Symmetries in crystal systems

Course description sheet

Basic information

Field of study Technical Physics	**Didactic cycle** 2025/2026
Major All	**Course code** JFTCS.IIi1.12381.25
Organisational unit Faculty of Physics and Applied Computer Science	**Lecture languages** Polish
Study level Second-cycle (engineer) programme	**Mandatoriness** Obligatory
Form of study Full-time studies	**Block** Major Modules
Profile General academic	**Course related to scientific research** Yes

Course coordinator	Radosław Strzałka
Lecturer	Radosław Strzałka

Period	**Method of verification of the learning outcomes**	**Number of ECTS credits**
Semester 1	Completing the classes **Activities and hours** Lectures: 15 Project classes: 30	4

Goals

C1	Zapoznanie studenta z podstawowymi symetriami w strukturze atomowej ciał stałych, w szczególności w kryształach periodycznych i aperiodycznych.
C2	Pokazanie związku symetrii (periodyczności) z budową atomową i konsekwencje tego związku dla metod analizy strukturalnej kryształów.
C3	Zapoznanie studenta z powszechnie stosowanymi narzędziami informatycznymi do analizy strukturalnej kryształów; wykorzystanie tych narzędzi do konkretnych zastosowań w krystalografii.

Course's learning outcomes

Code	Outcomes in terms of	Learning outcomes prescribed to a field of study	Methods of verification
Knowledge – Student knows and understands:			
W1	the concept of symmetry in the atomic structure and its influence on the atomic structure of crystals	FTC2A_W01, FTC2A_W03, FTC2A_W04	Activity during classes, Participation in a discussion
W2	features of the diffraction pattern, methods of its formation, and relationship with the atomic structure of crystals	FTC2A_W01, FTC2A_W03, FTC2A_W04	Activity during classes, Participation in a discussion
W3	the idea of structure refinement based on diffraction data, related problems, and examples of methods	FTC2A_W01, FTC2A_W03, FTC2A_W04	Activity during classes, Participation in a discussion
W4	what are periodic and aperiodic crystals, what are the differences in atomic structure, diffraction pattern, and crystallographic methods for their description	FTC2A_W01, FTC2A_W03, FTC2A_W04	Activity during classes, Participation in a discussion
Skills – Student can:			
U1	analyze the image of powder diffraction on the crystal using dedicated and self-developed tools	FTC2A_U01, FTC2A_U04	Execution of exercises, Project, Involvement in teamwork
U2	carry out the refinement of simple crystal structures using dedicated tools	FTC2A_U01, FTC2A_U04	Execution of exercises, Project, Involvement in teamwork
U3	perform a basic analysis of the diffraction pattern and atomic structure in aperiodic systems	FTC2A_U01, FTC2A_U04	Execution of exercises, Project, Involvement in teamwork
Social competences – Student is ready to:			
K1	take part in a discussion on a given problem and present the results of their own solutions to the problem in the forum of the group.	FTC2A_K01	Participation in a discussion, Involvement in teamwork
K2	collaborate in a small team or a larger group on a given issue, using their knowledge and skills to solve a complex problem	FTC2A_K02	Participation in a discussion, Involvement in teamwork

Program content ensuring the achievement of the learning outcomes prescribed to the module

Lectures on theoretical issues and discussing the available methods and tools in the structural analysis of crystals, as well as practical (design) classes aimed at familiarizing yourself with the functionality of these tools and independently applying them in given problems of crystal physics.

Student workload

Activity form	Average amount of hours* needed to complete each activity form
Lectures	15

Project classes	30
Preparation of project, presentation, essay, report	30
Preparation for classes	15
Realization of independently performed tasks	30

Student workload	**Hours** 120
Workload involving teacher	**Hours** 45

* hour means 45 minutes

Program content

No.	Program content	Course's learning outcomes	Activities
1.	Fundamentals of crystallography (reminder): symmetries, crystal structures, unit cell, structural factor, crystal diffraction, basics of structural analysis	W1	Lectures
2.	Symmetry in crystals: elements of symmetry; crystal lattices; point groups, space groups, Laue classes; crystallographic systems; multidimensional symmetries	W1	Lectures
3.	X-ray diffraction on crystals: crystal symmetry and diffraction pattern; structure solution, atomic density map; phase problem	W2	Lectures
4.	Fundamentals of methods for refining periodic structures: phase recovery; atomic structure model; iterative methods; examples of refinements	W3	Lectures
5.	Modulated structures: modulation vector, proportional and disproportionate modulation; diffraction pattern; the idea of the multidimensional method (superspace); examples	W2, W3, W4	Lectures
6.	Quasicrystals: atomic structure and diffraction pattern; quasicrystal families; basic properties and applications; modeling methods; refinement; multivariate method.	W1, W2, W3, W4	Lectures
7.	The statistical method of describing quasicrystals: the concept of the mean unit cell; disorder modeling; relationship with the multivariate method	W3, W4	Lectures

No.	Program content	Course's learning outcomes	Activities
8.	1. Modeling and visualization of the atomic structure (VESTA program) 2. Diffraction on crystals (powder and single crystals): indicating the diffraction pattern, solving the structure (CrysAlis, FullProf) 3. Refinement of monocrystalline structures (JANA2006 program) 4. Phase recovery, atomic density maps (structure solution): direct method, LDE method, charge flipping (Superflip program, lodemac) 5. Diffraction and structural analysis of quasicrystals: statistical and multivariate method (dedicated programs, QUASI package)	U1, U2, U3, K1, K2	Project classes

Extended information/Additional elements

Teaching methods and techniques :

Discussion, Group work

Activities	Methods of verification	Credit conditions
Lectures	Activity during classes, Participation in a discussion	none
Project classes	Activity during classes, Participation in a discussion, Execution of exercises, Project, Involvement in teamwork	participation in exercises and implementation of tasks, or project execution

Additional info

The lecture is theoretical and introduces the issues of structural analysis of crystals. As part of the project exercises, the student has the opportunity to apply theoretical knowledge and dedicated and own tools to analyze selected examples of crystal structures in two ways: (1) by participating in classes and performing exercises under the supervision of the tutor, or (2) by completing the project (independently or small teams). The path (1) of the student's participation in the exercises requires the student to use their own computer equipment (laptop). In path (2): project topics will be defined by the teacher at the beginning of the class. Projects can be submitted in the form of a study (essay, report + computer programs, if any), or during the presentation at the last class.

Conditions and the manner of completing each form of classes, including the rules of making retakes, as well as the conditions for admission to the exam

During the classes, the following are assessed:

- student activity during lectures and exercises (participation in discussions, involvement in work)
- implementation of tasks during exercises, including independence, the degree of mastery of tools, obtaining results (path (1))
- project, including the degree of advancement of the topic and correct implementation of the topic, method of presenting the result (path (2))

Method of determining the final grade

Assessment of the implementation of tasks during exercises (path (1)) or assessment for the project (path (2)) will be increased by activity during the lecture or exercises.

Manner and mode of making up for the backlog caused by a student justified absence from classes

Independent work on the issue raised during classes, consultation with the teacher in order to clarify doubts.

Rules of participation in given classes, indicating whether student presence at the lecture is obligatory

1. Participation in the lecture is optional (in accordance with the AGH Study Regulations)
2. Participation in the design exercises is:
    - compulsory, if the student chooses the path (1) of carrying out the classes (performing exercises recommended by the teacher on an ongoing basis)
    - optional, if the student chooses the path (2) of the course (project)

Literature

Obligatory

1. "Fundamentals of Crystallography", C. Giacovazzo, H.L. Monaco, G. Artioli, D. Viterbo, G.Ferraris, G. Gilli, G. Zanotti, M. Catti, z serii IUCr Texts on Crystallography, Oxford University Press 2002 (lub starsze/nowsze)
2. "Rentgenografia strukturalna monokryształów", P. Luger, PWN Warszawa 1989.
3. "Crystallography of Quasicrystals. Concepts, Methods and Structures", W. Steurer, S. Deloudi, Springer-Verlag Berlin Heidelberg 2009.
4. "Quasicrystals. A Primer", C. Janot, z serii Ofxord Science Publications, Oxford Univeristy Press, New York 1992.

Optional

1. Statistical approach to diffraction of periodic and non-periodic crystals – review / Radosław STRZAŁKA, Ireneusz BUGAŃSKI, Janusz WOLNY // Crystals [Dokument elektroniczny]. — Czasopismo elektroniczne ; ISSN 2073-4352. — 2016 vol. 6 iss. 9, [art. no.] 104, s. [1-19]. — Wymagania systemowe: Adobe Reader. — Tryb dostępu: http://www.mdpi.com/2073-4352/6/9/104/pdf [2016-09-27]. — Bibliogr. s. 17–19, Abstr.. — Publikacja dostępna online od: 2016-08-26
2. Model refinement of quasicrystals / Janusz WOLNY, Ireneusz BUGAŃSKI, Radosław STRZAŁKA // Crystallography Reviews ; ISSN 0889-311X. — 2018 vol. 24 no. 1, s. 22–64. — Bibliogr. s. 58–64, Abstr.. — tekst: https://www-1tandfonline-1com-15qtywsv0030c.wbg2.bg.agh.edu.pl/doi/pdf/10.1080/0889311X.2017.1340276

Scientific research and publications

Research

1. "Badania strukturalne kwazikryształów dekagonalnych i ikozaedrycznych - nieporządek atomowy, budowa klastrowa i własności fizyczne." - projekt NCN OPUS 2020-2022, kierownik prof. Janusz Wolny
2. "Badanie struktury kwazikryształów ikozaedrycznych - analiza dyfrakcyjna i modelowanie" - projekt NCN PRELUDIUM 2015-2017, kierownik dr Radosław Strzałka
3. "Własności strukturalne i mechaniczne metali - od prostych struktur do złożonych stopów metali na przykładzie kwazikryształów i innych układów międzymetalicznych" - projekt NCN OPUS 2014-2016, kierownik prof. Janusz Wolny

Publications

1. Model refinement of quasicrystals / Janusz WOLNY, Ireneusz BUGAŃSKI, Radosław STRZAŁKA // Crystallography Reviews ; ISSN 0889-311X. — 2018 vol. 24 no. 1, s. 22–64. — Bibliogr. s. 58–64, Abstr.. — tekst: https://www-1tandfonline-1com-15qtywsv0030c.wbg2.bg.agh.edu.pl/doi/pdf/10.1080/0889311X.2017.1340276
2. Statistical approach to diffraction of periodic and non-periodic crystals – review / Radosław STRZAŁKA, Ireneusz BUGAŃSKI, Janusz WOLNY // Crystals [Dokument elektroniczny]. — Czasopismo elektroniczne ; ISSN 2073-4352. — 2016 vol. 6 iss. 9, [art. no.] 104, s. [1-19]. — Wymagania systemowe: Adobe Reader. — Tryb dostępu:

http://www.mdpi.com/2073-4352/6/9/104/pdf [2016-09-27]. — Bibliogr. s. 17–19, Abstr.. — Publikacja dostępna online od: 2016-08-26
3. https://bpp.agh.edu.pl/autor/?idA=06874&fodR=0&fdoR=2021&fagTP=4&fagIF=0&fagPM=0&afi=1&vt=c#vtype

Learning outcomes prescribed to a field of study

Code	Content
FTC2A_K01	potrafi myśleć i działać w sposób kreatywny, doceniając rolę ciągłego dokształcania oraz właściwie określać priorytety stosując zasady etyki zawodowej
FTC2A_K02	potrafi współdziałać w środowisku interdyscyplinarnym oraz rozumie pozatechniczne skutki stosowania metod fizyki technicznej (w tym jej wpływu na środowisko) i związanej z tym odpowiedzialności za podejmowane decyzje
FTC2A_U01	potrafi zastosować metody i techniki z zakresu fizyki do rozwiązywania złożonych, interdyscyplinarnych problemów technicznych i naukowych, w sposób nieszablonowy, ze świadomością uwarunkowań ekonomicznych, prawnych i środowiskowych
FTC2A_U04	potrafi formułować i testować hipotezy związane z rozwiązywaniem złożonych zadań inżynierskich i prowadzeniem prac badawczych, w tym zastosować zaawansowane metody analizy statystycznej
FTC2A_W01	ma pogłębioną i rozszerzoną wiedzę z zakresu matematyki i fizyki niezbędną do zrozumienia podstawowych procesów zachodzących w przyrodzie
FTC2A_W03	ma pogłębioną wiedzę o trendach rozwojowych w wybranych działach fizyki oraz jej zastosowaniach we współczesnych technologiach
FTC2A_W04	dysponuje pogłębioną znajomością metod matematycznych i numerycznych niezbędnych do analizy procesów fizycznych i technologicznych