to the Rietveld method and LeBail. (2 hours)6. Mathematical basis of the Rietveld method. (2 hours)7. Package FullProf Suite. (6 hours)8. Neutron diffraction methods. (4 hours)9. Practical aspects of measurements of neutron and synchrotron (infrastructure, applying for beamtime, sample preparation, etc.). (2 hours)10. The future of diffraction methods. (2 hours)

Prerequisites and co-requisites

Basic knowledge in crystallography.

Assessment methods and criteria

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

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	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	Using Vesta software draw and then discuss the details of the structure of Mg10Ir19B16 compound.	
Work placement	Not applicable	