GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Computer modeling of materials, PG_00063398		
Field of study	Nanotechnology		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2026/2027
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	6.0
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 -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Szymon Winczewski	
	Teachers		

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	10.0	80.0	150

Subject objectives

The aim of the course is to familiarize students with methods of atomic-scale simulations, in particular with the method of molecular dynamics. The course consists of a lecture, which discusses various aspects of simulations from a theoretical perspective, and a laboratory, during which students gain practical experience with simulations and become acquainted with scientific software used in the field.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U02] can analyze and solve simple scientific and technical problems based on possessed knowledge, applying analytical, numerical, simulation and experimental methods.	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.	[SU5] Assessment of ability to present the results of task [SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment
[K6_W04] Has knowledge of IT tools (word processors, spreadsheets, etc.), preparing multimedia presentations, programming and computer graphics	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] has programming skills in a selected language, and is able to use basic software packages.	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

<table>
<tr><td>Subject contents</td><td>Lecture
1. The role and significance of computer simulation.
2. The molecular dynamics method - idea and outline.
3. Description of interactions. The Lennard-Jones potential. Interaction force.
4. Numerical integration of equations of motion. The basic and velocity Verlet algorithms.
5. Boundary conditions. Simulation boxes.
6. Identification of nearest neighbors. Potential cutoff. Cutoff radius.
7. Linked-cell method and the Verlet list method.
8. Starting a simulation. Selection of initial positions and initial velocities. Equilibration and sampling.
9. Calculation of basic thermodynamic parameters.

Computer labs
1. Defining and visualizing atomic systems.
2. Introduction to the VMD program.
3. Processing and presenting numerical results using gnuplot.
4. Introduction to the LAMMPS program.
5. Preparation, execution, and analysis of MD simulation results.
6. Study of vibrations of the Ar molecule based on MD simulations.
7. Determination of the specific heat of an argon single crystal using MD simulations.
8. Introduction to the OVITO program.
9. Determination of the bulk modulus of an argon single crystal using MD simulations.</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.</td></tr>
<tr><td>Supplementary literature</td><td>1. Dieter W. Heerman, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997.
2. Furio Ercolessi, A molecular dynamics primer.
3. Vasily Bulatov, Wei Cai, Computer Simulations of Dislocations, Oxford University Press, Oxford 2006.
4. Daan Frenkel, Berend Smit, Understanding molecular simulation: from algorithmsto applications, 2nd ed., Academic Press, 2002.
5. Andrew R. Leach, Molecular modelling: principles and applications, 2nd ed.,Prentice Hall, 2001.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
</table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td>1. Present a block diagram of the algorithm used in molecular dynamics simulations. Briefly discuss each of the steps performed.
2. Present (write down, explaining the symbols) the expression for the potential energy of a system of N atoms interacting via the Lennard-Jones potential. Explain the physical meaning of this expression.
3. Starting from the Taylor series expansion, derive the basic Verlet algorithm. Explain what disadvantages this method has and what causes them.
4. Explain how the application of periodic boundary conditions affects the MD simulation algorithm. Which aspects/stages of the algorithm require changes/modifications? What do these changes involve?
5. Discuss the problem of identifying nearest neighbors. What does it consist of? Why is it important? What methods are used to identify nearest neighbors?</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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