MSE235 Materials Structure & Properties Lab
Molecular dynamics laboratory: atomic mechanisms of plastic deformation

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What is in this lab?

• Background lecture
  • Lab objectives
  • Introduction to molecular dynamics (MD)
  • Tensile testing of materials

• Pre-lab lecture
  • How to run online MD simulations at nanoHUB.org
  • MD tensile “tests”

• Lab handout
  • Lab activities using nanoHUB
  • Questionnaire
  • Additional activities
Learning objectives

• Develop an atomic picture of plastic deformation in metals
• Understand the orientation of the active slip system with respect to the tensile axis
• Estimate the strength of perfect crystals and compare it to polycrystalline samples
• Strain hardening: difference between annealed and cold worked, and nanoscale samples
Nanoscale vs. macroscopic specimens

Platinum nanoscale bar

Diameter: 2.6 nm
Periodic length: 4.1 nm

Copper tensile bar
Line defects proposed in 1934 by Orowan, Polanyi, and Taylor
The motion of a dislocation on a slip plane caused a relative displacement of the material on either side of the plane
This relative displacement is called Burgers vector
Mechanical response

- Eng. Stress (MPa)
- Engineering strain

- Cold worked
  (30 mins. @ 500°C)

- Work hardening

- Annealed
  (30 mins. @ 650°C)

- Work softening
Nanoscale tensile tests: MD results

Eng. Stress (MPa)

Engineering strain

Initial

Strain: 0.075

Platinum nanowire
Radius 1.3 nm

Strain: 0.1
Nano vs. macro mechanical response

**Yield stress:**
- Typical values: 50 to 500 MPa
- Stress necessary to move existing dislocations

**Work hardening**
- Plastic deformation
  - Increase dislocation density
  - More obstacles for dislocation motion
  - Strengthening

**Work softening:**
- Dislocations do not stay inside the specimen (always a free surface nearby) ➞ no hardening
- Steps in surface make it easier to nucleate subsequent dislocations ➞ weakening

**Yield stress:**
- Pt nano-sample: ~6,000 MPa
- Stress necessary to nucleate a dislocation
Running MD: nanoMATERIALS simulation toolkit

nanoMATERIALS simulation toolkit @ nanoHUB
• General purpose tool for atomistic simulations of materials

Step 1: Go to the nanoHUB webportal nanohub.org
Step 2: Create an account
Step 3: Login
Step 4: Click on “All Tools” and select: nano-Materials Simulation Toolkit
Running MD with nanomaterials: step 1

Determine initial model for simulation

- Select a model from menu
- Click on Pt_nanowire_r13

Some possible operations

- Create supercell
- Modify the lattice parameters
Energy expression

How to calculate the total energy and atomic forces

For Pt atoms we will use a type of many body potential called Sutton Chen
Running MD with nanoMATERIALS: step 3

**Driver options**

**Ensemble**
- NVE constant volume and energy < select
- NVT constant volume and temperature
- NPT constant pressure and temperature

**Time-step** to integrate equation of motion
- Set to 0.004 ps (4 femtoseconds)

**Number of MD steps**
- Set to 4000

**Temperature** (initial value in NVE or target value for NVT and NPT)
- Set to 300 K
Strain per MD step
We will strain the nanowire along its axis
Input $0.00003$ in the Y direction
Strain rate is strain per step divided by MD timestep:

$$\dot{\varepsilon} = \frac{0.00003}{0.004 \cdot 10^{-12} s} = 7.5 \cdot 10^9 s^{-1}$$

Periodic tasks
How often (MD steps) to record data
• Entry to energy file (use default)
• Atomistic snapshot (500 steps)

Simulate
• Will submit your run – once finished (~5 min. in this example) the results will be displayed
Running the simulation

Molecular Dynamics Run
Initial Configuration

Energy Decomposition
vdW, EAM Energy: 0.
Electrostatic Energy: 0.
Total Energy: -365719.181

Stress (GPa) | 0.000544 | 0.000714 | -0.003525 |
Stress (GPa) | 0.000714 | -0.072042 | 0.003768 |
Stress (GPa) | -0.003525 | 0.003758 | -0.017505 |

# Energies in kcal/mol

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Viewing results with nanoMATERIALS

Select results to visualize
Viewing results with nanoMATERIALS

Select results to visualize

Molecular view
This lab

You will explore plastic deformation in metallic nanowires

- Visualize atomic snapshots to identify slip planes
- Explore individual slip events and the origins of the observed strain softening
- Study role of temperature on yield stress

- The laboratory handout will guide you through this steps