LUNDS UNIVERSITET
Lunds Tekniska Högskola

Course syllabus

Nanomekanik och flerskalig modellering
Nano Mechanics and Multiscale Modelling

FMEN25, 7,5 credits, A (Second Cycle)

Valid for: 2023/24
Faculty: Faculty of Engineering, LTH
Decided by: PLED M
Date of Decision: 2023-04-11

General Information

Main field: Nanoscience.
Elective for: F4, F4-bem, M4-bem, MNAV1, N4, N4-m, Pi4
Language of instruction: The course will be given in English on demand

Aim

Material properties emerge from phenomena on scales ranging from angstroms to meters. A multiscale treatment can provide a basis for an understanding of material behavior on different scales. The course addresses advanced undergraduate and graduate students. The purpose of the course is to present the theories and methods in multiscale modeling of materials and establish relations between atomistic descriptions and continuum mechanics. The course gives basic knowledge about the principles, concepts and methods in nanomechanics based on Euler-Langrange's, Hamilton's and Schrödinger's formulations of the mechanical laws. The general concepts and principles are presented and combined with interatomic potential functions for different materials. The course further involves the basics of classical statistical mechanics and quantum mechanics and provides a framework for further studies in molecular dynamics.

Learning outcomes

Knowledge and understanding
For a passing grade the student must

- acquire knowledge of the hierarchy of physical models
- apply the fundamental equations – Euler-Lagrange, Hamilton and Schrödinger
- explain and apply fundamental interatomistic potential functions
- acquire knowledge of the most important principals of molecular dynamics

- acquire knowledge about the relation between classical statistical mechanics, quantum mechanics and continuum mechanics.

Competences and skills
For a passing grade the student must

- identify relevant interatomistic potential functions for analysis of material systems
- be able to formulate and numerically solve simple problems in molecular dynamics
- be able to perform an analysis of a nanomechanical problem and to present the results in a well-written report

Judgement and approach
For a passing grade the student must

- adopt a critical and innovative attitude towards multiscale modelling
- be able to evaluate achieved results based on problem formulation and physical limitations

Contents

Introduction of hierarchy of physical models of materials. Fundamental continuum mechanics and thermodynamics. Lattices and crystal structures. Quantum mechanics. Empirical atomistic models of materials. Molecular statics. Atomistic foundations of continuum concepts: classical equilibrium, statistical mechanics, microscopic expressions for continuum fields, molecular dynamics. Multiscale methods: multi scale modelling, atomistic constitutive relations for multi lattice crystals, atomistic-continuum coupling: static methods, non-zero temperature and dynamics. Overview of fabrication techniques for today's nanostructures and modern experimental methods at the nano scale.

Examination details

Grading scale: TH - (U,3,4,5) - (Fail, Three, Four, Five)
Assessment: The examination of the course consists of written exam, compulsory hand in exercises and project work.

The examiner, in consultation with Disability Support Services, may deviate from the regular form of examination in order to provide a permanently disabled student with a form of examination equivalent to that of a student without a disability.

Admission

Assumed prior knowledge: Basic course in Continuum Mechanics
The number of participants is limited to: No

Reading list

- Ellad B. Tadmor and Ronald E. Miller: Modeling Materials: Continuum, Atomistic and Multiscale Techniques. Cambridge University Press, 2011, ISBN: 978-0-521-86698-0.

Contact and other information

Course coordinator: Prof. Aylin Ahadi, aylin.ahadi@mek.lth.se
Course homepage: http://www.mek.lth.se
Further information: The couse might be given in English.