Nanoscale tensile testing
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1. Objectives
In this computational lab you will perform online molecular dynamics (MD) simulations through nanoHUB of single-crystal copper nanowires under uniaxial tension of varying orientations and analyze the results in order to:

- Observe how slip planes in single-crystal nanowires are formed and explain plastic deformation at the atomic level in terms of dislocation motion and slip.
- Identify the characteristic features of stress-strain curves of nanoscale materials (i.e., elastic region, plastic region, Young’s modulus, yield stress)
- Differentiate plastic deformation for macro- versus nanoscale metals. Compare and contrast Young’s modulus, yield strength, and strain hardening between nanoscale, initially defect-free, single crystal samples and macroscale, polycrystalline samples
- Use critical resolved shear stress and crystallography to determine active slip systems

2. Background
Molecular dynamics (MD) is a popular simulation technique used in materials science and biology. The initial positions for all atoms must be defined, as well as a model for the energy of atom interaction \( F = \frac{\partial E}{\partial x} \). Atoms are assumed to be point particles, enabling \( F = ma \) to be integrated for each atom in the system. Thus, the technique predicts the structure and dynamics of materials from the atomic scale. Importantly, the model for how atoms interact is fit to experimental and quantum mechanical simulations, but electrons are not directly simulated. Many properties can be calculated with MD, including thermal, chemical, and mechanical.

In this computational lab, you will perform a series of tensile tests on copper nanowires using an MD tool on nanoHUB.org. The tool creates single-crystal copper nanowires of various crystallographic orientations (relative to the tensile axis) and deforms them to 25% engineering strain. In FCC metals, such as copper tested here, slip occurs on the closed-packed \{111\} planes along the close-packed \<110> directions in the slip plane. Using the MD simulations, you will be able to directly observe the formation of these slip planes in copper nanowires and how dislocation motion at the atomic level manifest as plastic deformation in copper at the macroscale.

Additional Resources:
  - “Mechanical Properties of Metals” (Chapter 6, Sections 6.1 – 6.7)
  - “Dislocations and Plastic Deformation” (Chapter 7, Sections 7.1 – 7.6, 7.10)
- nanoHUB-U: From Atoms to Materials (Sections 3–4) https://nanohub.org/courses/FATM
Related Resources:
This learning module uses the same simulation tool and setup and couples it with an experimental tensile testing lab.


3. Instructions

A. Login

1. Go to http://nanohub.org/ and log in with your username and password. Sign up for a free account if you do not already have one.
2. Go to the tool page “Nanomaterial Mechanics Explorer”. This can be searched among all nanoHUB tools, or directly accessed using: https://nanohub.org/tools/nanomatmech
3. Click the “Launch tool”. You should see the tool as shown in Figure 1.

B. Tensile test simulations (Quick-start)
To start, run a new tensile-test simulation of a copper nanowire oriented in the [100] direction. To do this, complete the steps outlined below:

1. As shown in Figure 1, select “Nanowire Tensile Test” from the “Experiment” dropdown
2. Then select “Copper [110]” from the “Nanowire Material and Orientation” dropdown
3. Click “Simulate” and wait for results. This simulation will take less than 30 minutes.

Figure 1: Simulation tool front page.
Note that the details of the simulation that you are running are given in the “Advanced options”. Results are shown while it runs, including the number of atoms in the system and the nanowire length over time.

**C. Multiple orientation nanowires**

Comparison of different orientations is one of the main objectives of this module. Follow the instructions from Section 3B to run two more orientations:

- [111]
- [100]

**D. Simulation results**

1. Review the simulation results. An example of available outputs is shown in Figure 2. The circled icon in Figure 2 next to the dropdown menu allows you to download any output.

![Figure 2: Simulation output options.](https://nanohub.org/resources/30014)

2. Focus on and/or save the following:
   a. Stress-strain data (both CSV data and image are available from “Stress vs strain”)
   b. Young’s modulus calculated by the tool (“Elastic modulus”)
   c. Notable images from the atomic structures (“Atomistic animation” from both the “All atoms” and “Defect atoms” views)
   d. Number of atoms in the system and simulation time (from the “Thermodynamic output file”)

3. The “Atomistic animation” outputs show the atom positions over time (strain) for the simulation. Figure 3 highlights this output’s slider to view different times. For each time you can zoom and rotate the structure; Figure 3 also shows the options menu to reset views and zoom. There are two versions of the atomistic animation: the first includes all atoms and the second includes only the atoms that are considered defects (i.e., meaning that they have different neighbors than the original crystal structure, in this case FCC). In these outputs, atoms that are colored **green** are FCC, **light blue** are BCC, **yellow** are HCP, and **dark blue** are unidentified crystal structure (e.g. atoms that are at the surface). It is important to note that, if there are not **dark blue** atoms at the surface, then that face is periodic: it interacts with the opposite side of the material as if it were within an infinite material.
Figure 3. Atomistic animation example.

4. Assignment

A. Useful reference
   - Copper data
     - Table 3.4 (Callister 9th ed. page 86)
     - Table 6.2 (Callister 9th ed. page 185)

B. While the simulation is running
   1. Is the Young’s modulus dependent on orientation?
   2. Is the yield stress or yield strain dependent on orientation?
   3. How many unique slip systems are active for these simulations?
   4. How will you identify the slip planes when looking at the atoms in this simulation?

C. After simulations have finished
   1. How do dislocations and slip within the nanowires impact its overall mechanical response (stress-strain curve)?
   2. For each property, how do the copper nanowires compare to macroscopic, experimental copper samples? What factors lead to similarities between the simulation and experimental Young’s moduli? What factors lead to differences?
      - Young’s modulus
3. How does the overall deformation response (stress-strain curve) compare between the copper nanowires with a macroscale, experimental copper sample?

4. Calculate all Schmid factors for the FCC slip system. What is the slip system(s) active for each orientation of the copper nanowires? What evidence corresponds to this matching or not matching the simulations?

5. **Additional simulations**

   **A. Custom size nanowire simulations**

   Section 3 shows how to run pre-built simulations. To become more familiar with the inputs and outputs, you can also create custom versions of the base tensile test. These instructions show how to run smaller (7x7 unit cell cross section) copper nanowire, which run faster than Section 3.

   1. Start from the “default” nanowire simulation, “Copper [110]”, instructions in Section 3B (choosing an option on the front page will automatically reset all inputs to that default).
   2. Enable “Advanced options” near the bottom of the tool and change the following inputs:
      a. Under the “Structure Details” tab switch from “Pre-built” to “Build new”
      b. Under the “Structure Details” tab, under “Main structure”:
         i. Change “Base orientation” (different for each run)
         ii. Change both the Y & Z “System size” from 11 to 7 (unit cells)
      c. Under the “Thermomechanics Details” tab review the inputs, comparing to details given above in the background
      d. Under the “Simulation Details” tab review the inputs
         (For example, the “Interatomic model” dropdown would allow you to choose a different model for the same material)
   3. Click “Simulate”. This should take about 10 minutes.

6. **Additional questions**

   1. What are the size effects at the nanoscale (comparing the same orientation)? Would you expect the same size effects in macroscale samples?
   2. Download the stress-strain data and calculate the Young’s modulus and yield stress (with any plotting software). How similar are the tool-reported yield stress and Young’s modulus values to those independently calculated from the stress-strain data?
   3. What does the model include (and what is the simulation therefore able to capture)?
   4. What does the model exclude?
   5. Choose a new interatomic model (See instructions in Section 5A)
      - How similar are the results?