Ductile and brittle failure in metals

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1. Objectives

In this computational lab you will perform online molecular dynamics (MD) simulations of nanoscale cracks under uniaxial tension through nanoHUB. Simulations with varying temperature and crystal structure will provide information to:

- Distinguish the atomistic mechanisms of ductile and brittle failure and the relationship with temperature
- Examine changes in crack propagation with crack length

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 samples containing nanoscale cracks using an MD tool on nanoHUB.org. Crack propagation is a main element of failure in metals and has caused many catastrophic events. The tool creates single-crystal systems with various temperatures and crystal structure (FCC and BCC) and deforms in tension to strain of 25% engineering strain. Using the MD simulations, you will be able to directly observe crack propagation at the atomic level and how this mechanical behavior at the macroscale.

Additional Resources:

- *Materials Science and Engineering: An Introduction* 9th ed. Callister & Rethwisch. Wiley.
  - "Failure" (Chapter 8, Sections 8.1 – 8.6)
- 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. Crack propagation simulations (Quick-start)

To start, run a new tensile-test simulation of a nickel system at 100K. To do this, complete the steps outlined below:

1. As shown in Figure 1, select "Crack Propagation" from the "Experiment" dropdown
2. Then select "Nickel (200K)" from the "Material and Temperature" dropdown
3. Click "Simulate" and wait for results. This simulation will take less than 30 minutes.

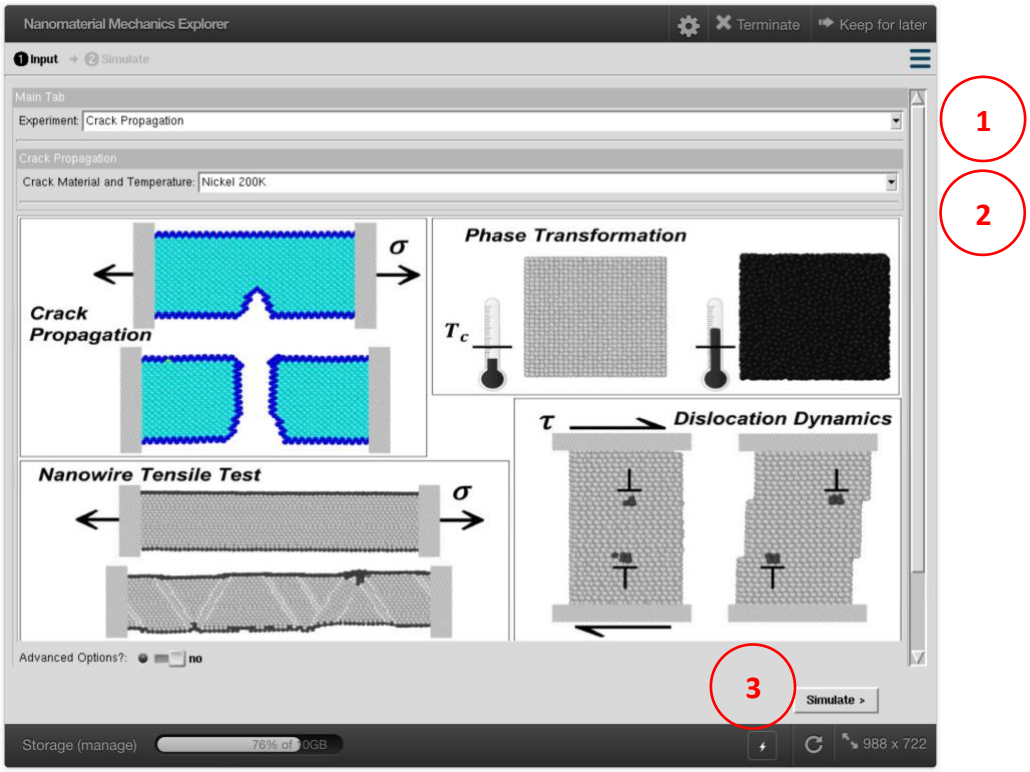

Figure 1: Simulation tool front page.

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 system length over time.

C. Multiple temperatures and crystal structures

Comparison of temperature and crystal structure are the main objectives of this module. Follow the instructions from Section 3B to run three more simulations:

- FCC (Nickel) 600K
- BCC (Iron) 100K
- BCC (Iron) 600K

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.

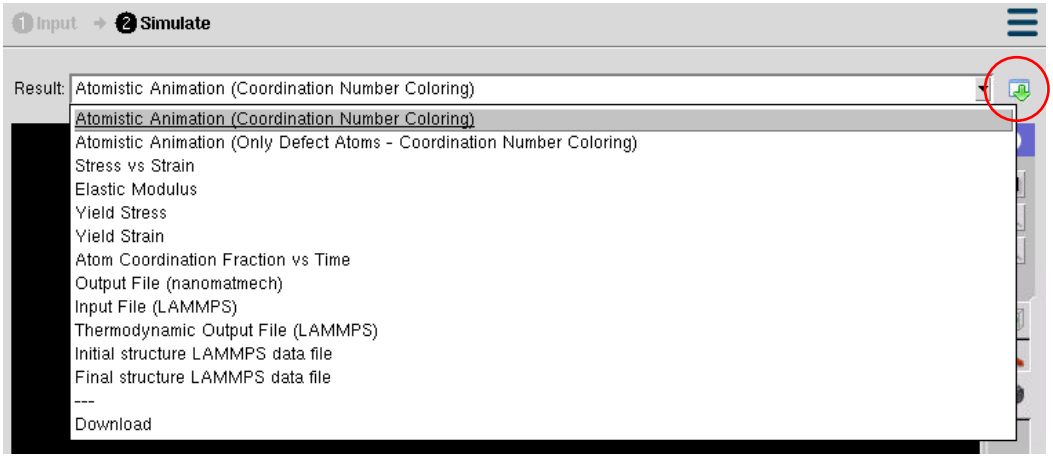

Figure 2: Simulation output options.

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.

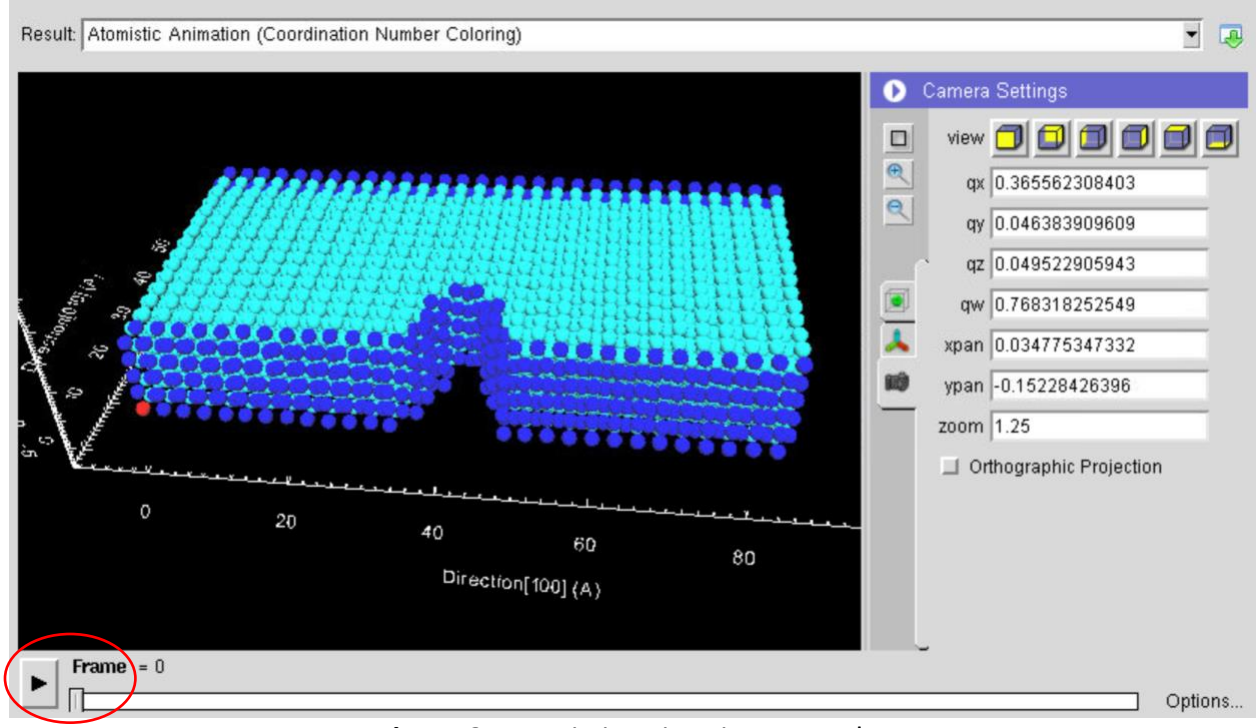

Figure 3. Atomistic animation example.

4. Assignment

A. While the simulations are running

1. Where is the applied stress concentrated in the material?

B. After simulations have finished

1. What are the distinguishing features between the ductile and brittle simulations? What are the stress relaxation mechanisms in each?
2. Why do we see a ductile-brittle transition? Or, when temperature changes, what changes for the stress relaxation mechanisms?
3. In BCC metals it is quite common to see a ductile-brittle transition, but not in FCC metals. Why are the results in these simulations different?

5. Additional simulations

A. Multiple crack lengths (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 crack propagation. These instructions show how to run with different sized cracks.

1. Start from the "default" crack simulation, "Nickel 200K", 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 "Modify structure":
        i. Change crack length from 5 to 2 (unit cells)
    c. Under the "Thermomechanics Details" tab review the inputs
        i. Change "Start Temperature" (different for each run)
    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 30 minutes.

6. Additional questions

1. How does varying the crack length affect the yield stress? How would you expect the crack length and yield stress to be related by theory?

2. What does the model include (and what is the simulation therefore able to capture)?
3. What does the model exclude?
4. Choose a new interatomic model (See instructions in Section 5A)
    - How similar are the results?