Lecturer: Dr. Igor Berinskii

Course name: Introduction to mechanics of solids with microstructure

Syllabus The course covers the analytical and computational methods to model and simulate mechanical behavior of materials taking their microstructure into account. Multiscale modeling from the atomistic level to the macro-level allows the description and prediction of the effective properties of materials. Nowadays it is highly important for nanostructures, composites, metamaterials, and foams. Also, multiscale methods are highly important for the study of fracture and dislocation mechanics, plasticity. This course allows us to understand some general concepts and use them to study different problems in the mechanics of solids.

Course plan:

1. **Introduction to the micro- and nanomechanics.** Scale levels. Classification of condensed matter. Structure of solids. Elements of crystallography: crystal lattice, symmetry groups, experimental methods in crystallography. Nanomaterials. Quasicrystals.
2. **Nature and types of interatomic bonds.** Chemical bond, energy and valence. Types of the bonds: ionic, covalent, metallic, Van-der-Waals, etc.
3. **Micromechanical defects in crystals.** Point defects. Dislocations. Cracks. Fracture of solids.
4. **Review of tensor calculus in solid mechanics.** Dyads, high-order tensors, dot product, vector product, trace, transpose, coordinates of the tensor.
5. **Empiric description of solids.** Potentials of interaction: Lennard-Jones, Stillinger-Weber and REBO, EAM. Force fields.
6. **Molecular statics and dynamics.** Verlet and leap-frog integration. Neighbors list. Boundary conditions.
7. **Atomistic foundations of continuum mechanics.** Micro-canonical ensembles. Total energy, kinetic energy, pressure, temperature.
8. **Tensors of stress and on strain at macroscopic level.** Hook's law for anisotropic solids.
9. **Linear deformation of crystal lattice.** Cauchy-Born rule. Tensor of stress at microscopic level. Examples: simple crystal lattices.
10. **Linear deformation of complex crystal lattice.** Nonlinear deformation of simple crystal lattice. Cauchy, Piola, virial, Hardy stress.
11. **Dynamics of 1D crystal.** Dynamics of 2 and 3-atomic molecule. Dynamics of simple crystal chain.
12. **Dynamics of two-atomic crystal.** 1D two-atomic chain and its generalization to 2D and 3D crystals. Acoustic and optical specter. Dispersion curves. Brillouin zone. Phonons.
13. **Nonlinear waves in crystals.** Bousinesq equation. Toda's chain.
14. **Atomistic-continuum coupling.** Quasicontinuum method. Representative cell method.

Grading:

30% - Home tasks

30% - Research project

40% - Final test

Literature:

- 620.112 TAD Ellad B. Tadmor and Ronald E. Miller, Modeling Materials: Continuum, Atomistic and Multiscale Techniques, Cambridge University Press, 2011.
- 620.105.4 LIU Liu, Wing Kam, Karpov, Eduard G., and Park. Harold S., Nano Mechanics and Materials: Theory, Multiscale Methods and Applications. John Wiley & Sons, Ltd, 2006.
- 539.102 CLE Cleland, Andrew N. Foundations of nanomechanics: from solid-state theory to device applications. Springer Science & Business Media, 2003.
- 539.2 ALL Allen, Mike P., and Dominic J. Tildesley. Computer simulation of liquids. Oxford university press, 1989.
- 539.102 RIE Rieth, Michael. Nano-engineering in Science and Technology: An Introduction to the World of Nano-design. Vol. 6. World Scientific, 2003.
- 620.105.4 LI Shaofan Li, Gang Wang. Introduction to micromechanics and nanomechanics. Singapore ; Hackensack, NJ : World Scientific. 2008.
- 620.11 LES LeSar , R. Introduction to computational materials science : fundamentals to applications
- Buehler, Markus J. Atomistic modeling of materials failure. Springer Science & Business Media, 2008.

Similar courses:

- Prof. E. Tadmor (University of Minnesota). Multiscale Methods for Bridging Length and Time Scales.
  http://www.aem.umn.edu/~tadmor/
- Prof. Wing Kam Liu (Northwestern University). Multi-scale Modeling and Simulation in Solid Mechanics
  http://www.mccormick.northwestern.edu/mechanical/courses/descriptions/417-multiscale-modeling-and-simulation-in-mechanics-I.html
- Prof. Markus J. Buehler (MIT). Multiscale materials design.
  http://professional.mit.edu/programs/short-programs/multiscale-materials-design
- Prof. Dennis Kochmann (ETH Zurich). Computational Multiscale Modeling. https://www.mm.ethz.ch/teaching.html