

# Online simulations via nanoHUB: Nanomaterial Mechanics Explorer

## First-time User Guide

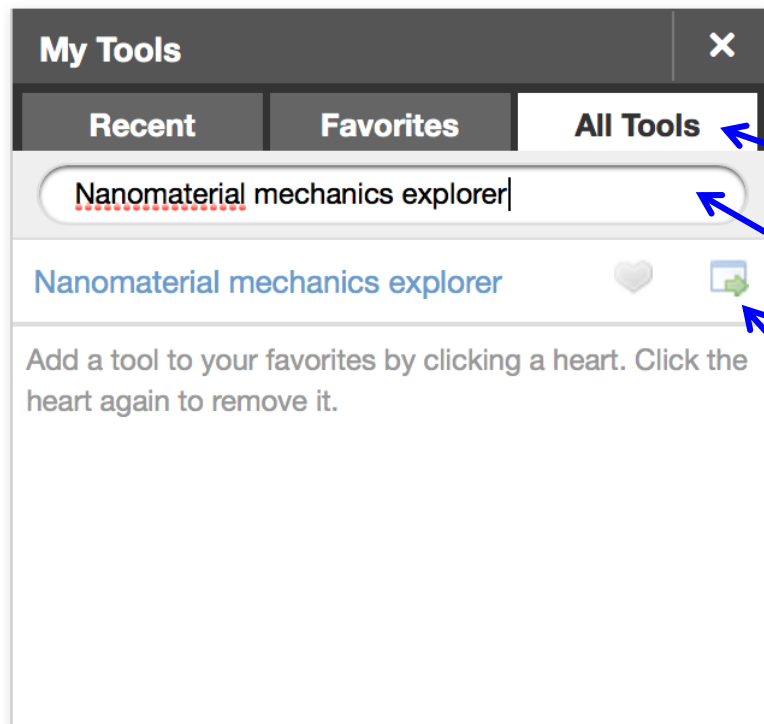
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School of Materials Engineering & Birck Nanotechnology Center  
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# 1) Launch the Nanomaterial Mechanics Explorer Tool

- 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/>



*My Tools on nanoHUB dashboard*

*All Tools tab*

*Search for “Nanomaterial mechanics explorer”*

*Launch the tool*

## 2) Front page and the default runs

- *Four main options –tutorials for each simulation type coming soon*

Nanomaterial Mechanics Explorer

⚙️ Terminate ▶️ Keep for later

1 Input → 2 Simulate

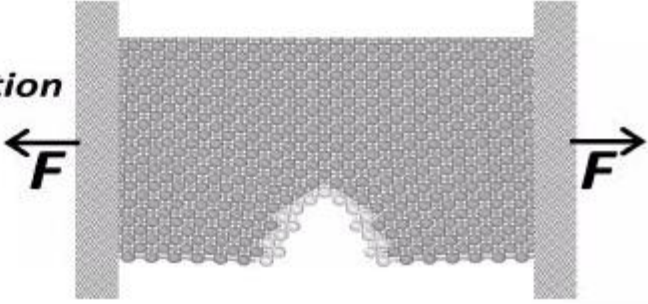
Main Tab

Experiment: Nanowire

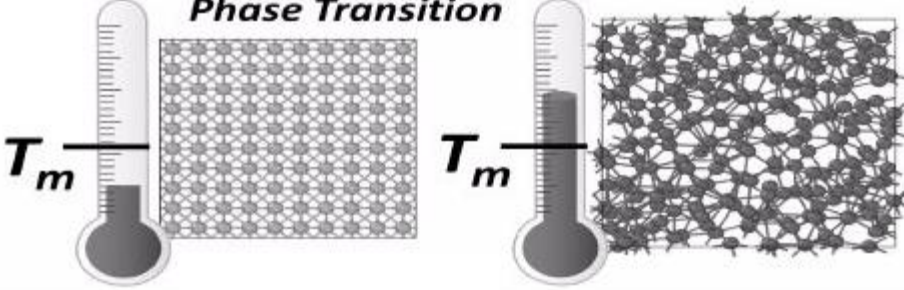
Nanowire

Nanowire Material and Orientation: Nickel [100]

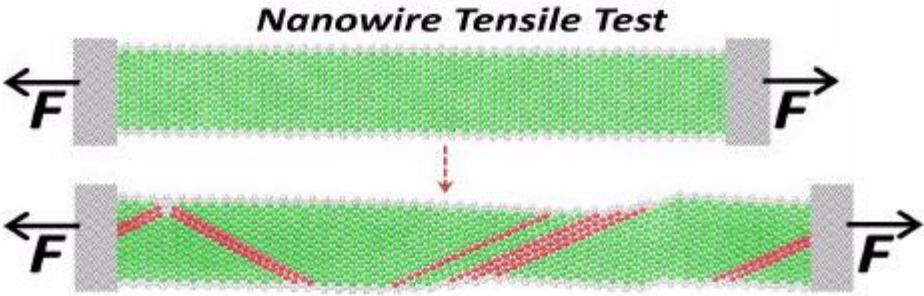
**Crack Propagation**



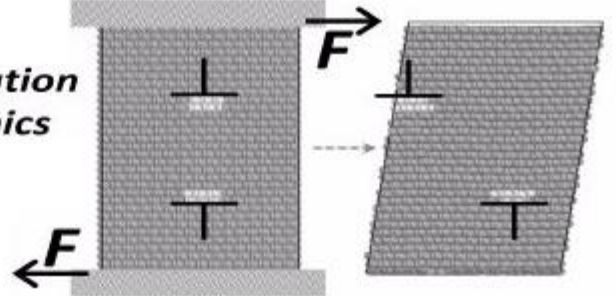
**Phase Transition**



**Nanowire Tensile Test**



**Dislocation Dynamics**



## 2) Run simulation

1. Select the test type:

Nanomaterial Mechanics Explorer

⚙️ Terminate ➡ Keep for later

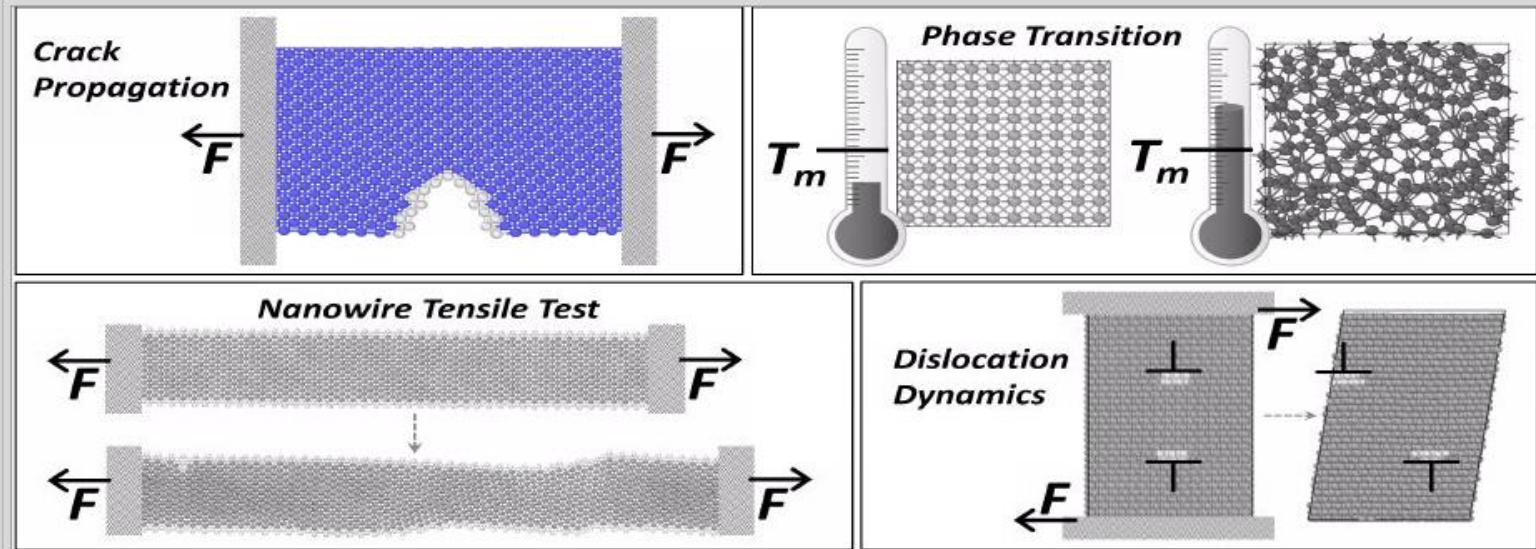
1 Input → 2 Simulate

Main Tab

Experiment: Crack Propagation

Crack Propagation

Crack Material: Nickel 300K



Advanced Options?:  no

2. Select provided example:

(The default runs will take 30 – 60 min)

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

Simulate >

Storage (manage) 60% of 10GB

⚡ ↻ 941 x 815

# (Advanced Options)

The screenshot displays the Nanomaterial Mechanics Explorer interface. The main window shows two simulation setups: "Crack Propagation" and "Nanowire Tensile Test". The "Crack Propagation" setup is selected, showing a material model with a crack and a force  $F$  applied. The "Nanowire Tensile Test" setup shows a nanowire under tension with force  $F$  applied. The "Advanced Options?" toggle is circled in red and set to "yes".

The "Advanced Options" panel is highlighted with a blue border and contains the following settings:

- Material: Nickel
- Element or Alloy?: Single Element
- Crystal Structure: FCC
- Lattice Parameter: 3.52Å

Annotations in blue boxes provide context:

- "Choosing details for the simulation *Material*" points to the material selection options.
- "With *Advanced Options*, all simulation inputs are customizable" points to the overall simulation configuration area.



# (Uncertainty Quantification with *Advanced Options*)

The screenshot displays the Nanomaterial Mechanics Explorer interface. The main window shows the 'Input' tab with 'Crack Propagation' as the experiment and 'Nickel 300K' as the crack material. A blue box highlights the 'Advanced Options?' section at the bottom left, where the 'yes' radio button is selected. A red circle highlights this section. A blue box highlights the 'Simulation Details' tab, which shows 'Total Run Time: 150ps'. A red circle highlights a distribution icon in the top right of this tab. A dialog box titled 'Total Run Time' is open, showing a 'gaussian' parameter value and a PDF plot. The dialog box contains the following fields: Mean: 150ps, Std Deviation: 15ps, Minimum: 105ps, and Maximum: 195ps. A blue box highlights this dialog box with the text 'Choosing distribution for Total Run Time'. The bottom of the interface shows a 'Simulate >' button and a storage indicator showing 60% of 10GB used.

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

The screenshot displays the Nanomaterial Mechanics Explorer interface. At the top, the title bar reads "Nanomaterial Mechanics Explorer" and includes buttons for "Terminate" and "Keep for later". Below the title bar, a progress indicator shows "1 Input" and "2 Simulate". The main content area displays the text "Running simulation..." followed by "You are running the Crack Propagation tool, the default case Nickel 300K. We expect the run to take less than 60 Minutes". A progress bar at the bottom of the main area shows "5%" completion. Below the progress bar is a button labeled "Abort". At the bottom left, there is a button labeled "< Input". The bottom status bar shows "Storage (manage)" with a progress indicator for "60% of 10GB", a power button, a refresh button, and a resolution indicator "941 x 815".

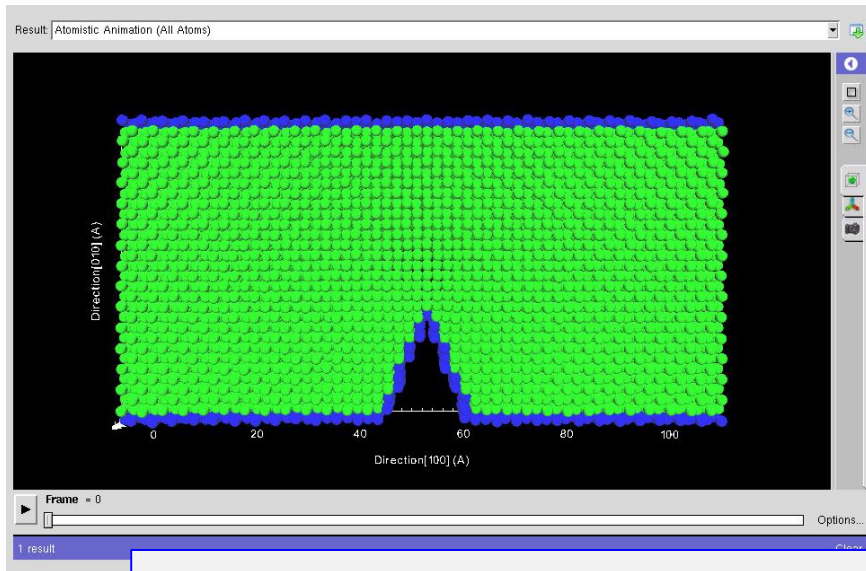
Notes about the simulation are shown while it runs

### 3) Explore simulation results

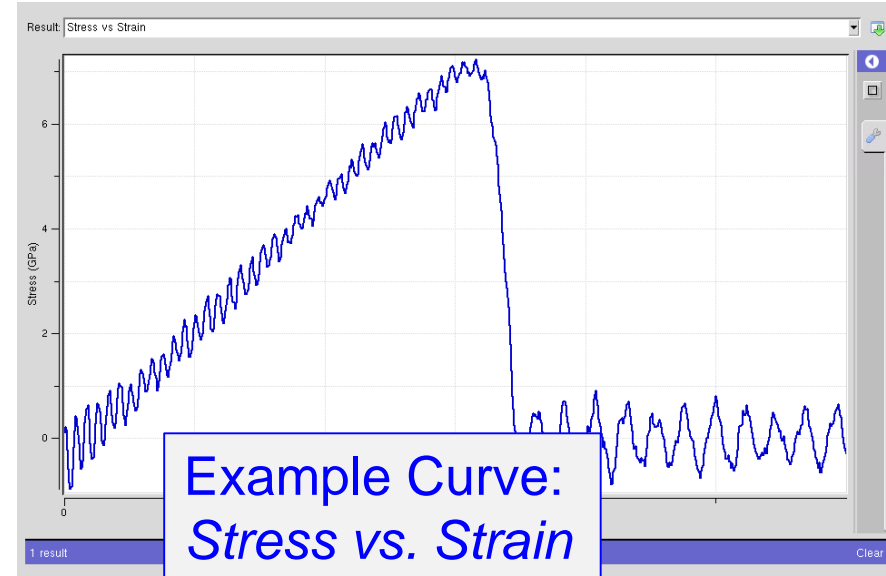
A. Atomistic animations

B. Curves

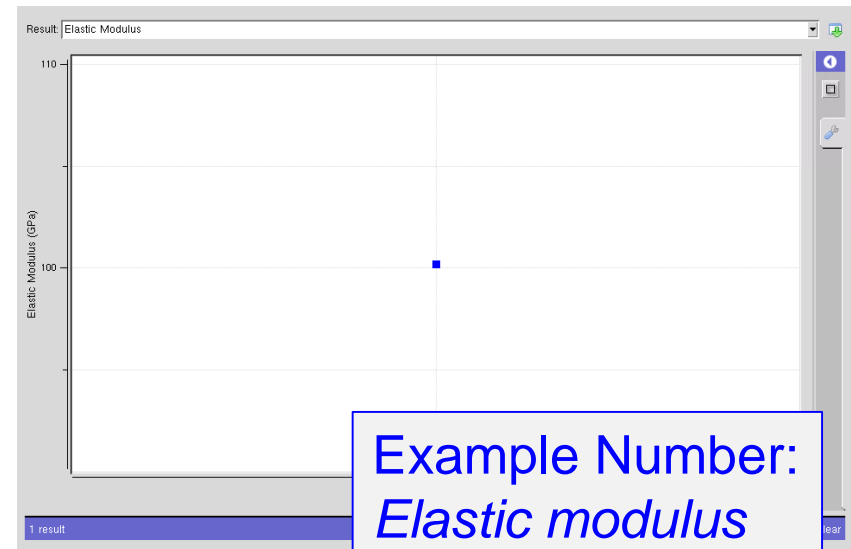
C. Numbers



Example Atomistic animation:  
*All atoms*



Example Curve:  
*Stress vs. Strain*



Example Number:  
*Elastic modulus*



# 3A) Atomistic Animation (All Atoms)

Nanomaterial Mechanics Explorer

1 Input → 2 Simulate

Result: Atomistic Animation (All Atoms)

Direction[010] (Å)

Direction[100] (Å)

Frame = 0

1 result

< Input

Storage (manage) 60% of 10GB

941 x 815

Select result with drop-down menu

Download the current result

Result: Atomistic Animation (All Atoms)

Direction[010] (Å)

Direction[100] (Å)

Frame = 42

Result: Atomistic Animation (All Atoms)

Direction[010] (Å)

Direction[100] (Å)

Frame = 45

Play, pause, select specific time

## 3A) Atomistic Animation (All Atoms)

Nanomaterial Mechanics Explorer

1 Input → 2 Simulate

Result: Atomistic Animation (All Atoms)

Camera Settings

view

qx 0.468991112929

qy 0.0096305078754

qz -0.0117957839065

qw 0.712999419777

xpan 0

ypan 0

zoom 3.81469726563

Orthographic Projection

Frame = 42

1 result Clear

< Input

Storage (manage) 60% of 10GB

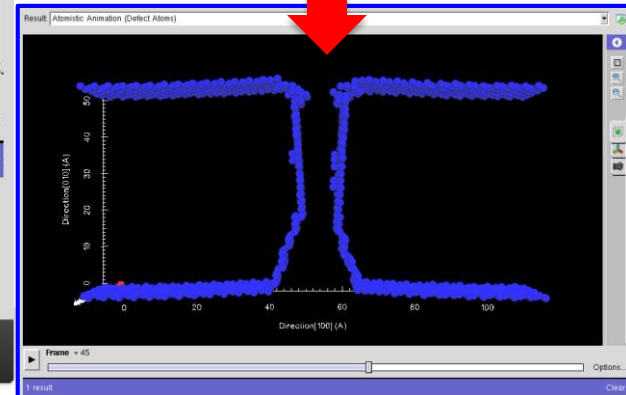
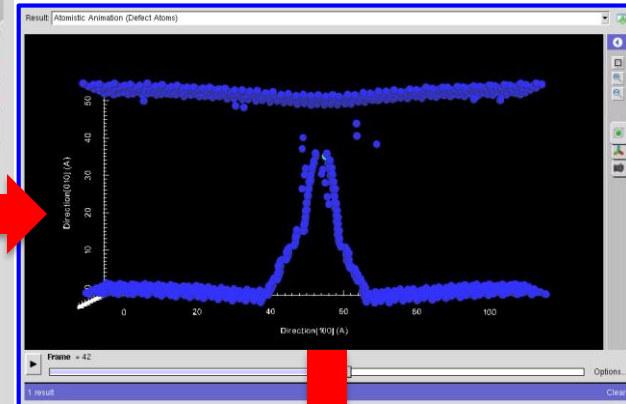
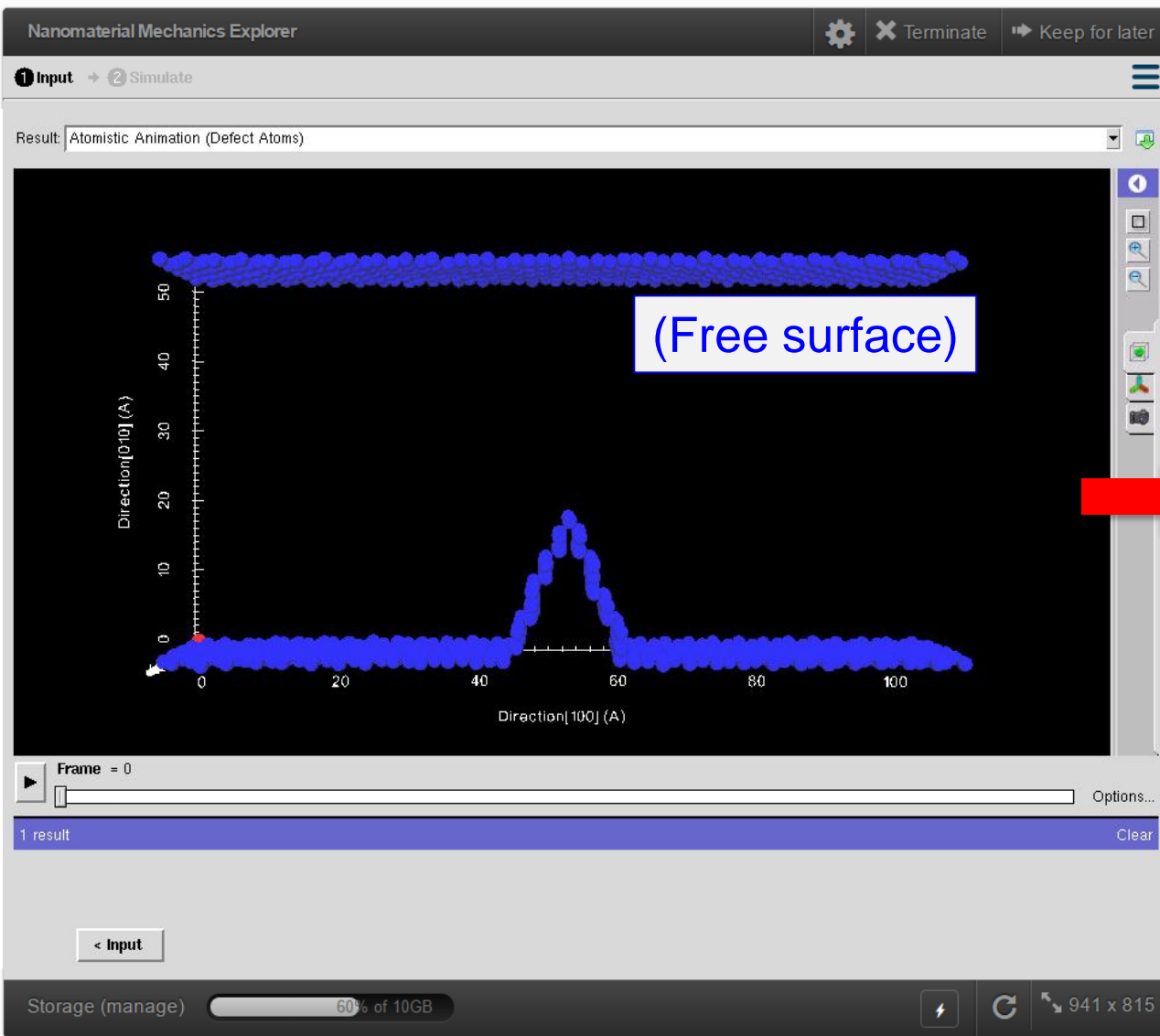
941 x 815

Can rotate,  
zoom, and move  
with mouse

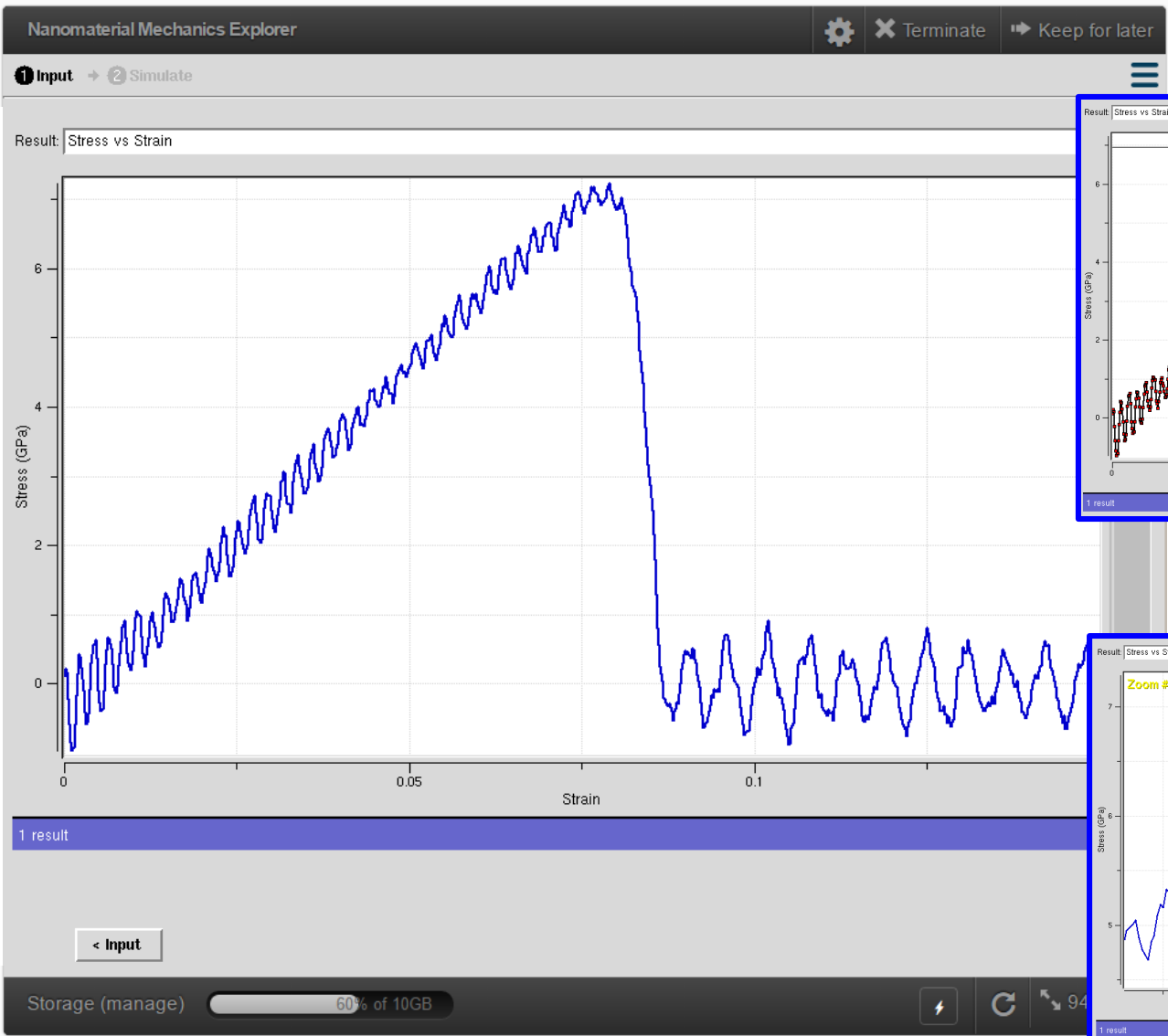
Side-bar allows  
changing all  
animation settings

# 3A) Atomistic Animation (*Defect Atoms*)

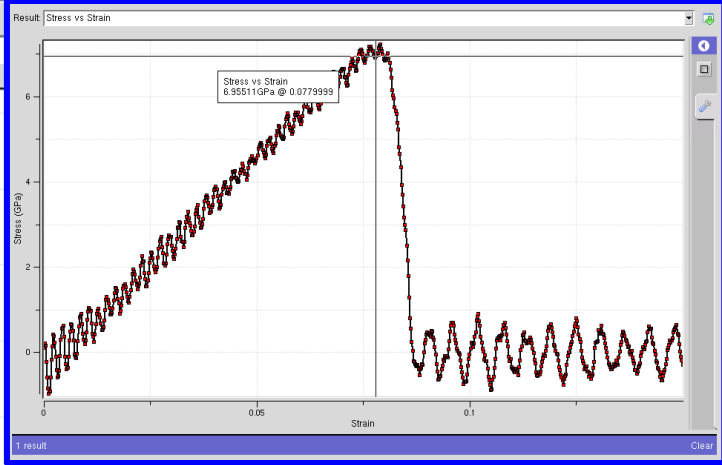
Similar to *All Atoms* output, but only shows atoms of a different crystal structure than the bulk material



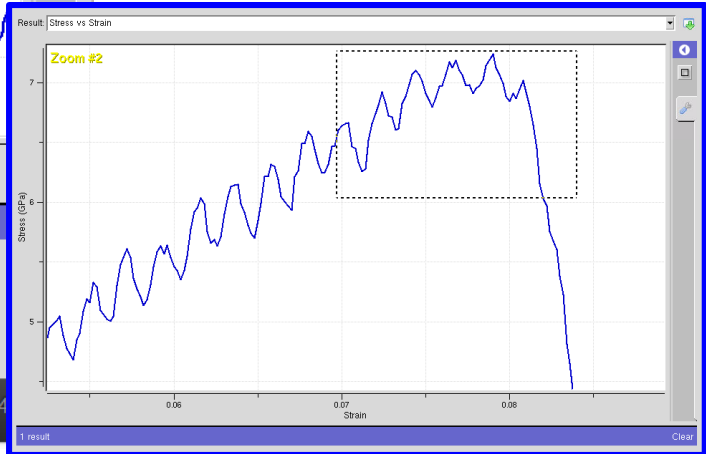
# 3B) Curve (Stress vs Strain)



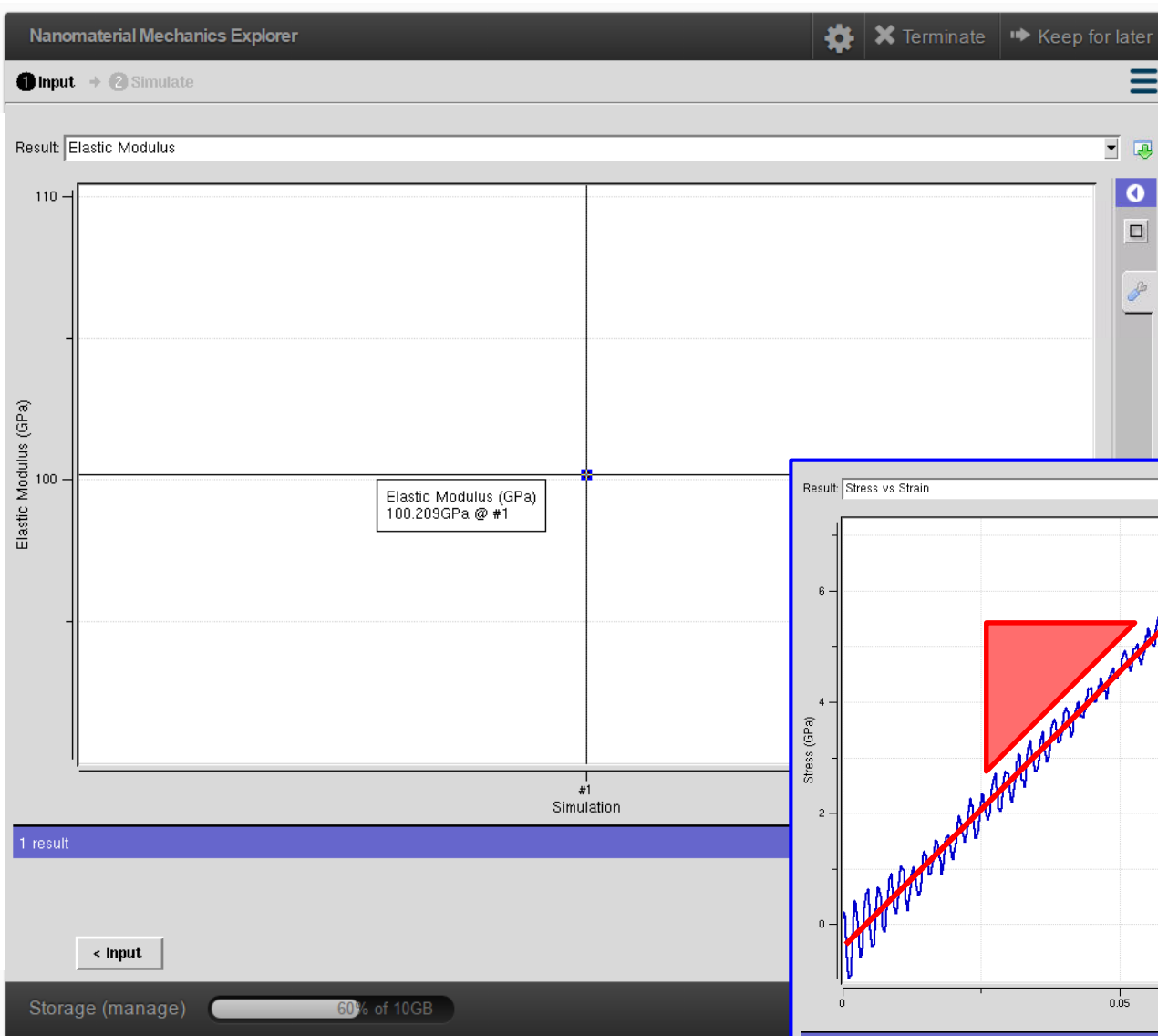
Mouse-over values



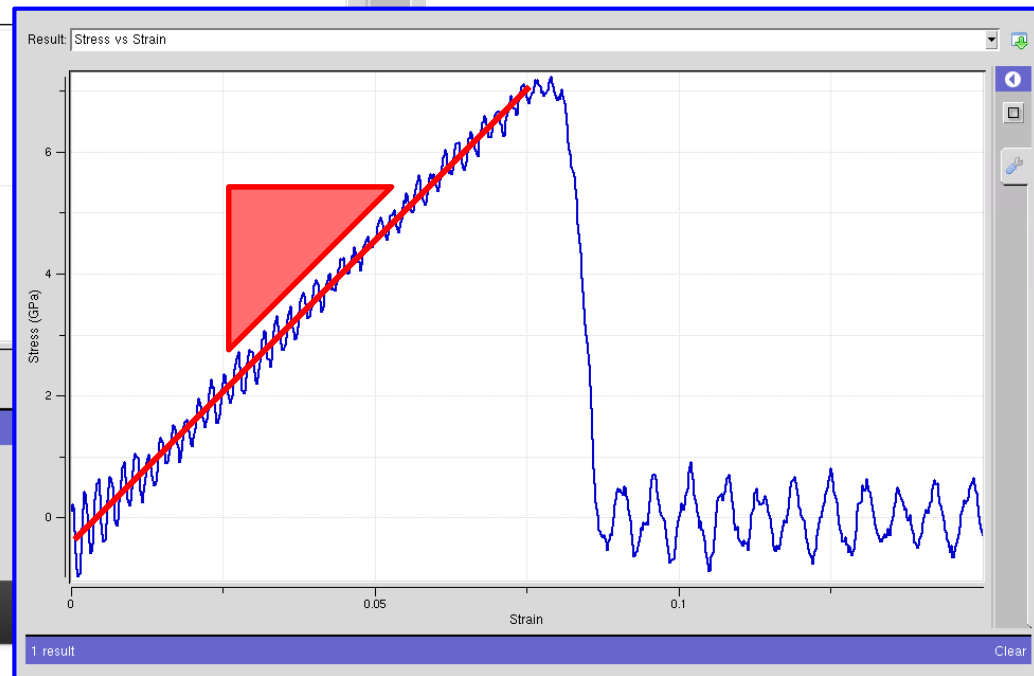
Zoom



## 3C) Numbers (*Elastic Modulus*)



(Calculated from  
*Stress vs Strain*  
curve elastic regime)





## 4) Run another!

Nanomaterial Mechanics Explorer

1 Input 2 Simulate

Result: Atomistic Animation (All Atoms)

Direction[010] (Å)

Direction[100] (Å)

Frame = 0

Options...

1 result Clear

< Input

Storage (manage) 60% of 10GB

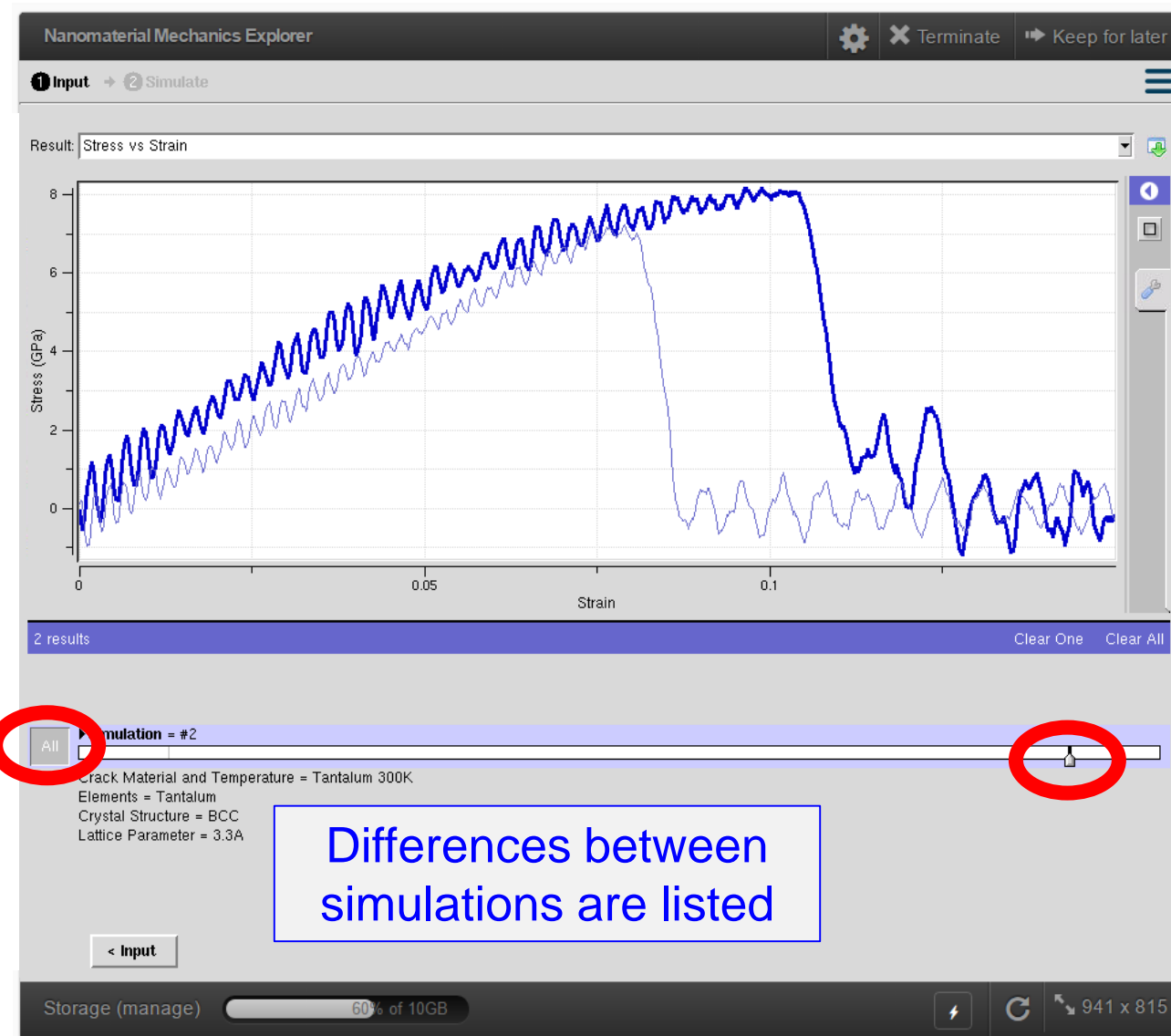
941 x 815

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

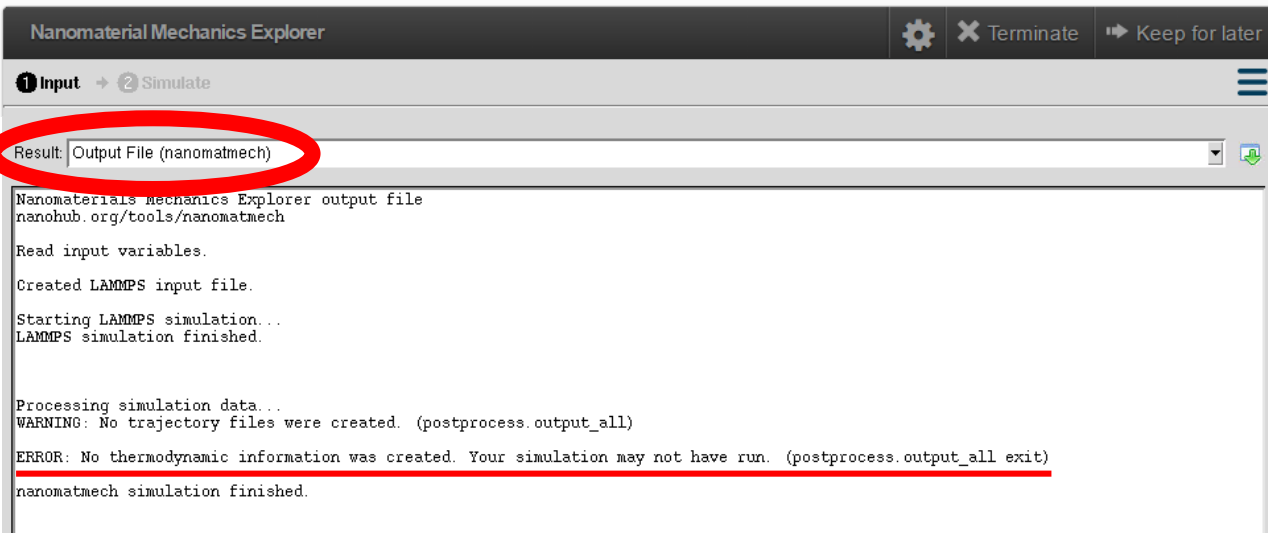
# Online simulations via nanoHUB: Nanomaterial Mechanics Explorer

## First-time User Guide: Extra tips

School of Materials Engineering & Birck Nanotechnology Center  
Purdue University  
West Lafayette, Indiana USA

# Errors!

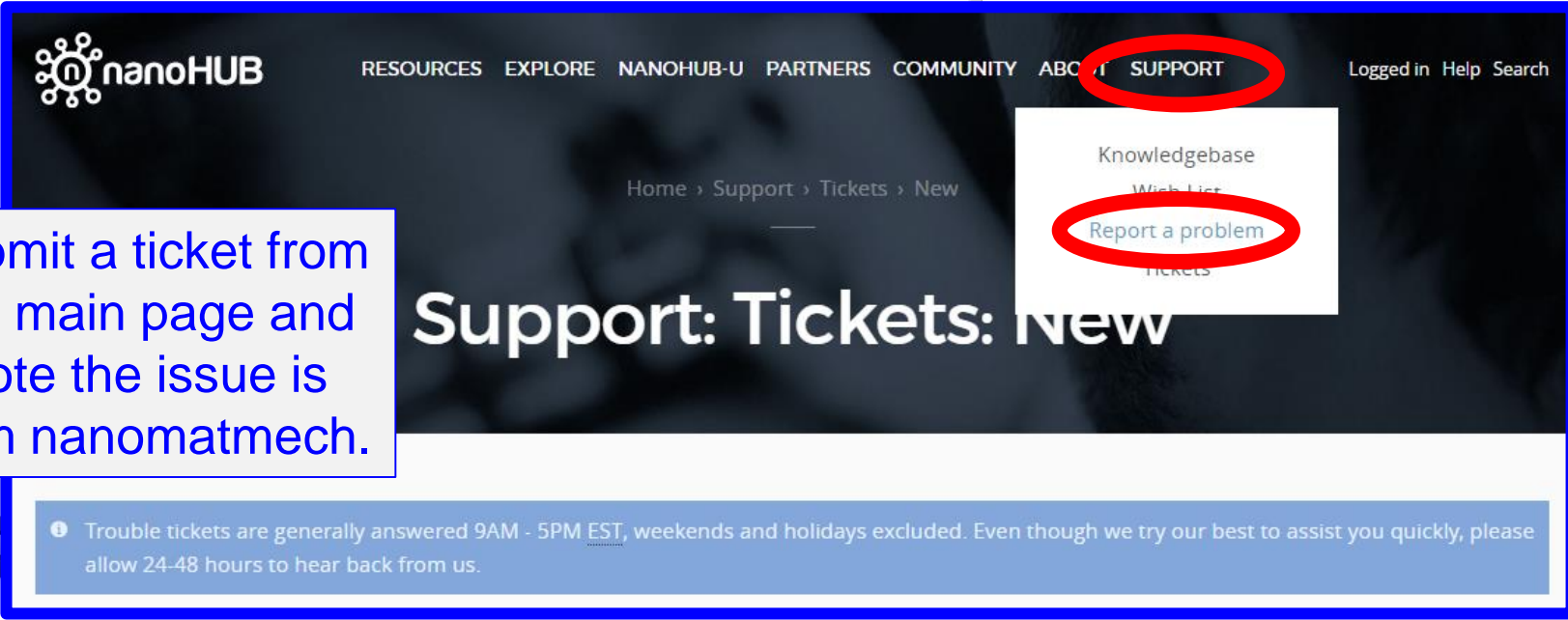
The simulations may not always work! Note the error in the tool, in the nanomatmech Output File, or Thermodynamic Output File.



```
Nanomaterial Mechanics Explorer output file
nanohub.org/tools/nanomatmech

Read input variables.
Created LAMMPS input file.
Starting LAMMPS simulation...
LAMMPS simulation finished.

Processing simulation data...
WARNING: No trajectory files were created. (postprocess.output_all)
ERROR: No thermodynamic information was created. Your simulation may not have run. (postprocess.output_all exit)
nanomatmech simulation finished.
```



RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT

Home > Support > Tickets > New

Report a problem

Support: Tickets: new

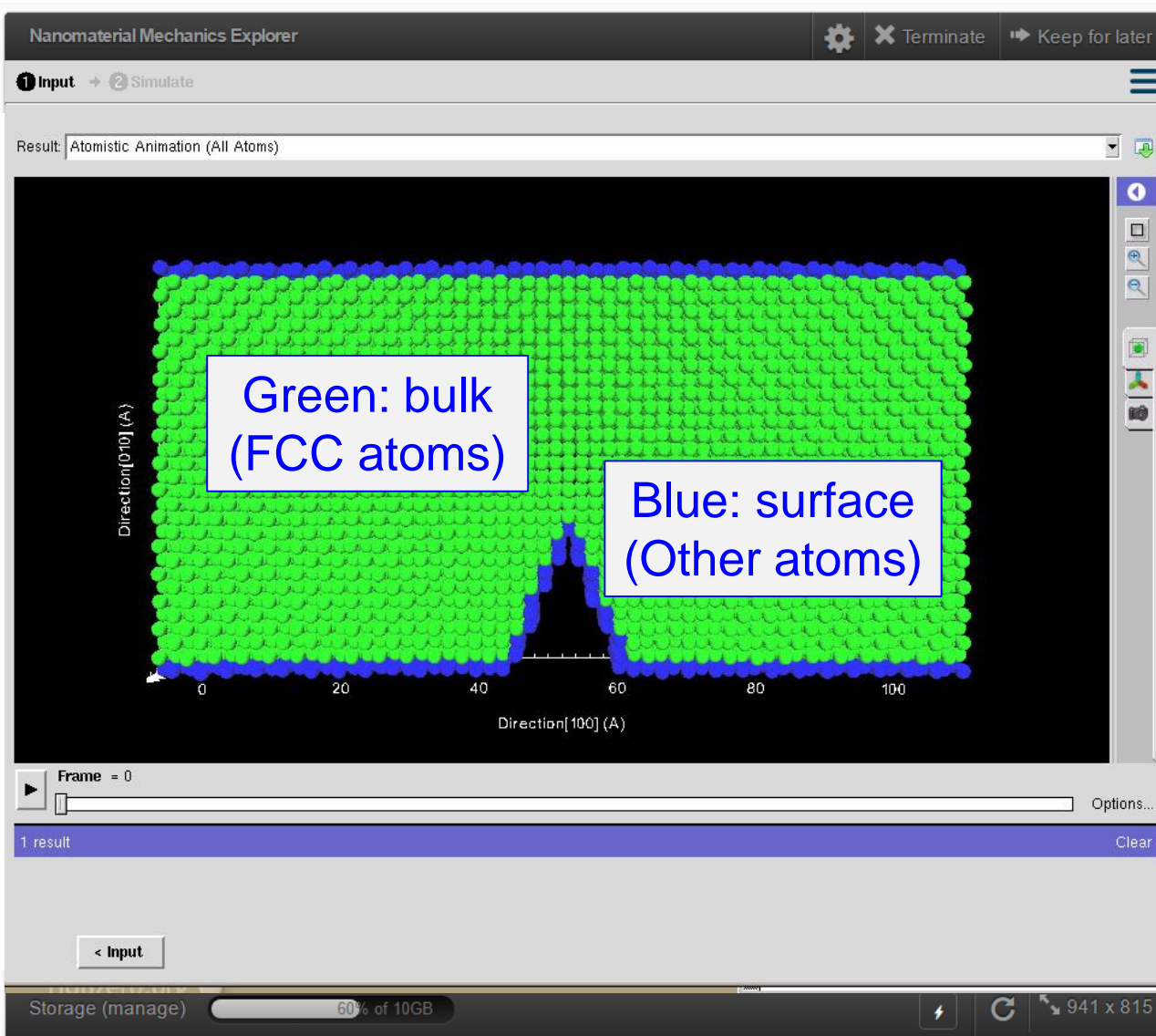
1 result

Storage (manage)





1 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.

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

# Atom colors



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

-  FCC atoms
-  BCC atoms
-  HCP atoms
-  Other atoms

# Origin marker

Nanomaterial Mechanics Explorer

⚙️ Terminate ▶️ Keep for later

1 Input → 2 Simulate

Result: Atomistic Animation (Defect Atoms)

Direction[010] (Å)

Direction[100] (Å)

Frame = 0

1 result Clear

< Input

Storage (manage) 60% of 10GB

⚡ ⌂ 941 x 815

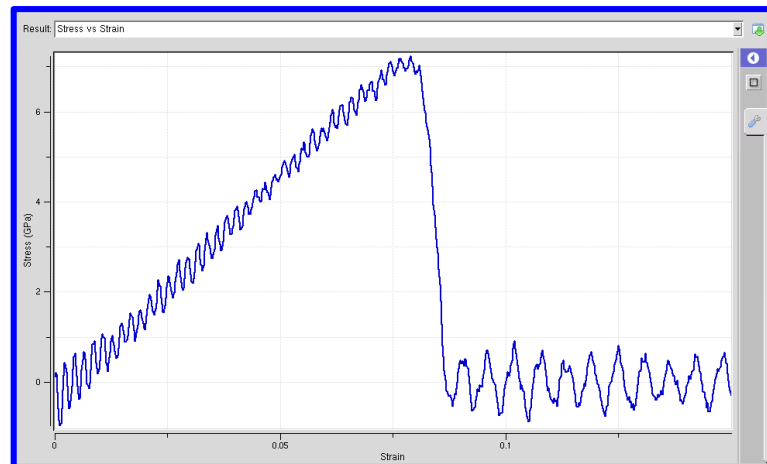
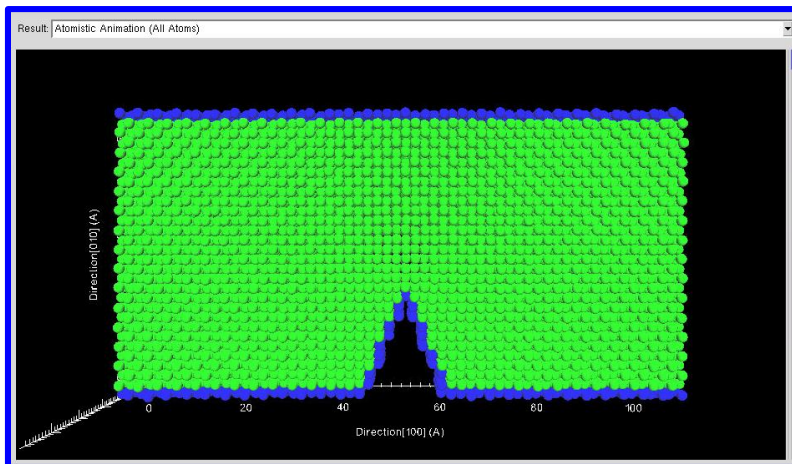
A single red  
“atom” marks  
the origin, but  
is not part of  
the simulation

# Multiple simulations

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

