Molecular dynamics laboratory: atomic mechanisms of plastic deformation

Laboratory objectives

In this lab students will perform online molecular dynamics (MD) simulations of metallic nanowires deformed uniaxially and analyze the results to:

- 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 polycrystalline samples
- Explore strain hardening focusing on the difference between annealed and cold worked macroscopic samples and nanoscale samples

Background

Molecular dynamics is a powerful simulation technique to explore materials behavior where the temporal evolution of every atom in a specimen is explicitly described. MD involves solving Newton's classical equations of motion ($F=ma$) numerically for every atom. In order to accomplish this one needs to know the forces acting on each atom, which arise from the interaction with other atoms and from external sources. Inter-atomic forces are described via an atomistic potential, or force field, that represents the total potential energy of the specimen as a function of atomic positions.

While approximations are involved in MD simulations (most importantly associated with the use of classical mechanics and the accuracy of interatomic potentials) it provides a very accurate description of materials. Those interested in learning more about MD simulations will find the following resources useful:

- M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids, Oxford Univ. Press, 1989
- D. Frenkel and B. Smit, "Understanding Molecular Simulation," Algorithms to Applications (Computational Science Series), 2nd ed., vol. 1, Academic Press, 2001
- Strachan, "MSE 597G An Introduction to Molecular Dynamics," 2008; http://nanohub.org/resources/5838

Procedure

The following two assignments should be performed individually or in small groups. The background and pre-lab lectures in this learning module provide the necessary background and a tutorial on how to perform the simulations using the nanoMATERIALS simulation tool available in the nanoHUB: http://nanohub.org/resources/1692.

Assignment 1: exploring the first plastic event. Follow the directions given in the pre-lab lecture to perform your first MD simulation of the deformation of a Pt nanowire with radius R=1.3 nm. Note that after you select the "Input model" locating the cursor over the selection will give you additional information about the model. The original length of this pre-built nanowire is

4.1 nm; you will duplicate the simulation cell two times along the y direction (parallel to the wire's axis) to increase its length to 8.2 nm. Remember to select the NVE "ensemble" in the "Driver specification" tab and set the strain per MD step, number of steps and timestep variables and make sure you write a snapshot every 500 MD steps.

Once the simulation is finished, explore the output plots and, if possible, discuss their meaning with your classmates. Focus on the temporal evolution of the stress along the wire, instantaneous temperature and potential energy. In the case of nanowires, the stress given by the simulation tool needs to be corrected, see Appendix. Download these three plots and paste them into a document or presentation file with a short description of what they represent. Indentify "interesting times" to explore atomic snapshots based on the stress-time curve. Analyze the atomic snapshots and identify the active slip planes and slip direction. Add snapshots before and after the deformation into your report file; before and after snapshots should have the same orientation.

Discuss the following questions with one or two classmates and provide a brief answer in your report.

- What is the orientation of the active slip plane(s) with respect to the tensile axis?
- How does the yield stress of the nanowire compare with those of annealed polycrystalline metals? What is the origin of this difference?
- Did you find a dislocation inside the sample (see cartoon of dislocation in pre-lab lecture) in any of the snapshots you analyzed? What does this tell you regarding how hard it is to nucleate a dislocation vs. how hard it is to move it?

Assignment 2: large deformations. Increase the number of MD steps to 10,000 (total simulation time: 10000x0.004ps = 40 ps). Analyze the plots and atomic snapshots as described in Assignment 1. What can you say about the nucleation of slip events? Is there a correlation between the location of one event and subsequent ones? Add plots and atomic snapshots from assignment 2 to your report and include a summary of your findings. Answer the following questions:

- Did the nanowire exhibit strain hardening? Why?
- Can you envision another case where the density of dislocation density does not increase during plastic deformation?

Additional suggested activities

Using the simulation tool you can explore other nanowire sizes, temperatures and strain rate. You can also perform simulations in compression by changing the sign of the strain per MD step.

Appendix:

The MD simulation code does not "know" that it is dealing with a nanowire and only a fraction of the cross-sectional area should be used to compute stress. Thus, the stress needs to be corrected to account for the difference of the cross-sectional area of the simulation cell and the actual cross-section of the wire. The stress the program outputs should be multiplied by the

cross-sectional area of the simulation cell (11.421nm x 12.237 nm) and divided by the cross-sectional area of the nanowire [π (1.3 nm)^2].