

Lab: deformation of nanoscale materials

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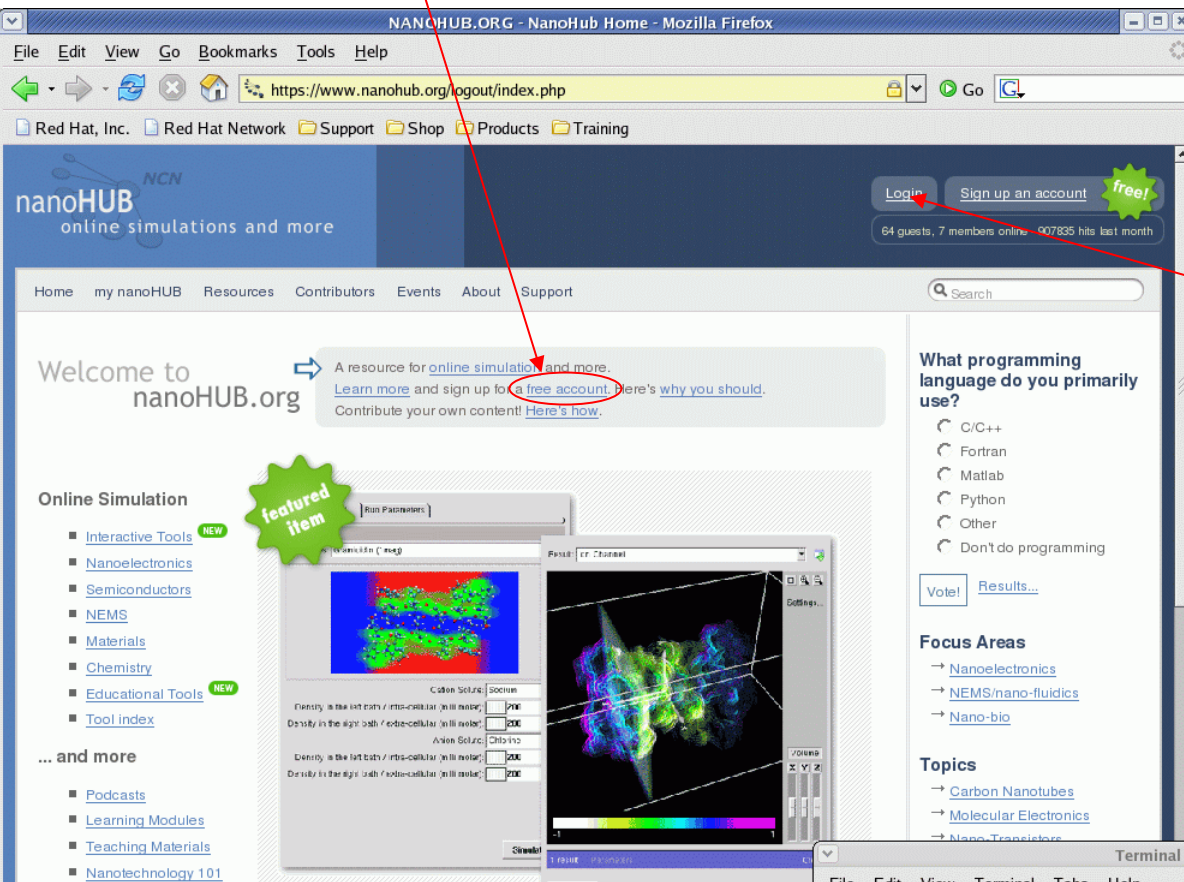
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nanoMATERIALS simulations toolkit

In order to run the nanoMATERIALS simulations toolkit you need to register as a user of the nanoHUB:

Go to www.nanohub.org
and click on:



The screenshot shows the nanoHUB website interface in a Mozilla Firefox browser. The address bar displays <https://www.nanohub.org/login/index.php>. The page header includes the nanoHUB logo and navigation links: Home, my nanoHUB, Resources, Contributors, Events, About, Support. A search bar is located in the top right. The main content area features a 'Welcome to nanoHUB.org' message and a 'Login' button. A red arrow points from the text 'and click on:' to the 'Login' button. Below the login button, there is a 'Sign up an account free!' button. The page also displays a 'What programming language do you primarily use?' poll with options: C/C++, Fortran, Matlab, Python, Other, and Don't do programming. A 'Focus Areas' section lists Nanoelectronics, NEMS/nano-fluidics, and Nano-bio. A 'Topics' section lists Carbon Nanotubes, Molecular Electronics, and Nano-Transistors. The 'Online Simulation' section is highlighted with a 'featured item' badge and shows a simulation interface with a 3D model and control panels.

Login and then click select
nanoMATERIALS tool

A simple MD runs with nanoMATERIALS

Determine initial model
for simulation

Select a model (Pt_nanowire)

Make a 5 5 5 supercell

NANOHUB.ORG - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

https://www.nanohub.org/index.php?optio

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nano-Materials Simulation Toolkit

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close

Input Model | Energy Expression | Driver Specification

Geometry to simulate: Pt_unitcell.bgf

Create Supercell

a direction: 5

b direction: 5

c direction: 5

Simulation cell parameters

Modify simulation cell parameters: no

Fixed atomic coordinates: Cartesian

Length a: 5A

Length b: 5A

Length c: 5A

Translate atoms

X direction: 0A

Y direction: 0A

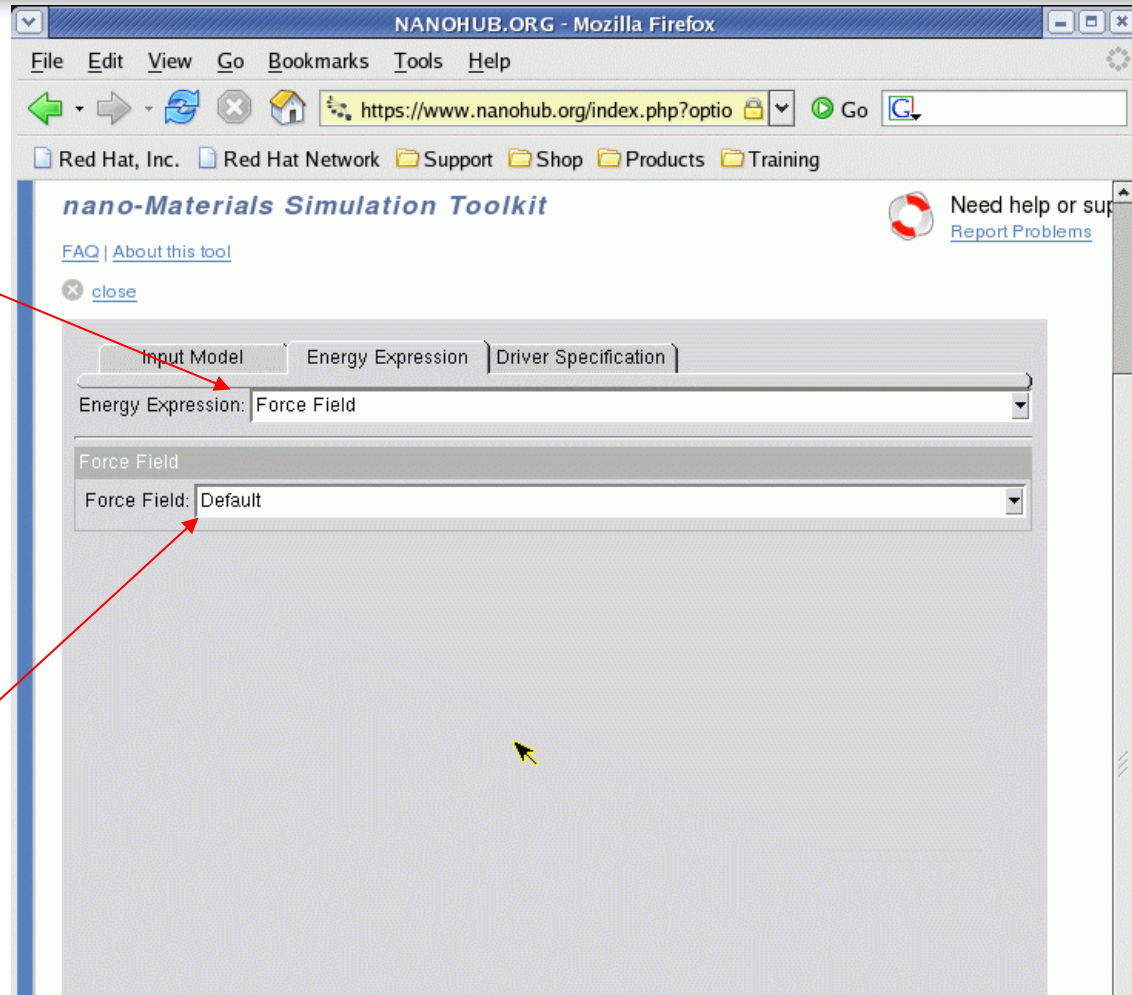
Z direction: 0A

A simple MD runs with nanoMATERIALS

Energy expression

Select how the energy (and derived quantities) of the system will be determined

We will let the program pick the force field for us (a many body Sutton Chen force field)



A simple MD runs with nanoMATERIALS

Driver options

What type of simulation?

Ensemble (NVE)

Time-step (5 fs)

Write a frame in the trajectory every 250 MD steps

Run simulation

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Input Model Energy Expression Driver Specification

Driver: Molecular Dynamics

Molecular Dynamics parameters

Ensemble: NVE

Time step: 0.005ps

Number of steps: 1000

Temperature: 300K

Temperature increment (K/ps): 0.00

Strain per MD step

X direction: 0

Y direction: 0

Z direction: 0

Periodic tasks

Write to energy file (steps): 10

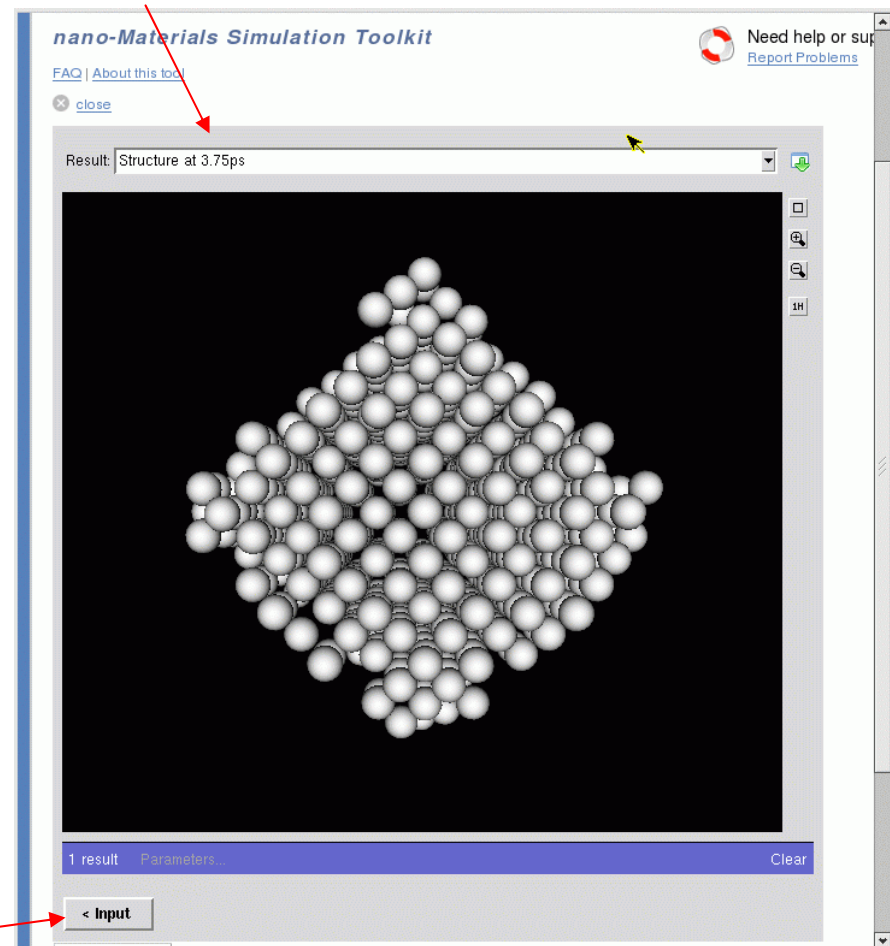
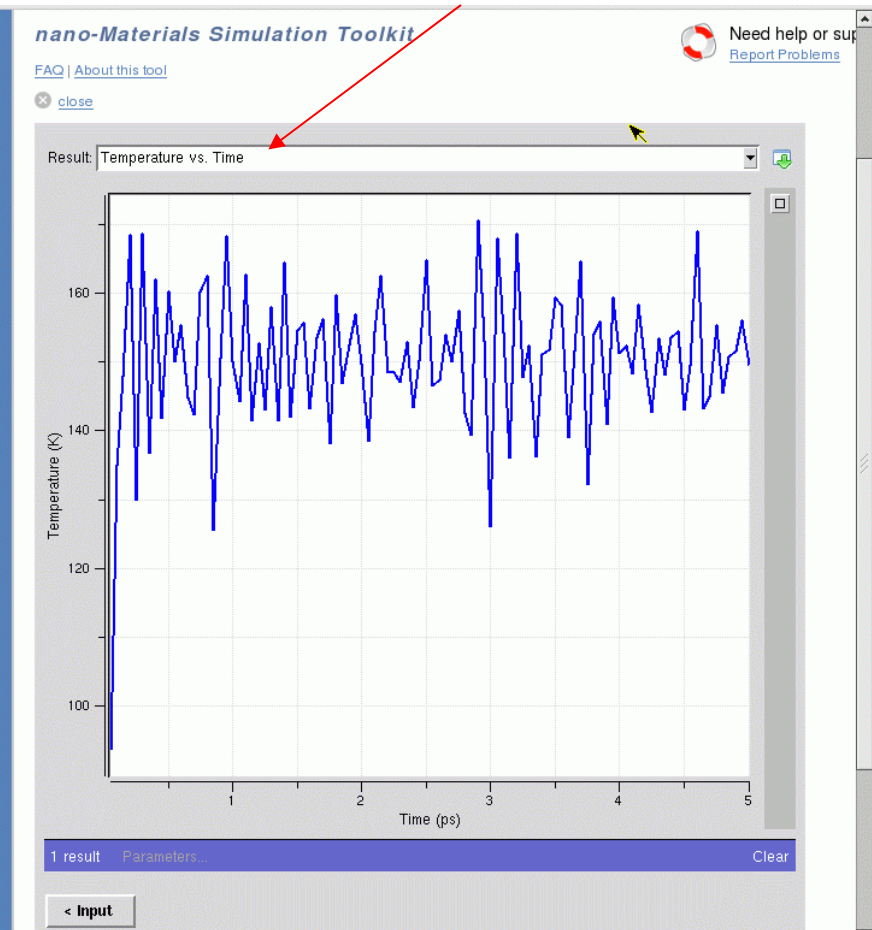
Write to trajectory (steps): 250

Update neighbor list (steps): 10

Simulate >

nanoMATERIALS: simulation results

Select the output to visualize (plots or snapshots)

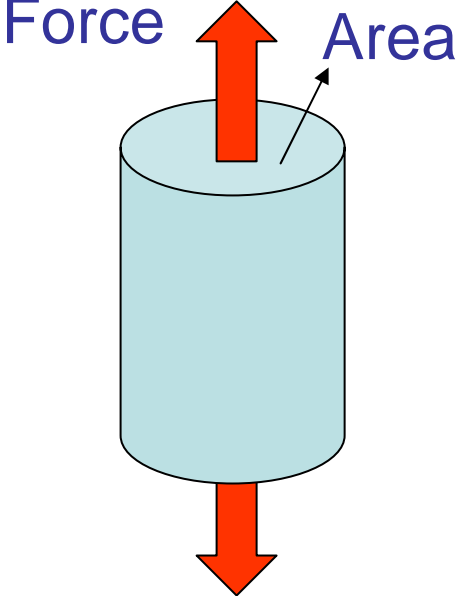


Back to input panels

Q: Why is the temperature about half of the input value?

Elements of Deformation & Failure

- Elastic deformation
 - Recoverable (if load is removed material goes back to original length)
 - Strain is proportional to strain
- Plastic deformation
 - Permanent shape change even after load is deformed
 - Material changed – atomic level rearrangement of neighbors
- Failure
 - Material separates in two
 - It usually follows “necking”



Force

Area

$$\text{Stress} = \frac{\text{Force}}{\text{Area}}$$

Length

Original length

$$\text{Strain} = \frac{L - L_0}{L_0}$$

Non-equilibrium MD: deforming a material

nano-Materials Simulation Toolkit

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 Need help?
[Report Problem](#)

Input Model | Energy Expression | Driver Specification

Input model: Pt_nanowire_r8_6.bgf

Create Supercell

a direction: 1
b direction: 1
c direction: 1

Simulation cell parameters

Modify simulation cell parameters: no

Fixed atomic coordinates: Cartesian

Length a: 5Å
Length b: 5Å
Length c: 5Å

- Select model Pt_nanowire_r8_6
- NO SUPERCELL (1 1 1)

Input Model | Energy Expression | Driver Specification

Driver: Molecular Dynamics

Molecular Dynamics parameters

Ensemble: NVE

Time step: 0.005ps

Number of steps: 2000

Temperature: 300K

Temperature increment (K/ps): 0.00

Strain per MD step

X direction: 0
Y direction: .00005
Z direction: 0

Periodic tasks

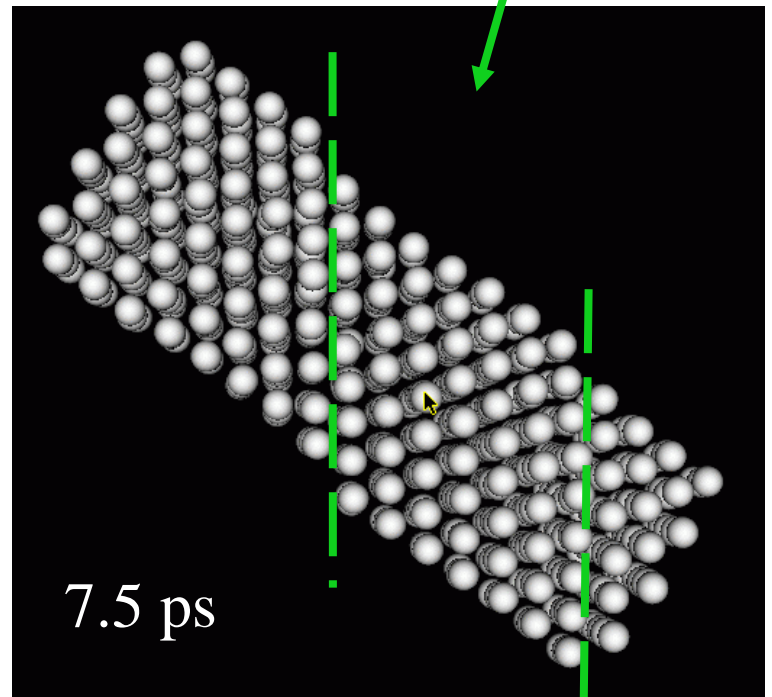
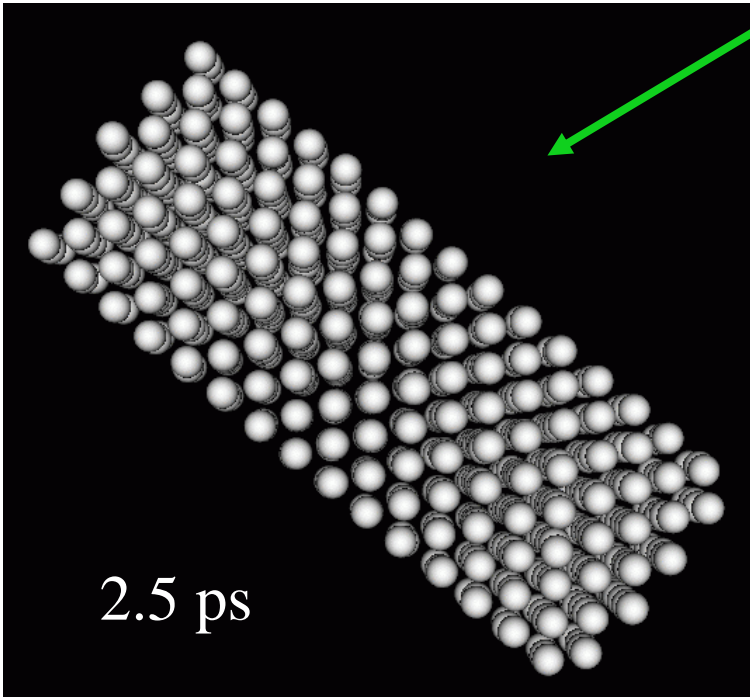
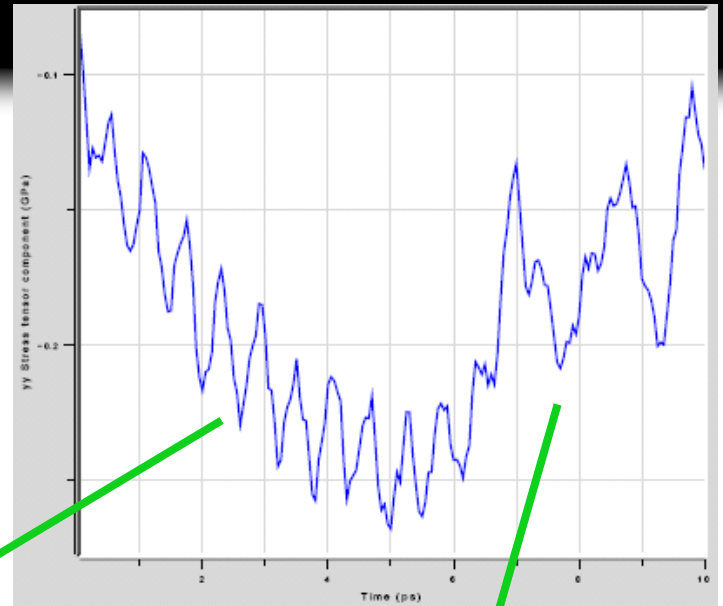
Write to energy file (steps): 5
Write to trajectory (steps): 500
Update neighbor list (steps): 10

[Simulate >](#)

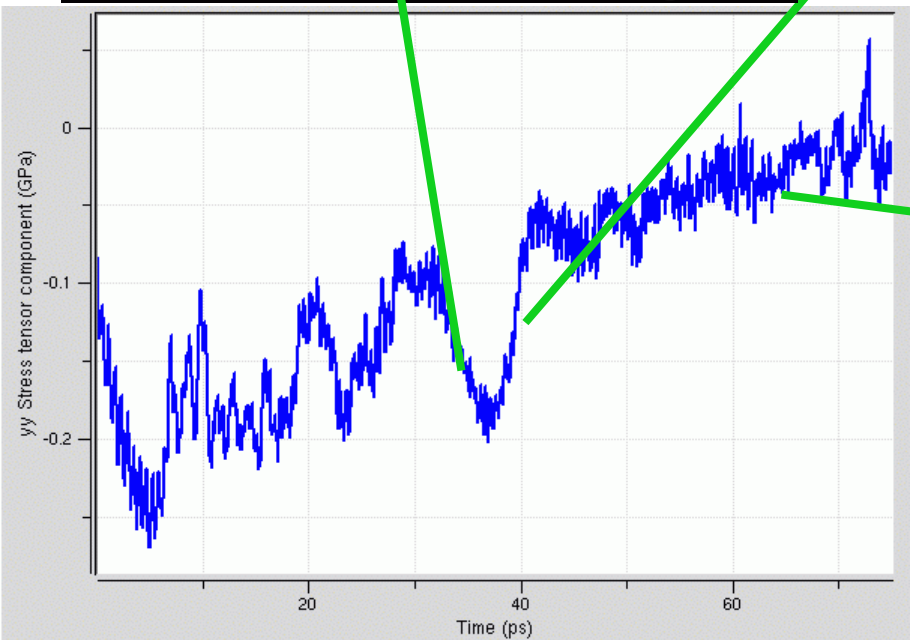
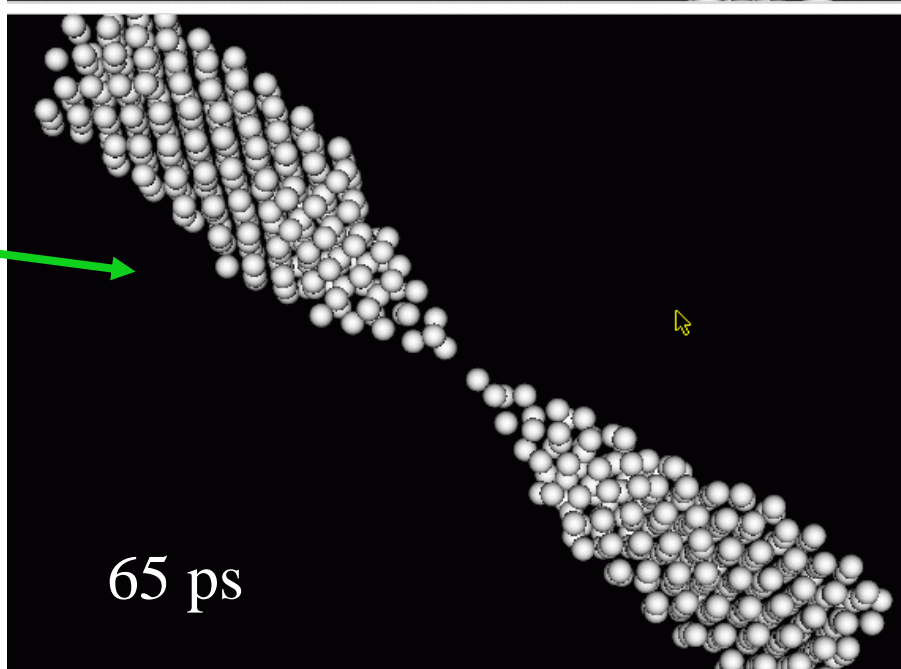
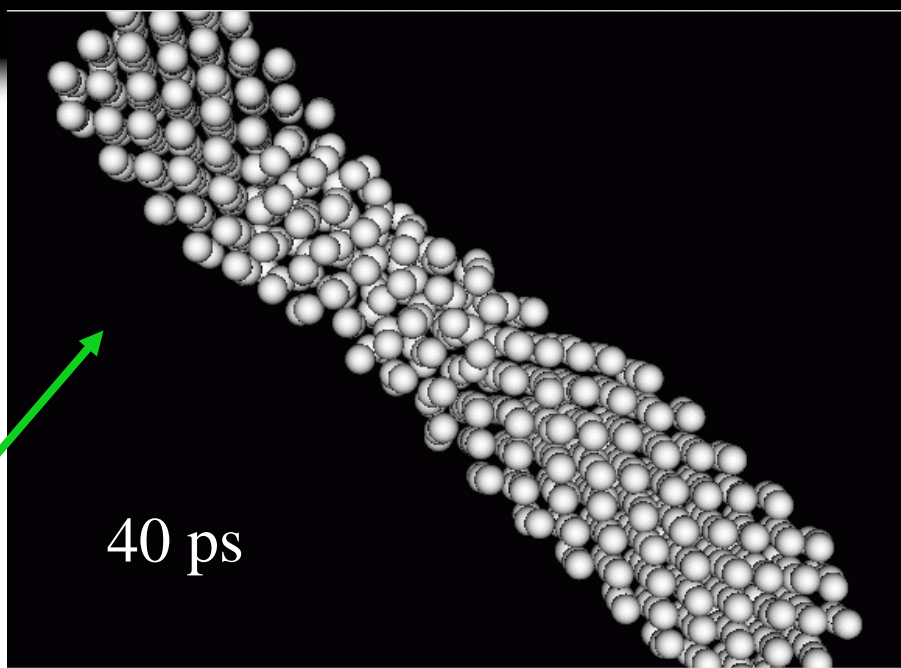
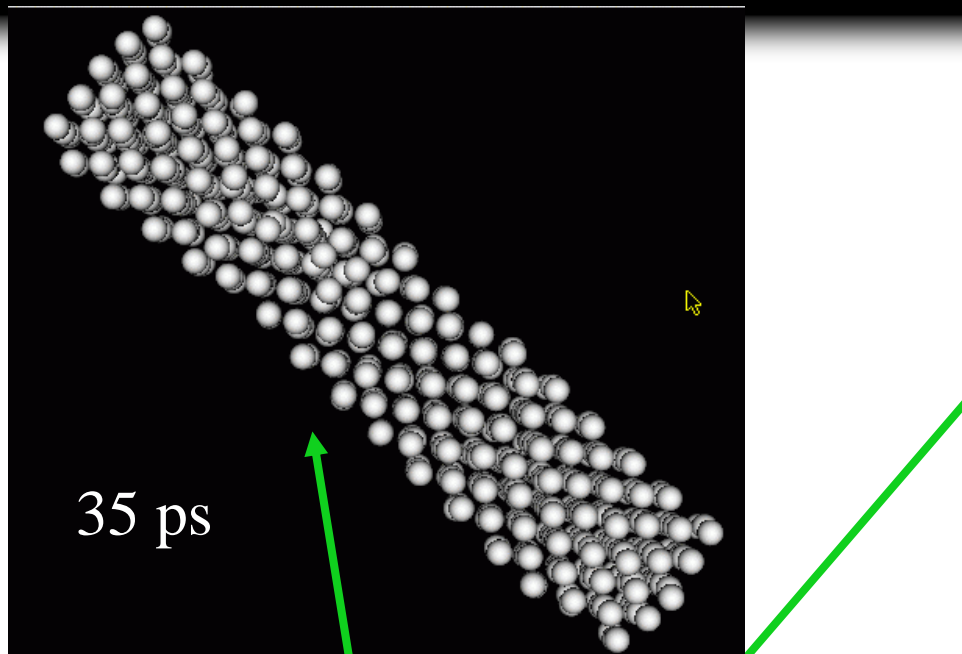
- Set to NVE
- Strain along the axis of the wire: 0.00005 (per step)

Results

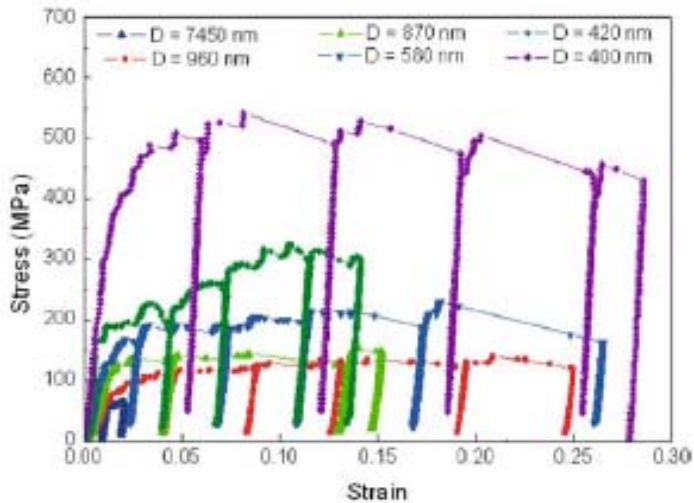
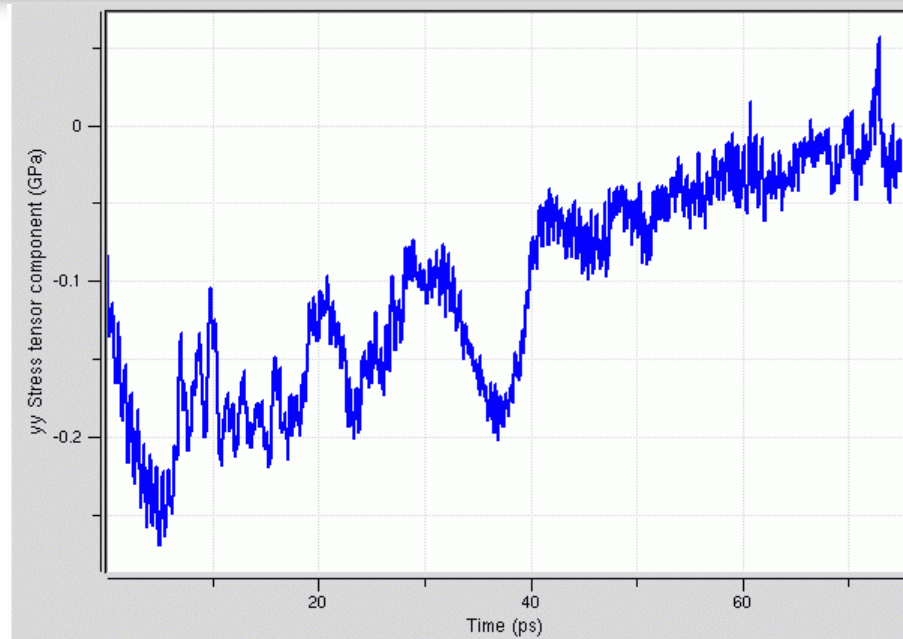
Elastic region up to about 5 ps
Plastic deformation leads to
significant stress relaxation



Results



Results



Gold nano-rods
Nix and collaborators, 2005

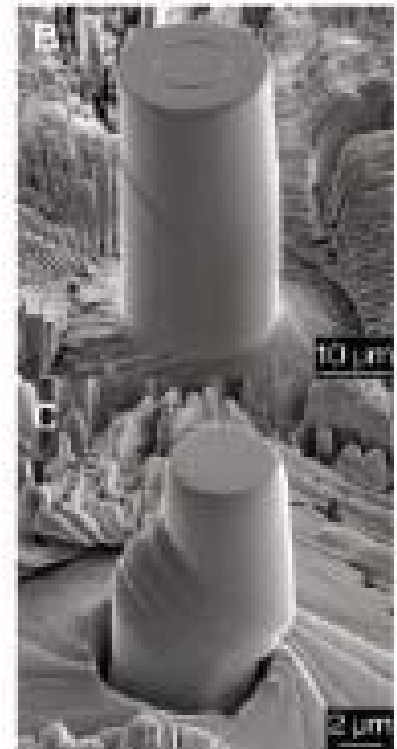


FIGURE 3 Stress-strain behavior of {001}-oriented pillars produced with a FIB: flow stresses increase significantly for pillars with the diameter of 500 nm or less

Suggested additional exercises

- What is the role of strain rate?
 - Half the strain per step and double the number of MD steps
 - Compare yield stress & maximum elongation
- Repeat for nano-wires with different sizes
 - Wires with radius 10.8 and 13 Å
 - Compare yield stress and maximum elongation

Note: there is a maximum allocated time and size for the simulations