GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	, PG_00052082		
Field of study	Nanotechnology		
Date of commencement of studies	October 2022	Academic year of realisation of subject	2024/2025
Education level	first-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	3	Language of instruction	Polish
Semester of study	6	ECTS credits	5.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Szymon Winczewski	
	Teachers	dr inż. Szymon Winczewski	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	45.0	0.0	0.0	60

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	60	6.0	59.0	125

Subject objectives

The main goal is to familiarise the students with atomistic simulation methods used in research on material qualities. During the course molecular dynamics methods are discussed. The goal is to familiarise the students with an array of simulation programs and other tools widely used in this field.

Learning outcomes

Course outcome	Subject outcome	Method of verification
K6_W04	The student knows the tools for analysing the results of numerical calculations. The student knows how to present the obtained results in a form of a research report.	[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge
K6_U03	The student is able to prepare and perform atomistic simulations using the programs presented during the course. The student is able to visualise the results of simulations using the graphical tools presented during the course.	[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment
K6_W06	The student understands the relation between microstructure and macroscopic properties of materials. The student knows, how the specificity of interatomic interactions influences the properties of materials. The student knows the basic thermodynamic response functions.	[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge
K6_U02	The student is able to critically analyse simulation results. The student is able to point out the limitations of the model used and propose corrections.	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject [SU5] Assessment of ability to present the results of task

<table>
<tr><td>Subject contents</td><td>1. Methods of defining atomic structures.

2. Methods of visualising atomic structures (VMD and Ovito programs).

3. Methods of describing interatomic interactions (Lennard-Jones potential, AIREBO force fields, multibody potentials).

4, Numerical methods for solving equations of motion (classic and velocity Verlet algorithm).

5. Simulation techniques: preparation and performance of simulations (LAMMPS program).

6. Processing and presentation of simulation results (Gnuplot program).

7. Statistical ensamble.

8. Thermodynamic response functions.

9. Methods of studying mechanical properties of atomic structures.

10. Structure analysis methods.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Student knows the basics of solid state physics and thermodynamics.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Test in theory</td><td>50.0%</td><td>25.0%</td></tr>
<tr><td>Written reports</td><td>50.0%</td><td>25.0%</td></tr>
<tr><td>Solving assignments</td><td>50.0%</td><td>50.0%</td></tr>
</table></td></tr>
<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>1. Dennis C. Rapaport, The Art of Molecular Dynamics Simulation, 2nd ed., Cambridge University Press, Oxford 2004.
2. Dieter W. Heerman, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997.
3. Furio Ercolessi, A molecular dynamics primer.
4. Vasily Bulatov, Wei Cai, Computer Simulations of Dislocations, Oxford University Press, Oxford 2006.
5. Daan Frenkel, Berend Smit, Understanding molecular simulation: from algorithmsto applications, 2nd ed., Academic Press, 2002.
6. Andrew R. Leach, Molecular modelling: principles and applications, 2nd ed.,Prentice Hall, 2001.</td></tr>
<tr><td>Supplementary literature</td><td>none</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:
Komputerowe Modelowanie Materiałów 2024/2025 - Moodle ID: 44693
https://enauczanie.pg.edu.pl/moodle/course/view.php?id=44693</td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>1. Defininig and visualizing of simple atomic systems.
2. Analysis and graphical presentation of the scientific data.
3. Properties of argon dimer.
4. Thermodynamical properties of argon crystal (heat capacity, melting temperature, thermal expansion).
5. Mechanical properties of argon crystal.</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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