

Nanoscale melting

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1. Objectives

In this computational lab you will perform online molecular dynamics (MD) simulations through nanoHUB to melt nickel samples and analyze the results in order to:

- Understand the process of melting at atomic scales
- Identify effects of surfaces and specimen size
- Describe differences between simulation and experiment

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 melting simulations using an MD tool on nanoHUB.org. The tool creates nickel systems and heats from room temperature above the melting point. Using the MD simulations, you will be able to directly observe the atomic movements during the melting phase transition, as well as the total system energy and structural changes.

Additional Resources:

- *Materials Science and Engineering: An Introduction* 9th ed. Callister & Rethwisch. Wiley.
 - “Mechanical Properties of Metals” (Chapter 10, Sections 10.1-10.4)
- nanoHUB-U: From Atoms to Materials (Sections 3–4) <https://nanohub.org/courses/FATM>

Related Resources:

Another learning module uses a different simulation tool (<https://nanohub.org/tools/matsimtk>), but is otherwise very similar.

- Strachan, A. Melting via molecular dynamics simulations. <https://nanohub.org/resources/22025>

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 bulk nickel system. To do this, complete the steps outlined below:

1. As shown in Figure 1, select “Melting” from the “Experiment” dropdown
2. Then select “Nickel Bulk” from the “Melting Material” dropdown
3. Click “Simulate” and wait for results. This simulation will take less than 60 minutes.

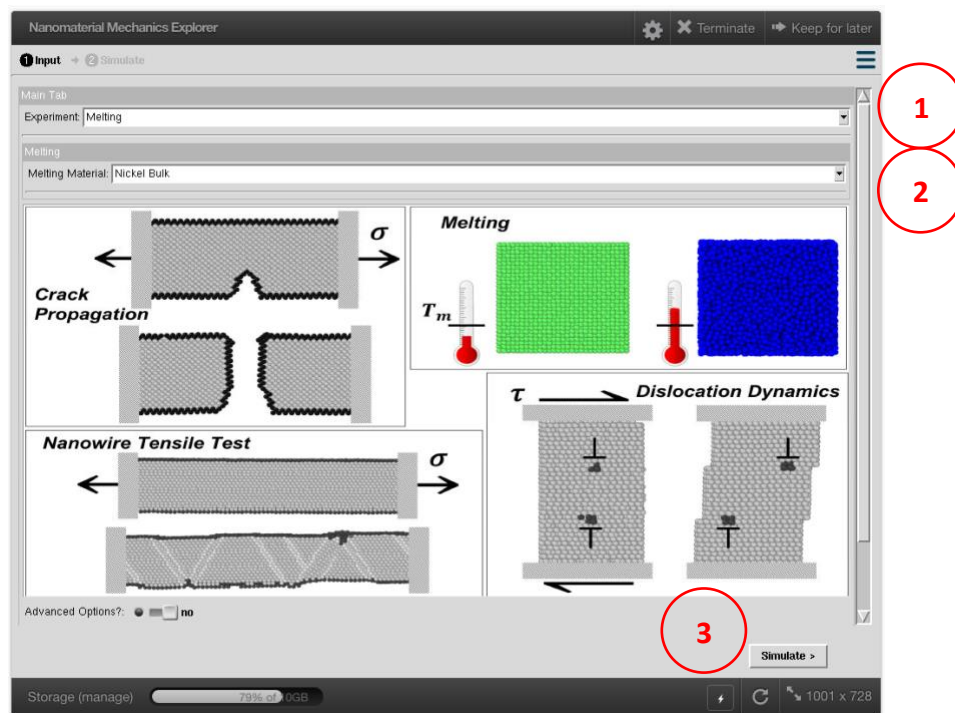


Figure 1: Simulation tool front page.

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 energy over time.

C. Bulk vs. nanoparticle

Comparison of boundary conditions is one of the main objectives of this module. Follow the instructions from Section 3B to run the second system:

- Nickel nanoparticle

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.

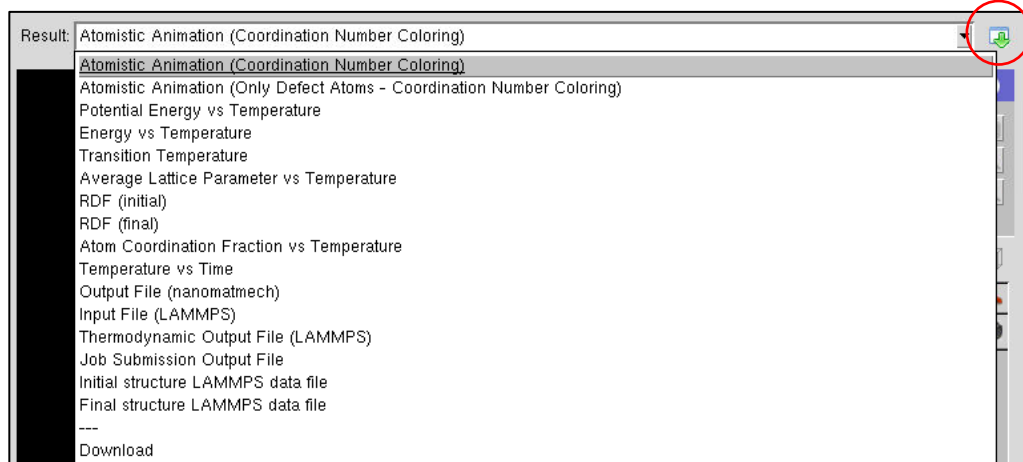


Figure 2: Simulation output options.

2. Focus on and/or save the following:
 - a. Lattice parameter vs. temperature data (both CSV data and image are available)
 - b. Potential energy vs. temperature data
 - Due to the latent heat, the potential energy increases sharply at a phase transition.
 - c. Phase transformation temperature calculated by the tool
 - d. Notable images from the atomic structures (“Atomistic animation” from both the “All atoms” and “Defect atoms” views)
 - e. 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 (temperature) 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.

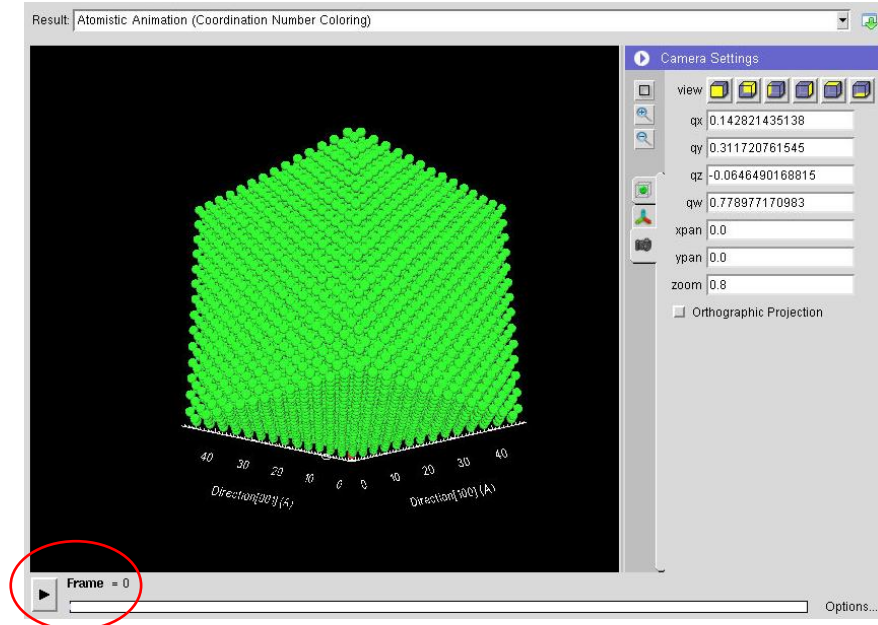


Figure 3. Atomistic animation example.

4. Assignment

A. While the simulation is running

1. What does the model include (and what is the simulation therefore able to capture)?
2. What does the model exclude?

B. After simulations have finished

1. Estimate the bulk melting temperature from the potential energy, lattice parameter, and atomic structure.
2. Compare this to the experimental melting point. What are possible reasons for differences?
 - In part, think about the concept of equilibrium and what happens when real materials melt and solidify.
3. As with Question 1, estimate the melting point for the nanoparticle.
4. Compare the melting process for the bulk and nanoparticle systems. Why are they different?

5. Additional simulations

A. Custom size nanoparticle 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 (7 unit cell) nanoparticle, which run faster than Section 3.

1. Start from the “default” simulation, “Nickel nanoparticle”, 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 both the X, Y, & Z “System size” from 14 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

3. What are the size effects at the nanoscale (comparing multiple nanoparticles)? Would you expect the same size effects in macroscale samples?
4. Choose a new interatomic model (See instructions in Section 5A)
 - How similar are the results?