GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Diffraction methods in nanotechnology, PG_00071200		
Field of study	Nanotechnology		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2026/2027
Education level	second-cycle studies	Subject group	Obligatory subject group in the field of study 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	1	Language of instruction	Polish
Semester of study	1	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		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	10.0	0.0	15.0	0.0	0.0	25

E-learning hours included: 0.0

eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=3977

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	25	1.0	24.0	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
[K7_U04] is able to formulate hypotheses, plan and conduct experimental research, critically analyze results, verify hypotheses, draw conclusions, and formulate well-founded opinions within nanotechnology and related physical and natural sciences. Recognizes economic and non-technical aspects of the activities performed	Both male and female students will formulate hypotheses, plan and conduct experimental research, critically analyze results, draw conclusions, and formulate opinions.	[SU5] Assessment of ability to present the results of task
[K7_U03] has enhanced abilities of using advanced specialist software packages	Both male and female students will acquire practical skills. They will learn to use the VESTA and GSAS II programs.	[SU4] Assessment of ability to use methods and tools
[K7_W04] has theoretical and practical knowledge of physical and chemical experimental methods in nanotechnology and understands the principles of their application in processes occurring throughout the life cycle of technical systems	Both male and female students will gain practical and theoretical knowledge of physical and chemical experimental methods in nanotechnology.	[SW2] Assessment of knowledge contained in presentation

Subject contents

Course content – lecture

1. Introduction to the course. (1/2 hour)
2. Diffraction techniques (techniques for testing single crystals, polycrystals, etc.). (2 1/2 hours)
3. Introduction to the ICSD/FindIt and CoD databases. Simulations using the PowderCell program (2 hours)
4. Imaging of crystallographic structures using VESTA software. (1 hour)
5. Introduction to the Rietveld and LeBail methods. (1 hour)
6. Mathematical foundations of the Rietveld method. (1 hour)
7. GSAS II package. (1 hour)
8. Summary. (1 hour)

Course content – laboratory

1. Simulations of diffractograms for various crystal structures.
2. Drawing unit cells using the VESTA program.
3. Indexing diffractograms.
4. Le Bail and Rietveld analysis of X-ray diffractograms.

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

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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