# Dislocation structure and propagation

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## 1. Objectives

In this computational lab you will learn about dislocations via online molecular dynamics (MD) simulations using nanoHUB. The simulations involve various types of dislocations in FCC and BCC crystals. During the learning module you will be able to:

- Distinguish edge and screw dislocations in FCC and BCC crystals
- Understand the propagation of both pure dislocation types, including Burger's vector, line direction, and slip plane

## 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 dislocation simulations using an MD tool on nanoHUB.org. The tool creates pairs of both edge and screw dislocations for both FCC and BCC crystals. In FCC metals, slip occurs on the closed-packed {111} planes along the close-packed <110> directions in the slip plane; similarly, for BCC materials the {110} planes with <111> directions are the primary slip systems. Using the MD simulations, you will be able to directly observe the motion of the dislocations, which ultimately causes plastic deformation in at the macroscale.

### Additional Resources:

- *Materials Science and Engineering: An Introduction* 9th ed. Callister & Rethwisch. Wiley.
  - "Dislocations and Plastic Deformation" (Chapter 7, Sections 7.1 – 7.4)
- nanoHUB-U: From Atoms to Materials (Sections 3–4) https://nanohub.org/courses/FATM

# 3. Main 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. Dislocation simulations (Quick-start)

To start, run a new simulation with edge dislocations in copper. To do this, complete the steps outlined below:

1. As shown in Figure 1, select "Dislocation Dynamics" from the "Experiment" dropdown
2. Then select "Copper Edge" from the "Dislocation Material and Type" dropdown
3. Click "Simulate" and wait for results. This simulation will take less than 30 minutes.

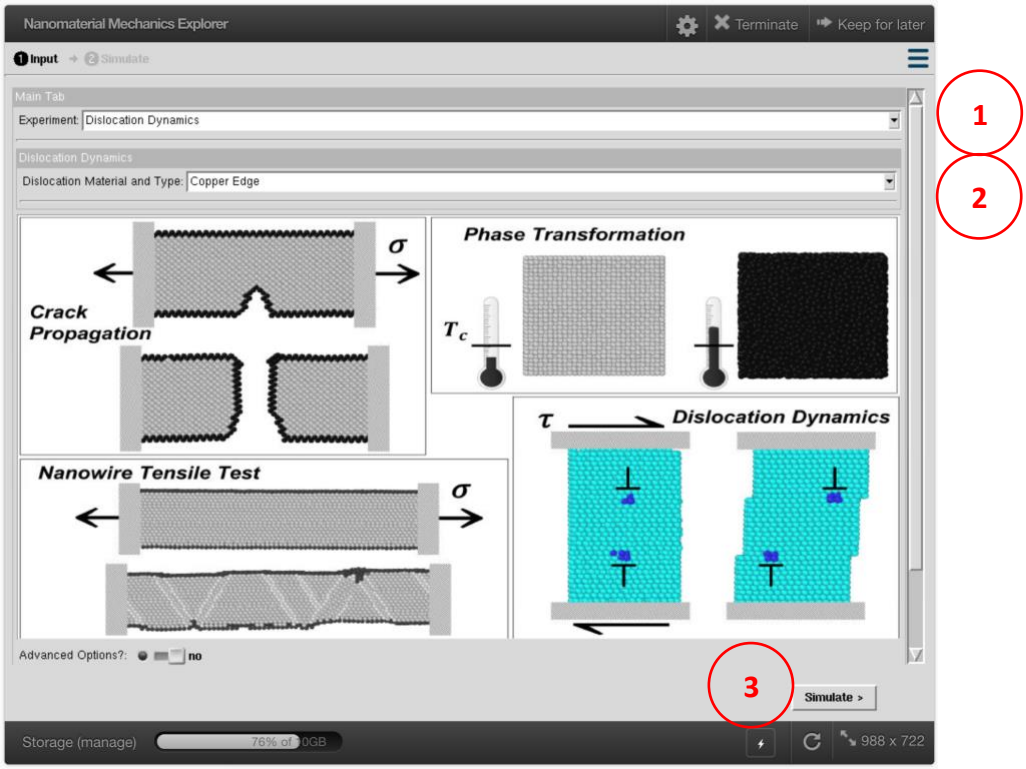


**Figure 1:** Simulation tool front page.

Note that the details of the simulation that you are running are given in the "Advanced options". In particular, the orientation of the system is:

- **x = [-110], y = [111], z = [11-2] with shear in the xy plane**

Results are shown while it runs, including the number of atoms in the system and the system length over time.

## C. Multiple dislocation types

Comparison of crystal structure and dislocation type is one of the main objectives of this module. Follow the instructions from Section 3B to run the following default cases:

- FCC (Copper) edge (dissociated)
  - x = [-110], y = [111], z = [11-2]
- FCC (Copper) screw (dissociated)
  - x = [111], y = [1-10], z = [11-2]
- BCC (Iron) edge
  - x = [111], y = [1-10], z = [11-2]
- BCC (Iron) screw
  - x = [-110], y = [111], z = [11-2]

In each case we will deform the simulation (in pure shear) to cause the motion of the dislocation.

## 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.

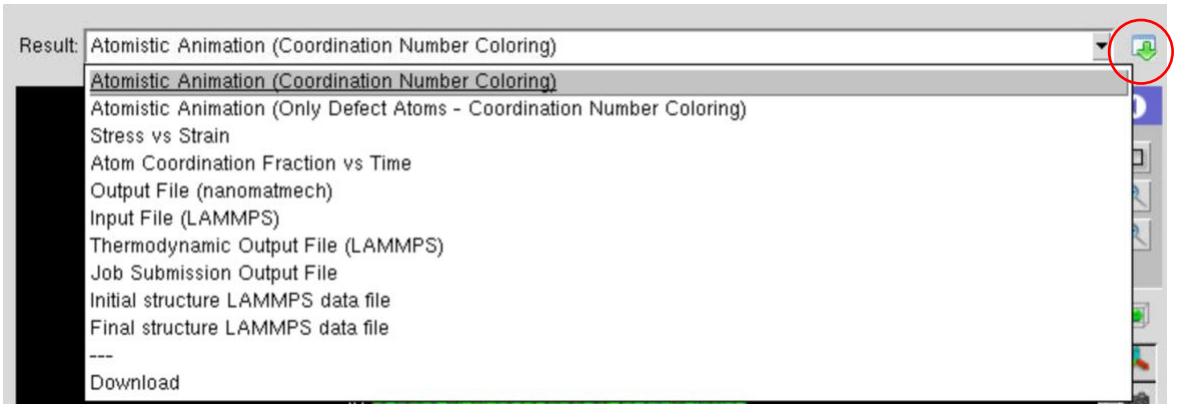


**Figure 2:** Simulation output options.

2. Focus on and/or save the following:
   a. Stress-strain data (both CSV data and image are available from "Stress vs strain")
   b. Notable images from the atomic structures ("Atomistic animation" from the "All atoms" view; "Defect atoms" may be helpful as well)
   c. 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.

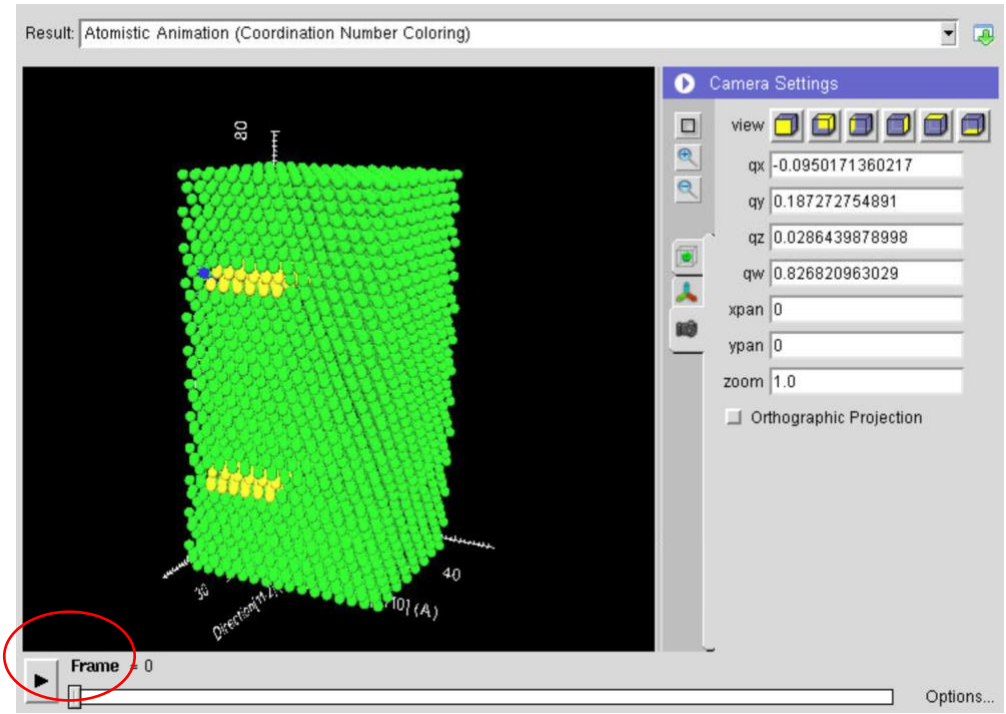


**Figure 3.** Atomistic animation example.

# 4. Assignment

## A. While the simulations are running

1. What are the definitions of Burger's vector, dislocation line, and slip plane?
2. Review the combinations of slip planes and directions for each combination of FCC/BCC and edge/screw dislocation.

## B. After simulations have finished

1. Annotate snapshots from each dislocation simulation (FCC & BCC, edge & screw), with the following information (use multiple simulation times):
    - Burger's vector,
    - Dislocation line direction, and
    - slip plane.

# 5. Additional simulations

## A. Multiple strain directions (Customized 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 dislocation simulation. These instructions show how to run with a different applied strain direction.

1. Start from the "default" dislocation simulation, "Copper Edge", 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 "Thermomechanics Details" tab
        i. Change the "Strain direction" to another shear option
    b. 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 under 30 minutes.

## B. Dislocation annihilation

One final pre-built simulation is available with the tool: FCC (Copper) screw annihilation. Run this from the front page (Section 3B).

# 6. Additional questions

1. What happens when the strain direction is changed? Show and describe changes from the atomic structure and/or stress vs. strain. How does this relate to Schmid factors and activated slip systems?
2. What is unique about FCC screw dislocations that allow the annihilation?

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?