Online simulations via nanoHUB: Nanomaterial Mechanics Explorer

First-time User Guide

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1) Launch the Nanomaterial Mechanics Explorer Tool

• Log in to nanoHUB

• From My Tools on nanoHUB dashboard, search for “Nanomaterial mechanics explorer” and launch the tool, or go directly to the tool at https://nanohub.org/tools/nanomatmech/
2) Front page and the default runs

- Four main options – tutorials for each simulation type coming soon
2) Run simulation

1. Select the test type:

   - Experiment: Crack Propagation
   - Crack Material: Nickel 300K

2. Select provided example:

3. Click *Simulate* to run with the default settings

(The default runs will take 30 – 60 min)
(Advanced Options)

With Advanced Options, all simulation inputs are customizable.
(Uncertainty Quantification with *Advanced Options*)

With *Advanced Options*, all *number* inputs can be input as a distribution to run multiple simulations at once, automatically.

Choosing distribution for *Total Run Time*
2) Wait for simulation results

Notes about the simulation are shown while it runs

Running simulation...

You are running the Crack Propagation tool, the default case Nickel 300K.
We expect the run to take less than 50 Minutes.
3) Explore simulation results

A. Atomistic animations

B. Curves

C. Numbers

Example Atomistic animation: *All atoms*

Example Curve: *Stress vs. Strain*

Example Number: *Elastic modulus*
3A) Atomistic Animation (All Atoms)

- Select result with drop-down menu
- Download the current result
- Play, pause, select specific time
3A) Atomistic Animation (All Atoms)

Can rotate, zoom, and move with mouse

Side-bar allows changing all animation settings
3A) Atomistic Animation (*Defect Atoms*)

Similar to *All Atoms* output, but only shows atoms of a different crystal structure than the bulk material (Free surface)
3B) Curve (Stress vs Strain)

Mouse-over values
Zoom
3C) Numbers (Elastic Modulus)

(Calculated from Stress vs Strain curve elastic regime)
4) Run another!

Run another simulation to compare to the current results

Choose another default run or change Advanced Options
4) Compare results (Default Ni & Ta runs)

Outputs can be compared by selecting “All”, or examined individually.

The selector bar chooses the primary result.

Differences between simulations are listed.
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First-time User Guide: Extra tips

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Errors!

The simulations may not always work! Note the error in the tool, in the nanomatmech Output File, or Thermodynamic Output File.

Submit a ticket from the main page and note the issue is from nanomatmech.

Trouble tickets are generally answered 9AM - 5PM EST, weekends and holidays excluded. Even though we try our best to assist you quickly, please allow 24-48 hours to hear back from us.
Atom colors

All atoms are colored by their local coordination (not by atom type)

- **Green**: bulk (FCC atoms)
- **Blue**: surface (Other atoms)
- **FCC atoms**
- **BCC atoms**
- **HCP atoms**
- **Other atoms**
Origin marker

A single red “atom” marks the origin, but is not part of the simulation.
Multiple simulations may show some strange animation views to accommodate each.

Multiple simulations may output different results, leading to some blank pages.

Crack propagation

Nanoparticle melting

(blank output)