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 2021		Academic year of realisation of subject		2023/2024		
Education level	first-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	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 dr inż. Michał Winiarski					

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_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
	K6_W07	The student is an expert in the physical and chemical basis of nanotechnology.	[SW2] Assessment of knowledge contained in presentation
	K6_K05	The student critically evaluates his own performance, constructively evaluates the results of the work of others.	[SK2] Assessment of progress of work

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
	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	Adresy na platformie eNauczanie: Dyfrakcyjne Metody Badań Strukturalnych - Moodle ID: 33551 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=33551

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