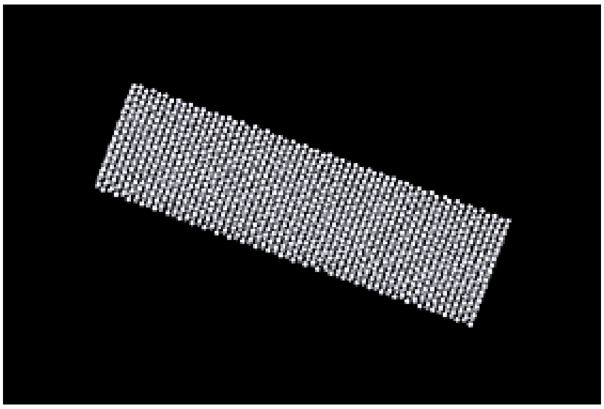
Learning Module: Atomic Picture of Plastic Deformation in Metals



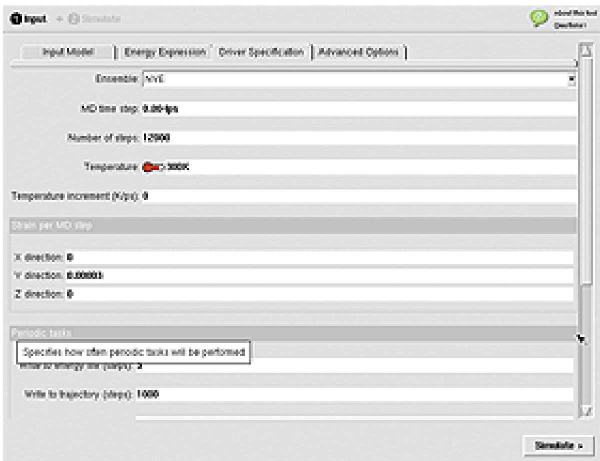
The main goal of this learning module is to introduce students to the atomic-level processes responsible for plastic deformation in crystalline metals and help them develop a more intuitive understanding of how materials work at molecular scales. *Image to the right shows plastic deformation of a metallic nanowire.*

The module consists of:

- Two introductory lectures (50 minutes each) available online as audiovisual presentations
  - [Overview Lecture]
  - [Prelab Lecture]
- Hands-on lab involving online molecular dynamics (MD) simulations via nanoHUB.org
  - [Lab Handout]

Jump directly to the learning module by clicking on the links above, or continue reading for the module's rationale, learning objectives, and target audience.

Why MD simulations?



MD provides a very detailed description of materials and its processes by describing the dynamics of each individual atom in a material. Such a realistic descript of materials has an enormous educational potential and, unlike simple toy models or cartoons, can help students understand how materials look and work at atomic scales. *Image to the right shows screenshots from the* [nano-Materials Simulation Toolkit](#)*.*

If you are interested in learning more about MD, see topics: [Molecular dynamics simulations of materials].

Learning objectives

Upon completion of this learning module most students will be able to:

- Compute stress strain curves of metallic nanowires using online MD simulations with the nano-Materials Simulation Toolkit and explore the role of size, temperature, and strain rate;
- Compute the strength of perfect nanowires and compare it with that of polycrystalline samples;
- Understand the role of pre-existing dislocations on the yield stress of metals;
- Understand the orientation of the active slip plane with respect to the tensile axis for uniaxial deformation;
- Understand the atomic displacements that lead to plastic deformation in single crystal nanoscale wires

Some students are expected to:

- Understand the difference in activation associated with dislocation nucleation and their propagation;
- Identify the active slip system (slip plane and slip direction) from the MD simulations
- Explore strain hardening focusing on the difference between annealed and cold worked macroscopic samples and nanoscale specimens;
- Explore and understand compressive vs. tensile asymmetry in uniaxial deformation of nanowires;

Instructors can build on this learning module to teach Schmid law and the calculation of Schmid factors for fcc crystals as well as the specimen rotation during single glide.

Audience

This learning module was designed for and used in an introductory course for second-year students of Materials Engineering at Purdue University. Students will find this learning module most useful if they are familiar with the following topics:

- Basic physics of classical mechanics;
- Mechanical response of metals (elastic and plastic deformation, yield strength, and work hardening)
- Basic knowledge of crystal structures (common crystal structures of metals, crystalline planes)

We expect this module to be useful in introductory and advanced courses of the mechanical response of materials and nanoscience at the undergraduate and graduate levels.