nanoMATERIALS simulation tool
First-time-user guide

Strachan Group
School of Materials Engineering and Birck nanotechnology Center
Purdue University
strachan@purdue.edu

This tool allows users to perform molecular dynamics simulations of metals and semiconductor structures. Properties and processes that can be studied include thermo-mechanical properties and thermal transport.

Addition information
• Topics page on MD simulations: 
  http://nanohub.org/topics/MD
• Lecture series on MD simulations of materials: 
  http://nanohub.org/resources/5838
• Publications:
Go to nanohub.org

Click here to Register

Register an Account

Complete all required fields and submit. A confirmation email will be sent.
Login

The link in the conformation email will direct you to the login screen

My HUB

Logging in will bring you to the “My HUB” page. Here you can view recently opened tools and any open sessions.
The Tool URL

Once you are logged in enter the URL for the tool as seen above.

Launching the Tool

Click here to open a session for this tool.
nano-materials Toolkit

The specifics of each simulation will be determined by the information entered on these tabs.

Note the scroll bar

When all necessary fields are completed, this button will begin simulation.

This button will open the tool in a separate window if desired.

My HUB Access

Now that you have accessed the tool, it is available from your “My HUB” page.

If you accidentally close the browser window or leave the website, your tool session will remain open. It can be accessed here.

New sessions of the nano-Materials Simulation Toolkit can now be opened in the recent tools tab.
The atomic model to be used. This is a Platinum (100) cell.

These values are the number of times that the unit cell is repeated in the model. This will produce a 10x10x10 unit cell structure.

Leave this checkbox as “no” and the Translate Atoms values as “0”.

This is the model by which the atomic interactions will be calculated. We use EAM (Embedded Atom Model).

nanoMATERIALS uses Embedded Atom Model (EAM) potentials for metals and Stillinger-Weber for Si.
Driver Specification Tab

This is the time step (Δt). This simulation will be in .004 ps increments.

The number of total time steps.

The simulated temperature.

These values represent the number of steps between recorded values. For example, out of the 3000 total time steps, the trajectory data will be recorded six times: once every 500 steps.

Advanced Options Tab

The “Advanced Script” region is where any extra commands will be written in code.

Lines beginning with a “#” are comment lines. They will be ignored as the program runs. These lines are already present when you load the tool and give some instructions for additional code.

The following slides provide examples of how to create nanostructures using the advanced options tab.
Advanced Options: creating a sphere

Step 1. Create a Pt 10x10x10 supercell. Simulation cell length: 10a₀=3.95 nm

Step 2. Select a sphere of desired radius, invert selection (select all atoms outside sphere) and delete selected atoms

In Advanced Tab:

Note: to avoid spheres from interacting with periodic images the simulations cell length should be larger than the radius diameter + potential cutoff distance

Advanced Options: creating a nanowire between slabs

1 - The first line selects all atoms in the supercell from a height of 11.575 to a height of 27.27

2 – The second line inverts that selection.

3 - The third line selects a cylinder of radius 11.875 centered at (19.625,19.625). This is in addition to the selection from 2.

4 – The fourth line inverts the entire selection. This will result in a ring shape.

5 – The fifth line deletes all selected atoms leaving just the nanowire with a substrate on top and bottom.
Simulate

After all variables and code is entered correctly, click “Simulate” in the bottom right corner of the tool.

The tool will now run the code. Data will be calculated and displayed on the screen. This can take several minutes depending on the size/type of the supercell and the number of time steps.

Clicking “Abort” will halt the simulation.

Output

Drop down menu for each result.

Click Structure to view the structure snapshots at various times throughout the test.

To go back and try different parameters click “Input”.

After multiple tests in the same session, this slider will appear allowing you to go back to previous results. Changes from test to test are indicated in the light blue area.
Structure Results

Holding the left mouse button anywhere on the image will allow you to manipulate the view.

This button will bring you back to the original view.

This will change from a perspective projection to an orthoscopic projection. Give it a try.

Orthoscopic vs. Perspective Projections

Orthoscopic  Perspective
Comparing Structures at Different Times

Structure at 2.0 ps

Structure at 10.0 ps

Exporting an Image

Once you are satisfied with your image, click here to save.

Make sure “Image File” is selected and click “Download”.

You may have to set your browser to allow pop-ups from nanohub.org and try again. A new browser window will pop up and allow you to save the .png image file.