



## 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 2024		Academic year of realisation of subject		2025/2026		
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	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 -> Wydział Politechniki Gdańskiej						
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	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_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		
	[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_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		
Subject contents	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
	Final test	60.0%	60.0%
	Practical test	60.0%	40.0%
Recommended reading	Basic literature	<ol style="list-style-type: none"><li>1. FullProf manual: <a href="https://www.psi.ch/sinq/dmc/ManualsEN/fullprof.pdf">https://www.psi.ch/sinq/dmc/ManualsEN/fullprof.pdf</a></li><li>2. L.B. McCusker, et al. <i>Rietveld refinement guidelines</i>, J. Appl. Cryst. (1999) vol. 32, 36-50</li><li>3. B. H. Toby, <i>R-factors: how good is good enough?</i>, Powder Diffraction (2006) vol. 21, 67-70</li><li>4. D. S. Sivia, <i>Elementary Scattering Theory For X-ray and Neutron Users</i>, Oxford University Press (2014)</li><li>5. H. M. Rietveld, A profile refinement method for nuclear and magnetic structures, Journal of Applied Crystallography (1969) vol. 2, 65-71 <a href="http://epswww.unm.edu/media/pdf/Rietveld-1969-ProfileRefinement.pdf">http://epswww.unm.edu/media/pdf/Rietveld-1969-ProfileRefinement.pdf</a></li></ol>	
	Supplementary literature	<ol style="list-style-type: none"><li>1. G. Will, <i>Powder Diffraction: The Rietveld Method and the Two Stage Method to Determine and Refine Crystal Structures from Powder Diffraction Data</i>, Springer (2006) <a href="http://link.springer.com/book/10.1007/3-540-27986-5">http://link.springer.com/book/10.1007/3-540-27986-5</a></li></ol>	
	eResources addresses		
	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		

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