MSE235 Materials Structure & Properties Lab
Molecular dynamics laboratory:
atomic mechanisms of plastic deformation

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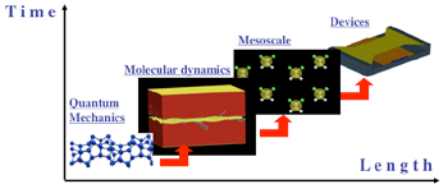

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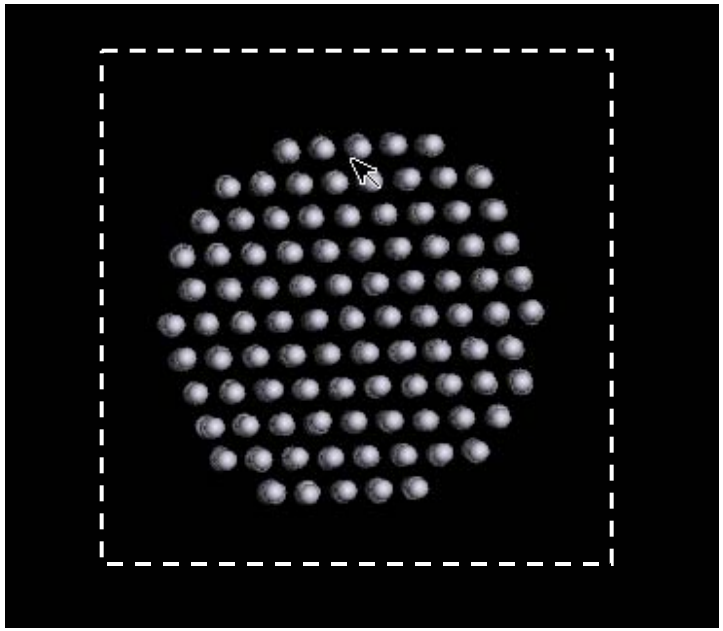
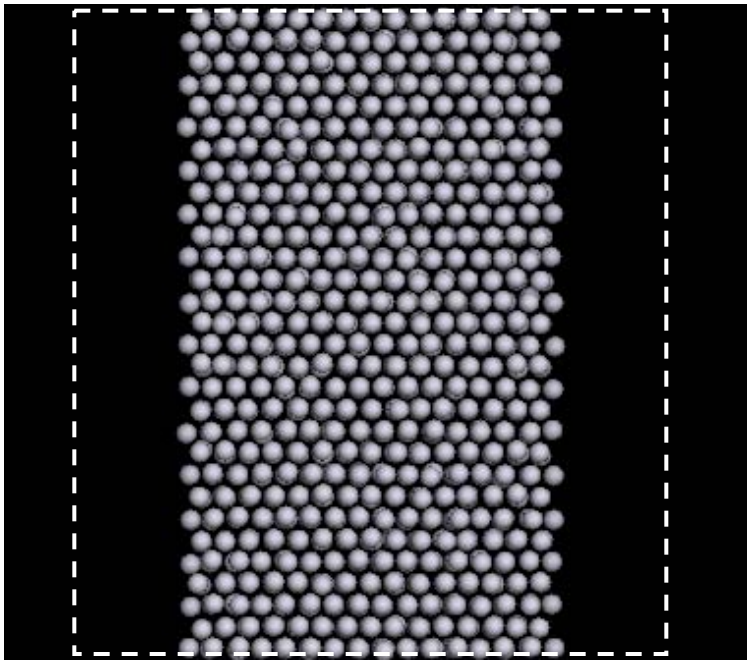
What is in this lab?

- Background lecture
  - Lab objectives
  - Introduction to molecular dynamics (MD)
  - Tensile testing of materials
- Pre-lab lecture
  - How to run online MD simulations at nanoHUB.org
  - MD tensile “tests”
- Lab handout
  - Lab activities using nanoHUB
  - Questionnaire
  - Additional activities

Learning objectives

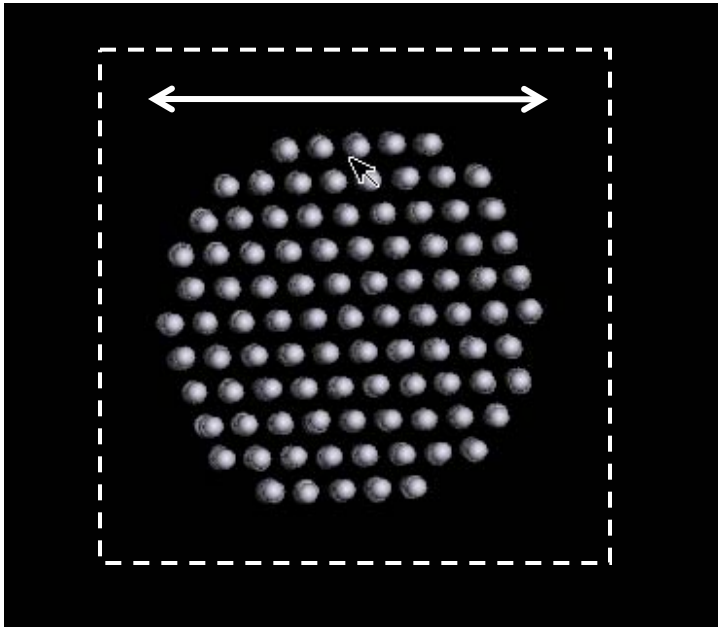
- Develop an atomic picture of plastic deformation in metals
- Understand the orientation of the active slip system with respect to the tensile axis
- Estimate the strength of perfect crystals and compare it polycrystalline samples
- Strain hardening: difference between annealed and cold worked, and nanoscale samples



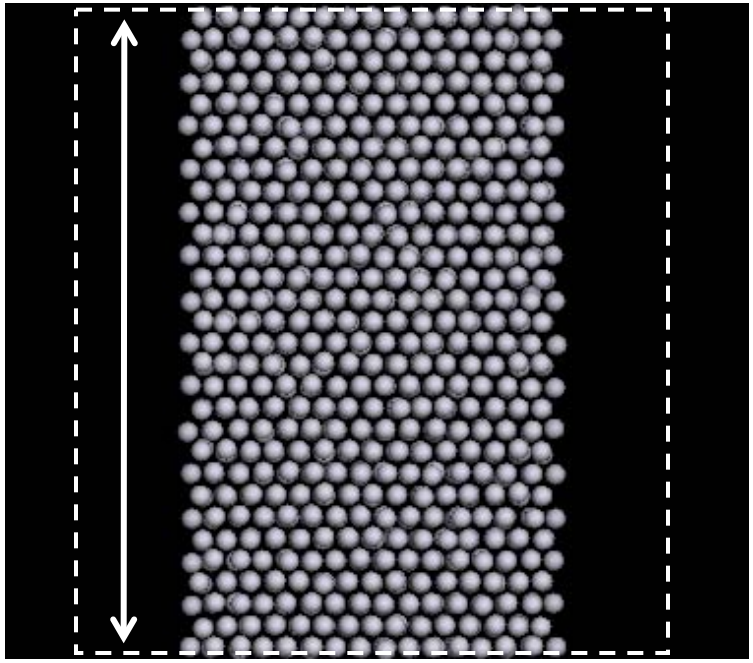


Nanoscale vs. macroscopic specimens

Diameter: 2.6 nm



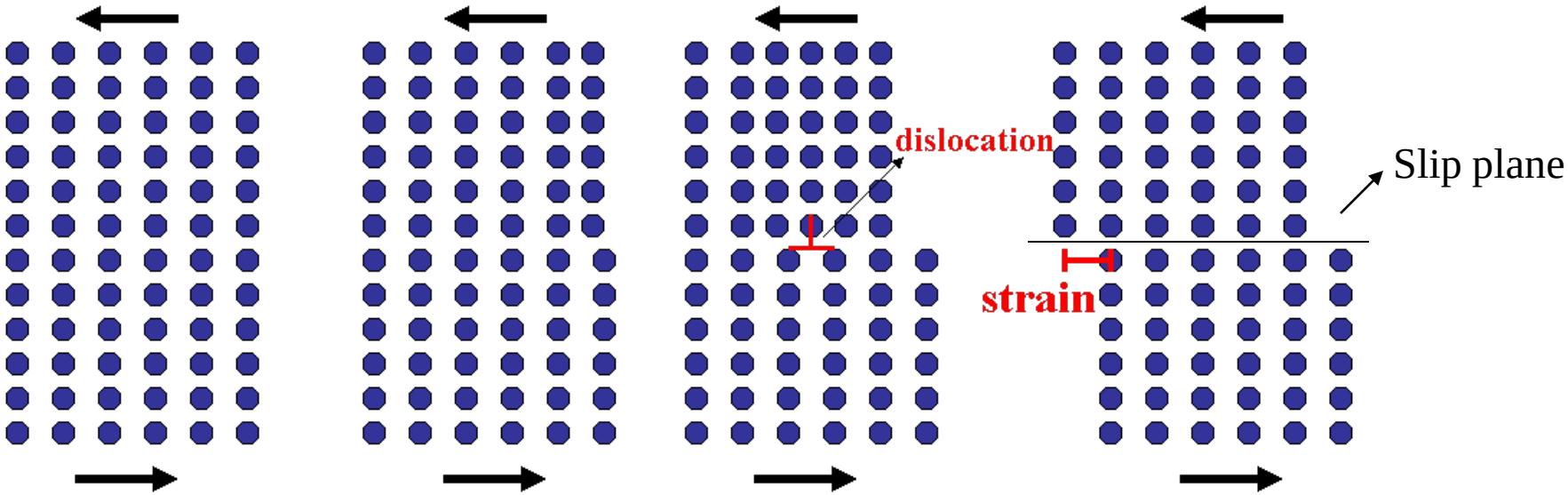
Periodic length: 4.1 nm



Platinum nanoscale bar

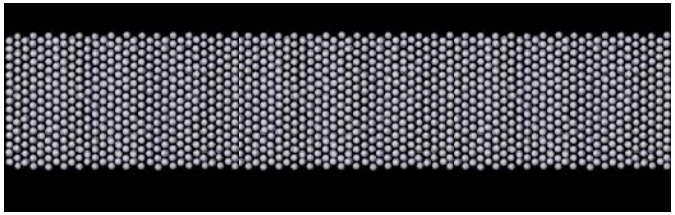
Copper tensile bar

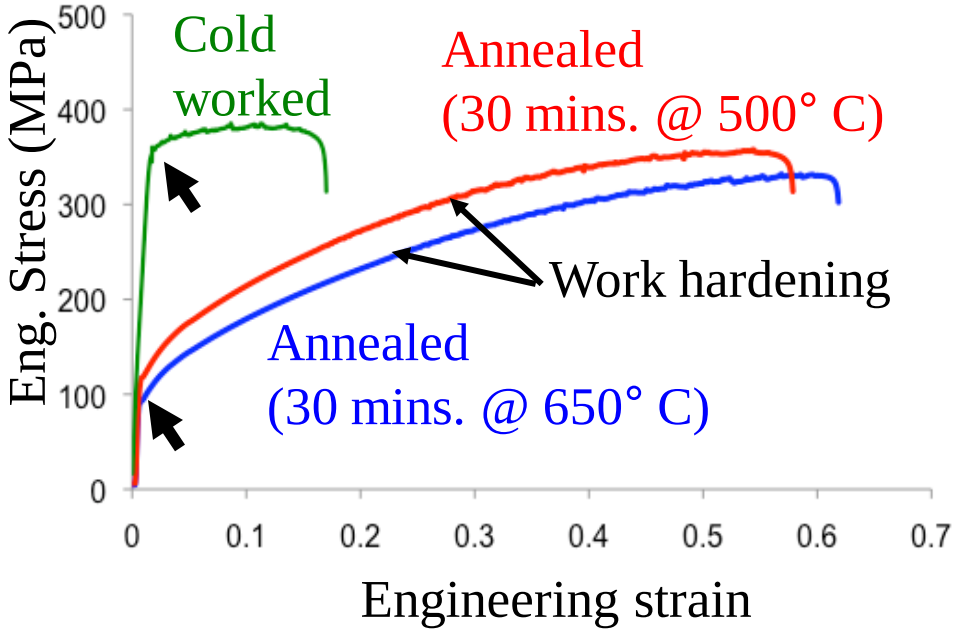
Plasticity carriers in metals

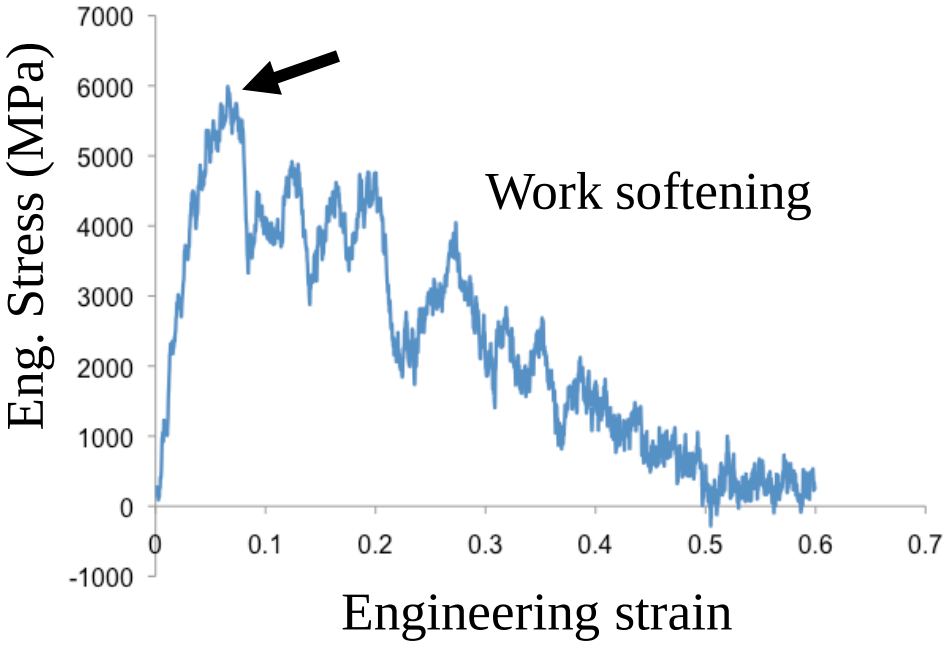


- Line defects proposed in 1934 by Orowan, Polanyi, and Taylor
- The motion of a dislocation on a slip plane caused a relative displacement of the material on either side of the plane
- This relative displacement in called Burgers vector

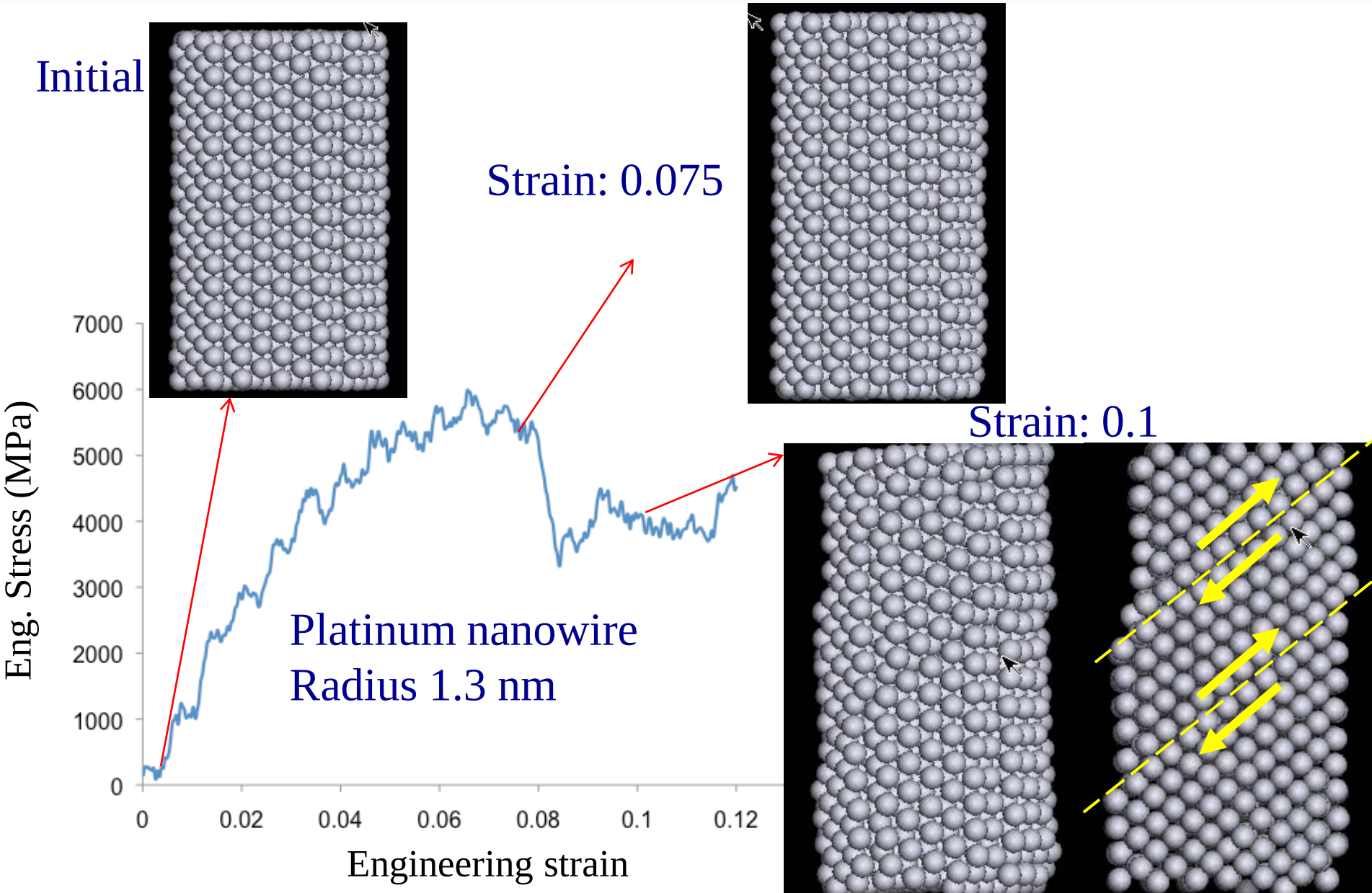
Mechanical response







Nanoscale tensile tests: MD results



Nano vs. macro mechanical response

Yield stress:

•Typical values: 50 to 500 MPa

•Stress necessary to move existing dislocations

Work hardening

Plastic deformation

↓

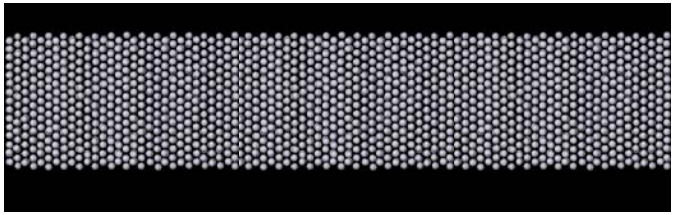
Increase dislocation density

↓

More obstacles for dislocation motion

↓

Strengthening



Yield stress:

•Pt nano-sample: ~6,000 MPa

•Stress necessary to nucleate a dislocation

Work softening:

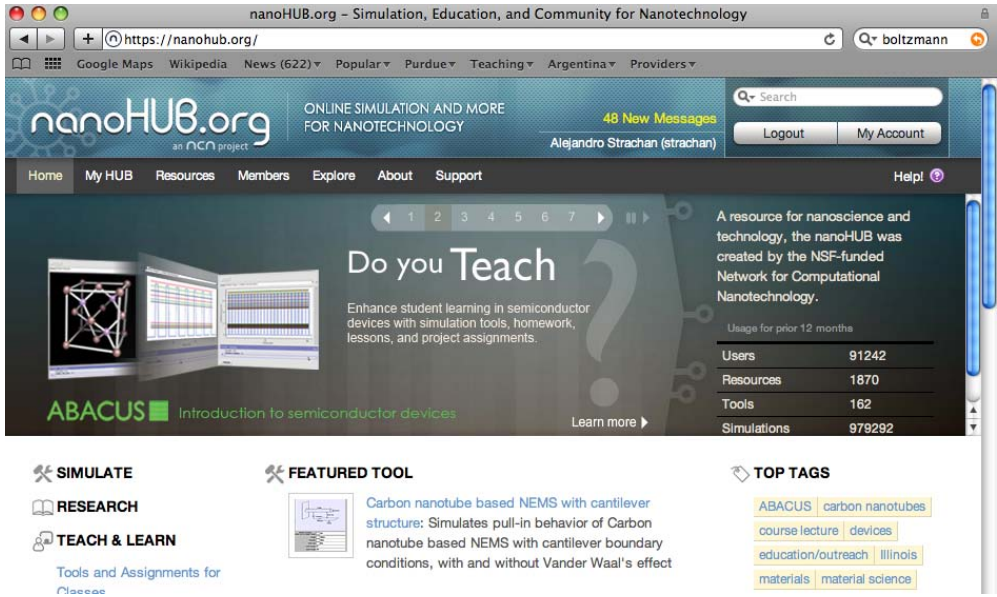
•Dislocations do not stay inside the specimen (always a free surface nearby) → no hardening

•Steps in surface make it easier to nucleate subsequent dislocations → weakening

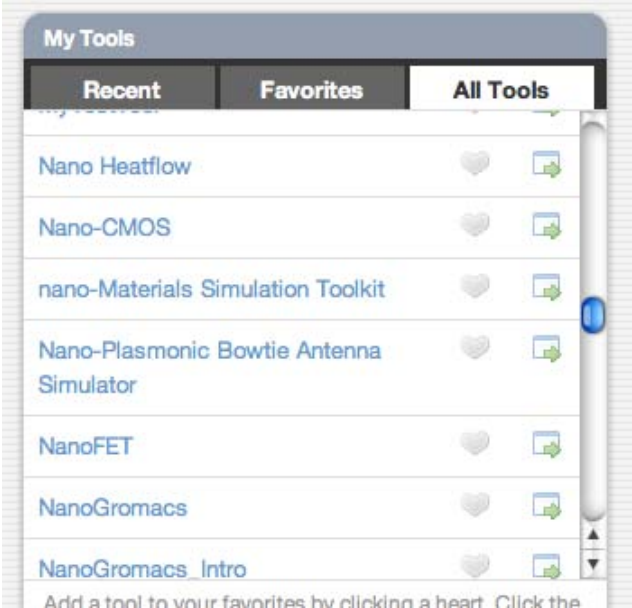
Running MD: nanoMATERIALS simulation toolkit

nanoMATERIALS simulation toolkit @ nanoHUB

- General purpose tool for atomistic simulations of materials



Step 1: Go to the nanoHUB webportal nanohub.org
Step 2: Create an account
Step 3: Login
Step 4: Click on "All Tools" and select:
nano-Materials Simulation Toolkit



Running MD with nanoMATERIALS: step 1

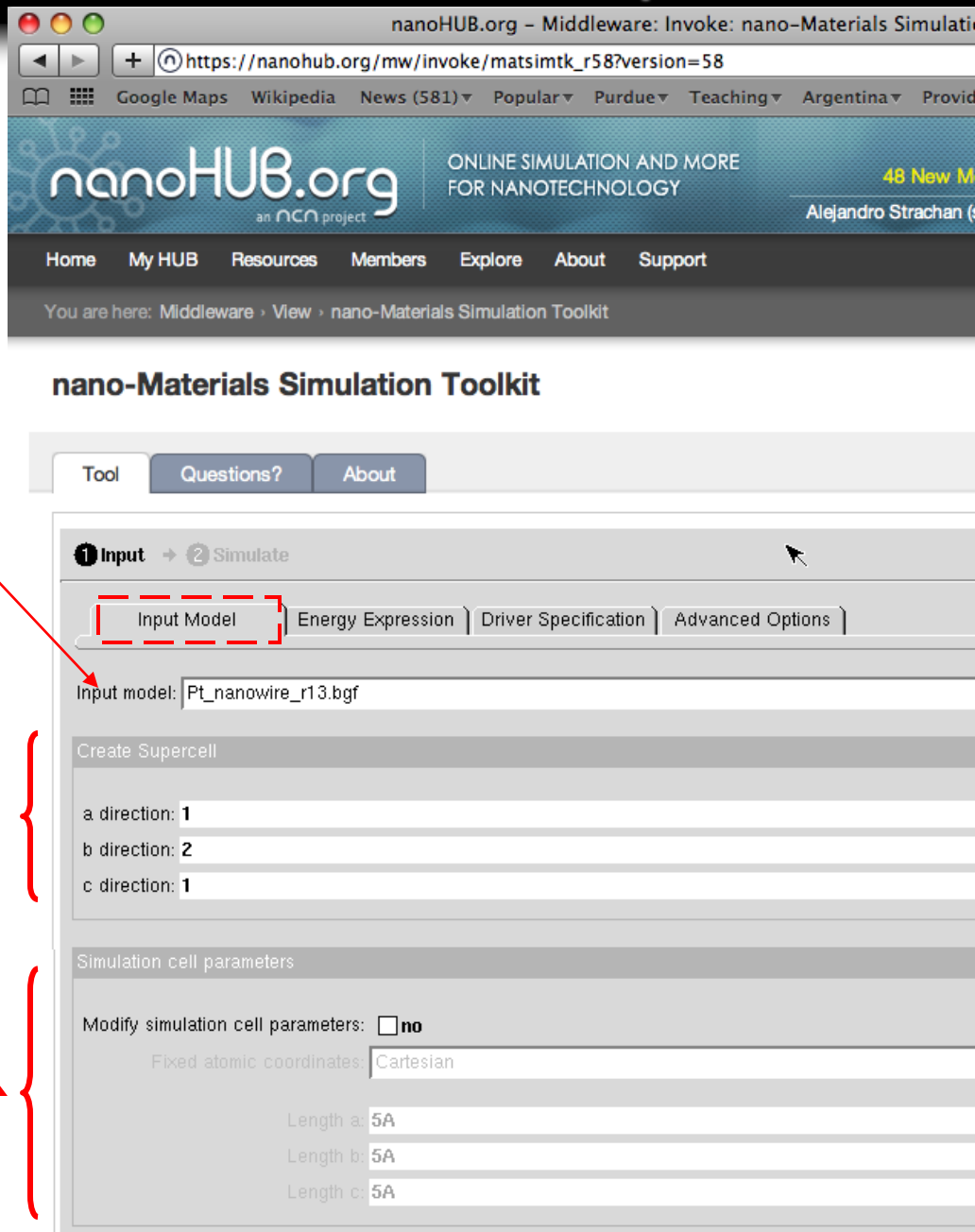
Determine initial model for simulation

- Select a model from menu
  Click on Pt_nanowire_r13

Some possible operations

- Create supercell

- Modify the lattice parameters

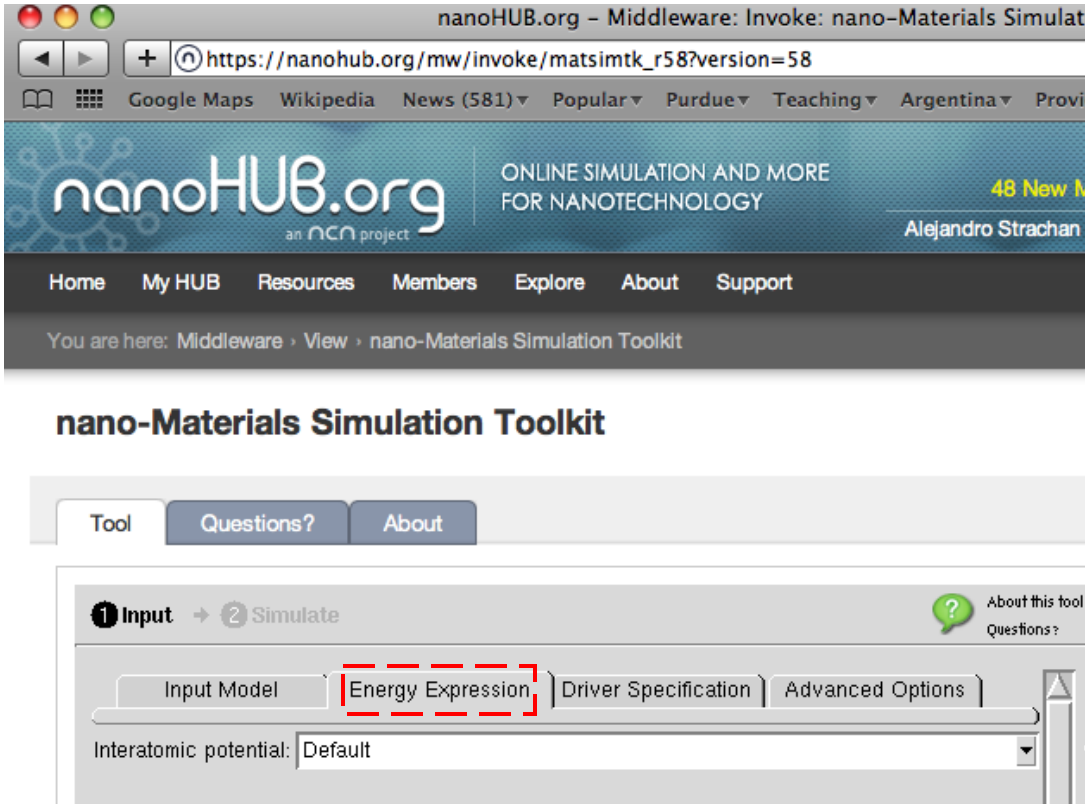


Running MD with nanoMATERIALS: step 2

Energy expression

How to calculate the total energy and atomic forces

For Pt atoms we will use a type of many body potential called Sutton Chen



Running MD with nanoMATERIALS: step 3

Driver options

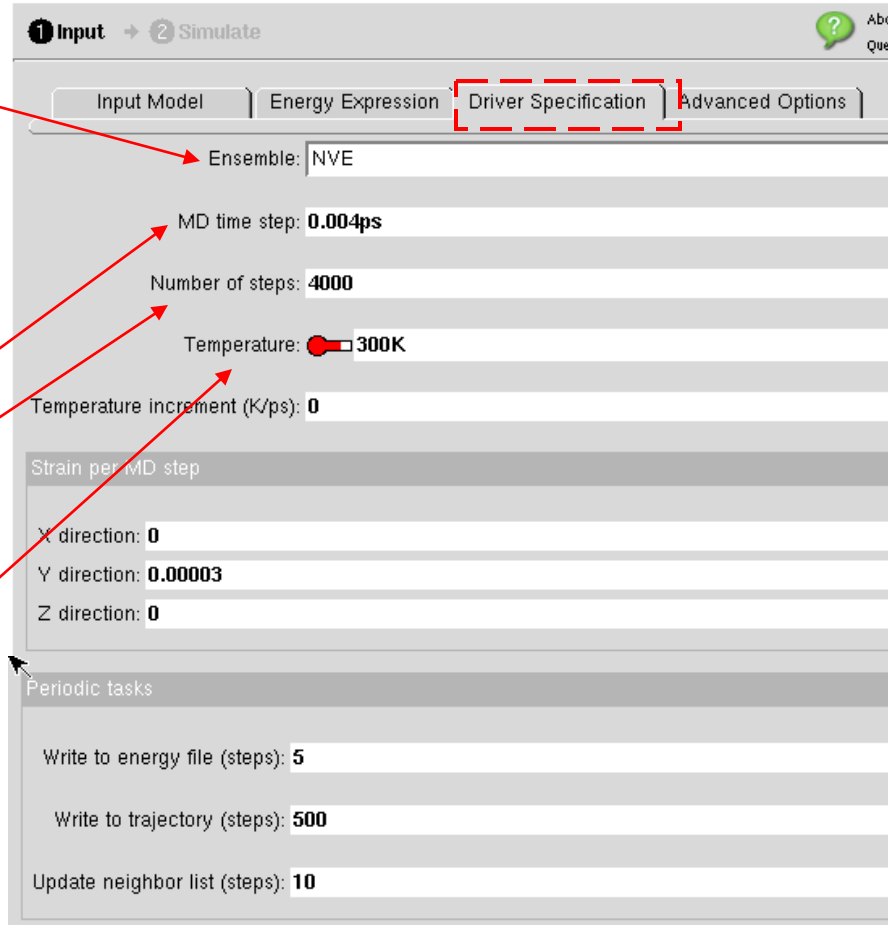
Ensemble

NVE constant volume and energy < select
NVT constant volume and temperature
NPT constant pressure and temperature

Time-step to integrate equation of motion
Set to 0.004 ps (4 femtoseconds)

Number of MD steps
Set to 4000

Temperature (initial value in NVE or target value for NVT and NPT)
Set to 300 K



Running MD with nanoMATERIALS: step 3

Driver options Part B

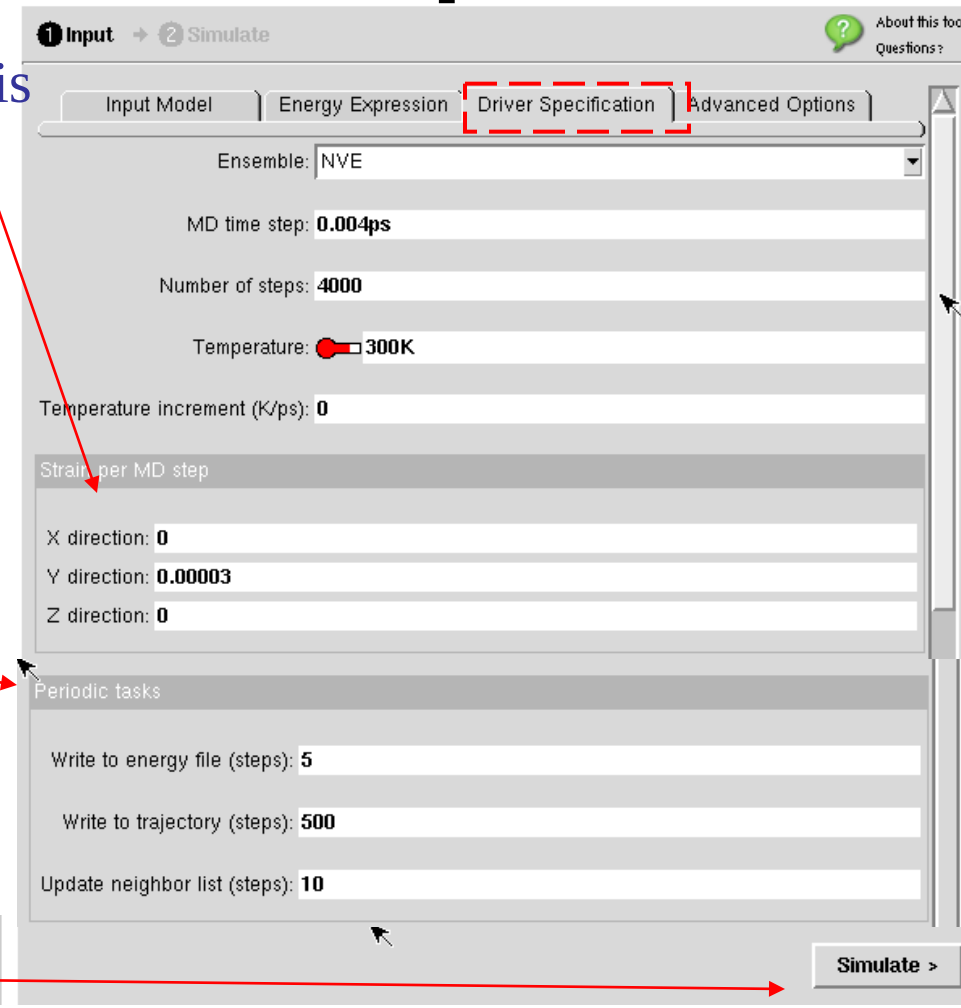
Strain per MD step

We will strain the nanowire along its axis

Input 0.00003 in the Y direction

Strain rate is strain per step divided by MD timestep:

$$\dot{\varepsilon} = \frac{0.00003}{0.004 \cdot 10^{-12} s} = 7.5 \cdot 10^{9} s^{-1}$$



Periodic taks

How often (MD steps) to record data

- Entry to energy file (use default)
- Atomistic snapshot (500 steps)

Simulate

- Will submit your run – once finished (~5 min. in this example) the results will be displayed

Running the simulation

nanoHUB.org – Middleware: Invoke: nano-Materials Simulation Toolkit

https://nanohub.org/mw/invoke/matsimtk_r58?version=58

Google Maps | Wikipedia | News (683) | Popular | Purdue | Teaching | Argentina | Providers

1 Input → 2 Simulate

About this tool
Questions?

Simulate

About this tool
Questions?

```
 Initial kin temp:    2549.93917   300.357507   300.

 ____________________________________________
 MOLECULAR DYNAMICS RUN
 INITIAL CONFIGURATION

   ENERGY DECOMPOSITION
     vdW, EAM ENERGY:              0.
     ELECTROSTATIC ENERGY:    0.
   TOTAL ENERGY:           -365719.181

  Stress (GPa)  |     0.000544    0.000714   -0.003525 |
  Stress (GPa)  |     0.000714   -0.072042    0.003768 |
  Stress (GPa)  |    -0.003525    0.003768   -0.017605 |
 ____________________________________________

# Energies in kcal/mol
#      Time        Pot. Ener.          Kin. Ener.        Total E.          Temp. (K)        Press. (GPa)
      0.0200       -365707.429591          2537.833038       -363169.596552           298.931526
      0.0400       -365697.610306          2532.543592       -363165.066715           298.308481
      0.0600       -365703.881489          2544.494161       -363159.387328           299.716140
      0.0800       -365714.403068          2561.305254       -363153.097813           301.696320
      0.1000       -365701.978737          2555.845908       -363146.132829           301.053263
      0.1200       -365676.536605          2537.799156       -363138.737449           298.927535
      0.1400       -365656.127359          2524.798761       -363131.328599           297.396217
      0.1600       -365660.568256          2536.018853       -363124.549403           298.717833
      0.1800       -365683.059326          2564.057050       -363119.002276           302.020454
      0.2000       -365695.635246          2581.063035       -363114.572212           304.023
```

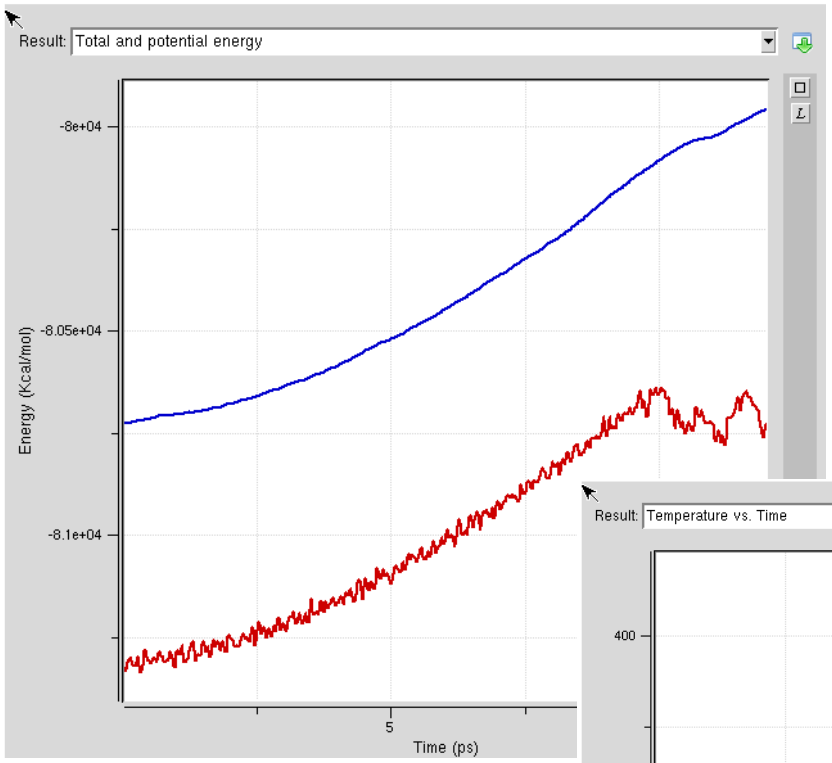
Abort

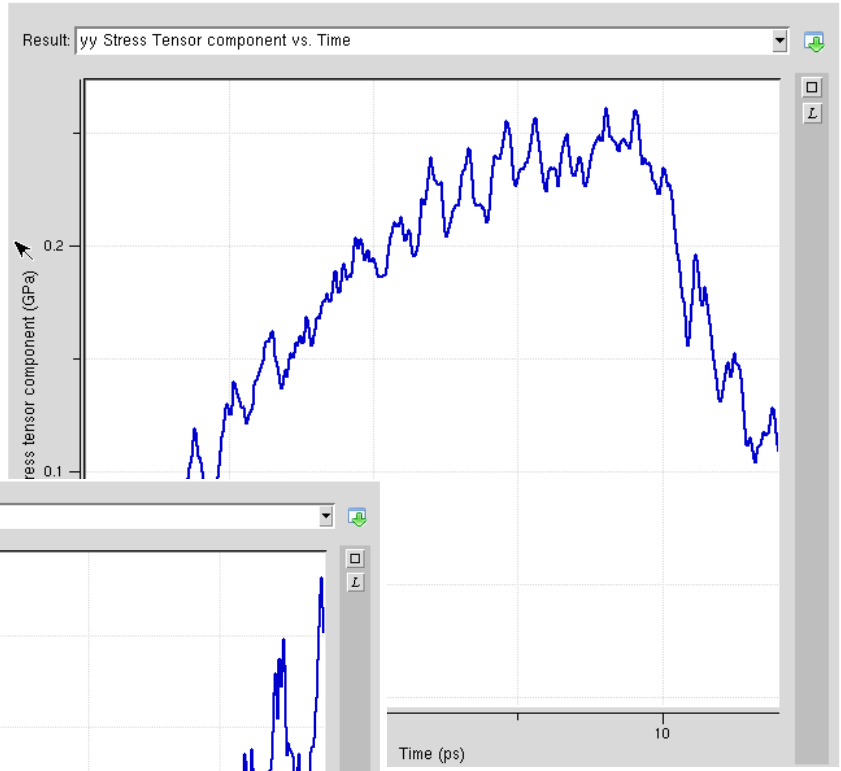
< Input

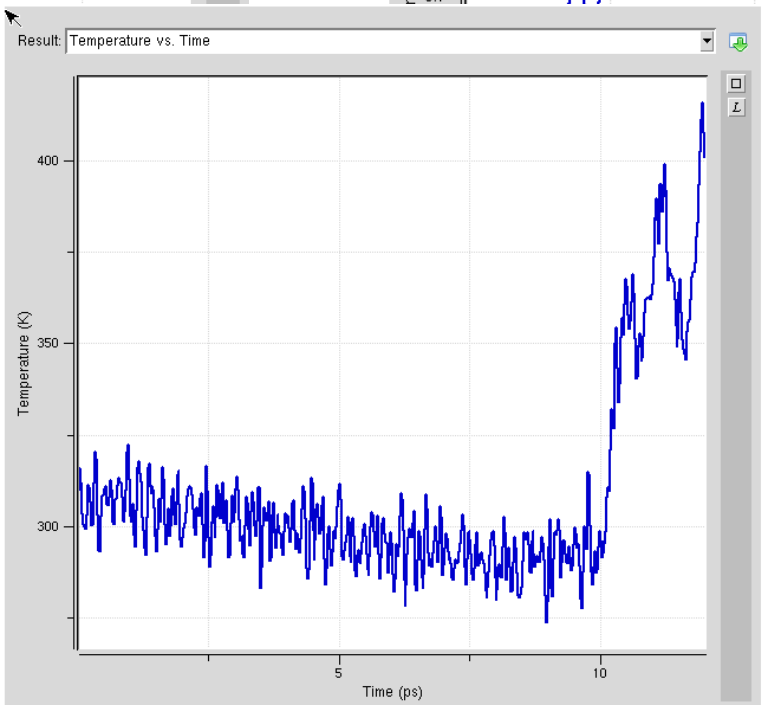
780 x 600

Viewing results with nanoMATERIALS

Select results to visualize

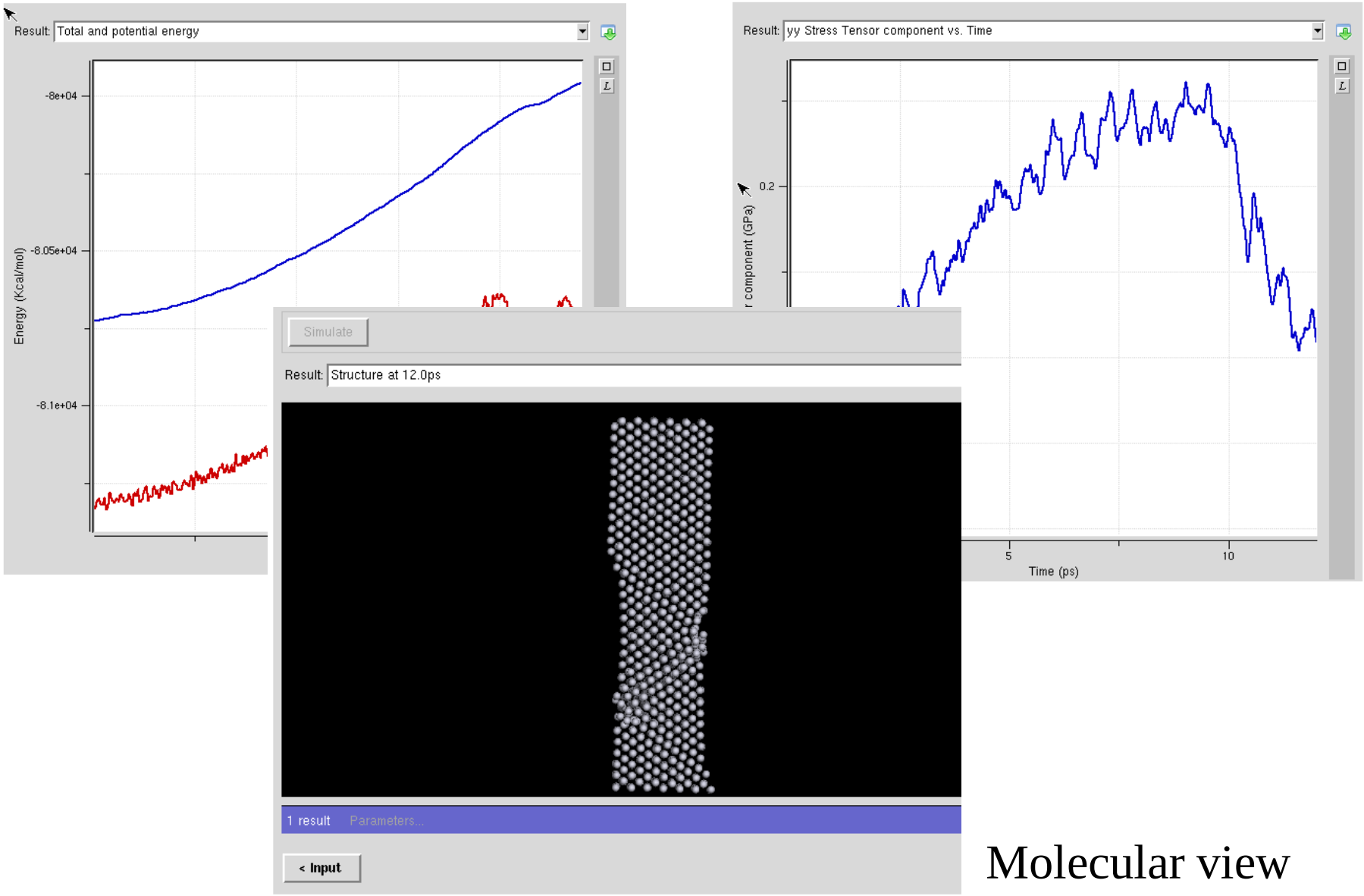






Viewing results with nanoMATERIALS

Select results to visualize



Molecular view

This lab

You will explore plastic deformation in metallic nanowires

- Visualize atomic snapshots to identify slip planes
- Explore individual slip events and the origins of the observed strain softening
- Study role of temperature on yield stress

- The laboratory handout will guide you through this steps

Question & Answer 1