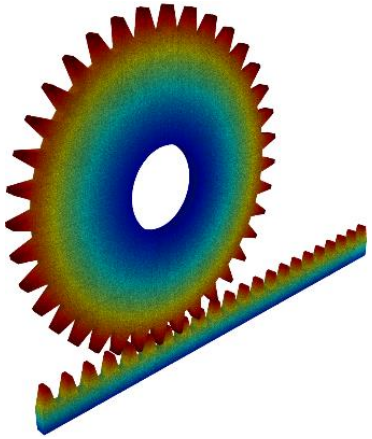
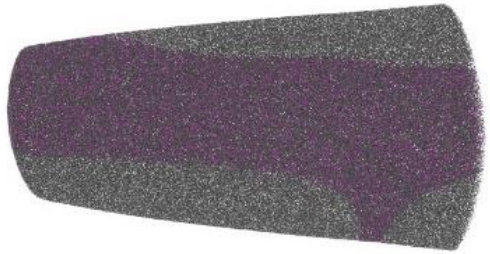
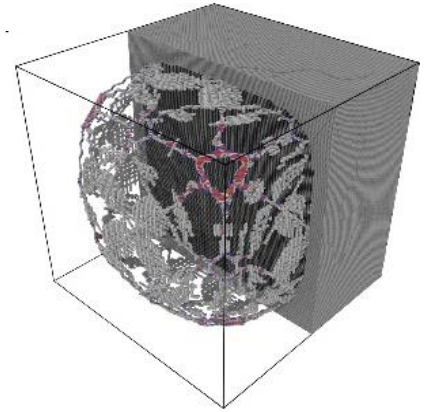
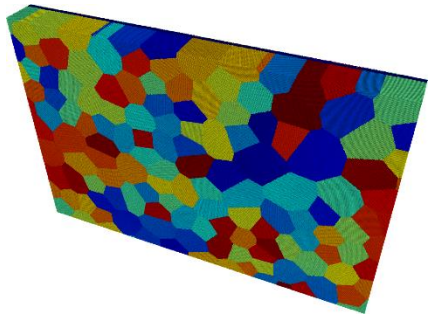
TECHNISCHE UNIVERSITÄT
BERGAKADEMIE FREIBERG
Die Ressourcenuniversität. Seit 1765.

M5 Micro-Mechanics & Multiscale Materials Modeling

Theory, Modeling and Simulation of Microstructures

Dr. Arun Prakash

Micro-Mechanics & Multiscale Materials Modelling (M^5) Group

TU Bergakademie Freiberg

NOTE: These lecture notes and slides are for use within the course only!
Redistribution in strictly prohibited!

Recording of the lecture or the tutorial is prohibited by law. Failure to comply with these regulations may have legal consequences and can lead to exmatriculation

Details of the course

- Lecture: Thursday, 08:00 – 09:30
- Exercise: Two slots
  - ~~Tuesday, 11:30 – 13:00~~
  - Wednesday, 08:00 – 9:30

- OPAL course: https://bildungsportal.sachsen.de/opal/auth/RepositoryEntry/

- Enrolment to the OPAL course is mandatory
- Lecture slides will only be posted in OPAL
- Please use the “Contact Supervisor(s)“ link in the course to mail queries pertaining to the course
- Critique is welcome. Make sure that you inform me of it in time!

QR code for OPAL course

More stuff about the lecture …

- For exercises, you can use the CAE-pool remotely via x2go-client
- You can activate remote visualization using Turbovnc.
  (See subsequent slide for more details).
- For the exercises, Mr. Mohammed Saad Qureshi will be the teaching assistant
- The computers in the pool will only be accessible for the duration of the exercise!
- PVL: Turn in your assignments in time. This is a prerequisite for the exam!
- Lecture slides will be uploaded to OPAL after the lecture
- Not everything we discuss during the lecture will be found in the slides.
  Your own notes are necessary and important
- These slides are provided to you as a part of the lecture only.
  Redistibution is prohibited!

Course syllabus

1. Introduction
    i. What is this lecture about?
    ii. Modeling techniques at different length and time scales
    iii. Modeling and the nanoscale
    iv. Atomistic simulations: The why and the how
    v. Some examples
2. Atomistic structure generation
    i. Basic machinery of atomistic simulations
    ii. List of tools/toolkits for sample generation
    iii. Generating a single crystal
        i. Basis vectors and rotation
        ii. Periodicity
    iv. Defect structures: Types of defects
    v. Generating samples with vacancies and pores
    vi. Sculpting samples with surfaces
    vii. Inserting dislocations
        i. A quick recap on dislocations
        ii. Inserting infinite straight dislocations
        iii. Inserting dislocation loops
    viii. Generation of complex structures
        i. Generation of Voronoi polycrystals
        ii. Nanosculpt: Generation of arbitrary shapes
3. Boundary conditions
    i. Typical BC used in atomistic simulations
    ii. Influence of BCs: idealized vs. realistic structures
    iii. FE2AT: imposing arbitrary BC from FE onto atomistic configurations
4. Interatomic potentials
    i. Introduction
    ii. Born-Oppenheimer approximation
    iii. Which potential energy function to use?
    iv. Pair potential
    v. Pair functionals
    vi. Many body potentials
    vii. Transferability of different methods
    viii. Which potential for which material

Course syllabus

5. Molecular statics
   i. Simulation types with molecular statics
   ii. Concept of the potential energy surface
   iii. Optimization: General remarks, classification and convergence criteria
   iv. Algorithms:
      i. Bracketing procedures
      ii. Parabolic schemes
      iii. Line descent algorithms
      iv. Quasi-Newton methods
      v. Quenched dynamics
   v. Implementing molecular statics
      i. Basic algorithm
      ii. Neighbor lists
      iii. Binning
   vi. Molecular statics for crystals and defects
      i. Cohesive energy and lattice constant
      ii. Vacancies
      iii. Surfaces and interfaces
      iv. Stacking fault energies
      v. Elastic constants

6. Analysis and visualization
   i. Preliminary considerations
      i. Why visualization and analysis?
      ii. Which quantities are readily available and what to visualize?
      iii. List of useful software
   ii. Analysis of crystalline structures
      i. Structure identification methods
      ii. Template matching methods
      iii. Analysis of dislocation and slip
      iv. Topological characteristics in polycrystals
      v. Continuum metrics with atomistic simulations
   iii. Analysis of complex crystals: $L1_2$
      i. Super dislocation and defect types
      ii. Examples
   iv. Analysis of amorphous materials
      i. Bond angle distribution
      ii. Ring statistics
      iii. Coordination polyhedral
      iv. Bond statistics
      v. Stereographic projections

Course syllabus

7. Molecular dynamics
    i. Some preliminary considerations
    ii. The generic MD algorithm
    iii. Time integration
        i. Numerical time integration schemes
        ii. Criteria for choosing a time integrator
        iii. Choice of time step
    iv. Ensembles in MD
    v. Typical steps in MD simulation
8. Application of molecular statics: Grain boundaries
    i. Introduction
    ii. Characterization of GBs
        i. Geometric description
        ii. Atomistic description
    iii. Tilt and twist GBs
    iv. GB energy
    v. Special and general grain boundaries
        i. Concept of the CSL
        ii. Example of $\Sigma 5$ GB
    vi. Structure of GBs
    vii. Atomistic simulations of GBs
        i. Main purpose and types of study
        ii. Generating atomistic GB structures
        iii. Example of $\Sigma 3$ (111) twin boundary in fcc materials

Lecture schedule

Date	Topic
03.04.2025	Introduction
10.04.2025	Basics of simulations + Structure generation - I
17.04.2025	Sample generation – II + Boundary conditions – I
24.04.2025	Boundary conditions – II + Interatomic potentials – I
01.05.2025	Holiday (Labor day)
08.05.2025	Interatomic potentials - II
15.05.2025	Molecular statics – I: PES and Optimization
22.05.2025	Molecular statics – II: Implementing MS
29.05.2025	Holiday (Ascension day)
05.06.2025	Molecular statics – III: Application to crystals and defects
12.06.2025	Visualization + Analysis – I: Basics, fundamental quantities, simple analysis methods
19.06.2025	Visualization + Analysis – II: Advanced analysis methods, amorphous materials, alloys
26.06.2025	Molecular dynamics
03.07.2025	Grain boundaries
10.07.2025	Buffer

Exercise schedule

Date	Topic
01.04 / 02.04	No Exercise
08.04 / 09.04	Introduction to LAMMPS
15.04 / 16.04	Structure generation – I
22.04 / 23.04	Structure generation – II
29.04 / 30.04	Static relaxation / MS – I
06.05 / 07.05	Visualization + Analysis - I
13.05 / 14.05	Static relaxation / MS – II
20.05 / 21.05	Static relaxation / MS - III
27.05 / 28.05	Buffer for finishing exercises
03.06 / 04.06	Visualization + Analysis – II, Dislocation analysis, Thompson tetrahedron
10.06 / 11.06	Buffer for finishing exercises
17.06 / 18.06	No Exercise (Dies Academicus)
24.06 / 25.06	Molecular dynamics: Lattice constant at temperature and time increment
01.07 / 02.07	Grain boundaries – I (GB creation)
08.07/09.07	Grain boundaries – II (GB energy)

Exercises

Task

- Compute the elastic constants (C11,C12,C14) for the potential assigned to you. Compute the bulk and shear moduli.
- Write down the complete elasticity matrix using the computed elastic constants
- How anisotropic is the material? Can you quantify this?