AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Module name: Computational Theory of Diffraction

Academic year: 2019/2020 Code: ZSDA-3-0121-s ECTS credits: 3

Faculty of: Szkoła Doktorska AGH

Field of study: Szkoła Doktorska AGH Specialty: —

Study level: Third-cycle studies Form and type of study: Full-time studies

Lecture language: English Profile of education: Academic (A) Semester: 0

Course homepage: —

Responsible teacher: Mitura Zbigniew (mitura@metal.agh.edu.pl)

Module summary

Theory of diffraction is presented in the context of running computer simulations to plan experiments and analyze their results. The module can be useful for students working with diffraction methods who want to understand such methods in detail. Computational examples are given for light, x-ray and electron waves. Students should prepare own simple computer codes and/ or run existing software. The module should be interesting for materials engineers, physicists and chemists.

Description of learning outcomes for module

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Connections with FLO	Method of learning outcomes verification (form of completion)
Social competence: is able to			
M_K001	Student can actively read scientific publications on modelling of diffraction	SDA3A_K01, SDA3A_K03	Activity during classes
Skills: he can			
M_U001	Student potentially can analyze experimental results using numerical methods of diffraction	SDA3A_U06, SDA3A_U03, SDA3A_U02, SDA3A_U01	Execution of a project
M_U002	Student can execute computer simulations before conducting any actual experiments	SDA3A_U07, SDA3A_U06, SDA3A_U04	Execution of a project
Knowledge: he knows and understands			
M_W001	Student has general knowledge on theory being the basis for development of computer software for simulations of diffraction phenomena	SDA3A_W03, SDA3A_W02	Project

Number of hours for each form of classes

	Form of classes										
Suma	Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
30	15	0	0	15	0	0	0	0	0	0	0

FLO matrix in relation to forms of classes

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Form of classes										
		Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
Social competence: is able to												
M_K001	Student can actively read scientific publications on modelling of diffraction	-	-	-	+	-	-	-	-	-	-	-
Skills: he can												
M_U001	Student potentially can analyze experimental results using numerical methods of diffraction	-	-	-	+	-	-	-	-	-	-	-
M_U002	Student can execute computer simulations before conducting any actual experiments	-	-	-	+	-	-	-	-	-	-	-
Knowledge: he knows and understands												
M_W001	Student has general knowledge on theory being the basis for development of computer software for simulations of diffraction phenomena	+	-	-	+	-	-	-	-	-	-	-

Student workload (ECTS credits balance)

Student activity form	Student workload
Udział w zajęciach dydaktycznych/praktyka	30 h
Preparation for classes	15 h
przygotowanie projektu, prezentacji, pracy pisemnej, sprawozdania	30 h
Contact hours	5 h
Summary student workload	80 h
Module ECTS credits	3 ECTS

Additional information

Module content

Lectures

1. Basic features of wave phenomena (discussed for light, x-rays and electrons)
2. Maxwell’s equation and the scalar wave equation
3. Fresnel and Fraunhofer approximations for diffraction of light waves
4. Analysis of x-ray diffraction for small crystals
5 Simulations of x-rays spectra for multilayers
6. Description of electron diffraction with the use the Schrödinger equation
7. Simulations of transmission electron microscopy images

Project classes

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Teaching methods and techniques:

Lectures: oral presentation,
multimedia presentation
Project classes: oral presentation,
multimedia presentation

Warunki i sposób zaliczenia poszczególnych form zajęć, w tym zasady zaliczeń poprawkowych, a także warunki dopuszczenia do egzaminu:

Lectures:
Student’s presence is obligatory during lectures.

Project classes:
It is expected that a student will complete three small projects strictly related to the material presented during the lectures. The basic part of each project should be the preparation a short computer code by himself or the proper use of scientifically recognized codes available in the literature or the Internet.

Zasady udziału w poszczególnych zajęciach, ze wskazaniem, czy obecność studenta na zajęciach jest obowiązkowa:

Lectures:
– Attendance is mandatory: Yes

– Participation rules in classes: Students take part in lectures and get knowledge according to Syllabus. Discussion of problems is recommended during lecture classes. Audiovisual registration requires permission.
Project classes:
– Attendance is mandatory: Yes
– Participation rules in classes: Students take part in classes and prepare projects according to materials advised by a teacher.

Method of calculating the final grade
The scores from three projected completed within project classes will be summed up and then rounded to the nearest grade allowable.

Sposób i tryb wyrównywania zaległości powstałych wskutek nieobecności studenta na zajęciach:
a single absence is allowable without consequences,
multiple absences: self-solution of specified problems is required

Prerequisites and additional requirements
It is assumed that a student has basic knowledge on preparation of own computer codes (in any programming language).

Recommended literature and teaching resources
Birkholz M. – Thin Film Analysis by X-Ray Scattering – Wiley-VCH, Weinheim, 2006.

Kirkland E.J. – Advanced Computing in Electron Microscopy. Second Edition -Springer, New York, 2006.

Lauterborn W., Kurz T. and Wiesenfeldt M.- Coherent Optics. Fudamentals and Applications – Springer, Berlin, 1993.

Peng L.-M., Dudarev S.L. and Whelan M.J. – High-Energy Electron Diffraction and Microscopy – Oxford University Press, Oxford, 2004.

Scientific publications of module course instructors related to the topic of the module
G. Gładyszewski, Z. Mitura and M. Subotowicz, 1990, Ion beam mixing in Au-Cu compositionally modulated alloys, Materials Letters, 9, 325-327.

Z. Mitura, 2015, Theoretical analysis of reflection high-energy electron diffraction (RHEED) and reflection high-energy positron diffraction (RHEPD) intensity oscillations expected for the perfect layer-by-layer growth, Acta Crystallographica Section A (Foundations and Advances), 71, 513-518.

Z. Mitura and P. Mikołajczak, 1988, Computer simulation of X-ray spectra of metallic superlattices, Journal of Physics F: Metal Physics, 18, 183-195.

P.Mazurek, K.Paprocki and Z.Mitura, 2006, Investigation of Si-Au vicinal surfaces using scanning tunnelling microscopy and reflection high-energy electron diffraction, Journal of Microscopy, 224, 125–127.

Additional information
None