1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2018

Recitation #5

Fitting interatomic potentials:
Cu FFC cell stretching vs Cu Nanowire Tensile

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Massachusetts Institute of Technology

Review from last week

- Interatomic potentials

$$\phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - M_{ij}\left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \quad ?$$

$$\phi(r_{ij}) = D\exp\left(-2\alpha(r_{ij} - r_0)\right) - 2D\exp\left(-\alpha(r_{ij} - r_0)\right) \quad ?$$

Let's solve it together

- QM calculations provide de following data for Cu-Cu interactions.

Cu – Cu distance (Å)	Interaction Energy (eV)
2.4	0.9
2.6	0.04
2.8	-0.18
3	-0.19
3.2	-0.17
3.4	-0.11
3.6	-0.1
4	-0.06
4.4	-0.03
5	-0.02
5.8	-0.007

- Use stretch FCC to study the deformation of a Cu nanowire in which the Cu – Cu interactions fit the QM data

- Are the results different from those obtained in the Tensile deformation lab made in Pset #1? If so, why?

First step: fitting

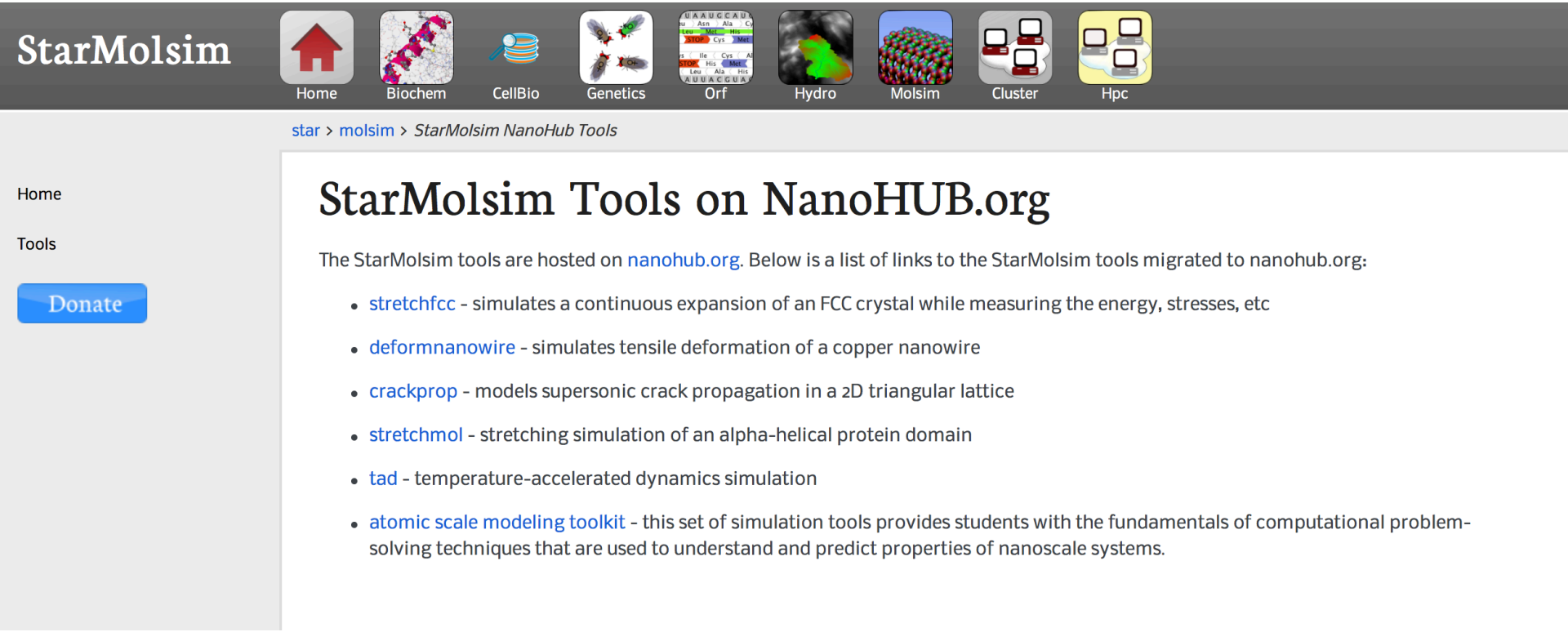
- What are the LJ parameters that better describe this Cu-Cu interaction?
- Use MS excel to do the fitting.
- Would a Morse potential work as well? With what parameters?

$$\phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - M_{ij}\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

$$\phi(r_{ij}) = D\exp\left(-2\alpha(r_{ij}-r_0)\right) - 2D\exp\left(-\alpha(r_{ij}-r_0)\right)$$

2nd step: run stretchfcc lab

Simulation index (MIT tools for IM/S):
http://star.mit.edu/molsim/nanohub/index.html



Collect

Stretching Simulation of FCC Crystal

By Markus Buehler[1], Justin Riley[1], Joo-Hyoung Lee, Jeffrey C Grossman[2]

1. Massachusetts Institute of Technology (MIT) 2. Massachusetts Institute of Technology

This tool simulates a continuous expansion of an FCC crystal while measuring the energy, stresses, etc

Launch Tool

Version 1.2 - published on 03 Sep 2014

doi:10.4231/D35717P48 cite this

View All Supporting Documents

Tool Audience Unrated

262 users, detailed usage

0 Citation(s)

1 question (Ask a question)

0 review(s) (Review this)

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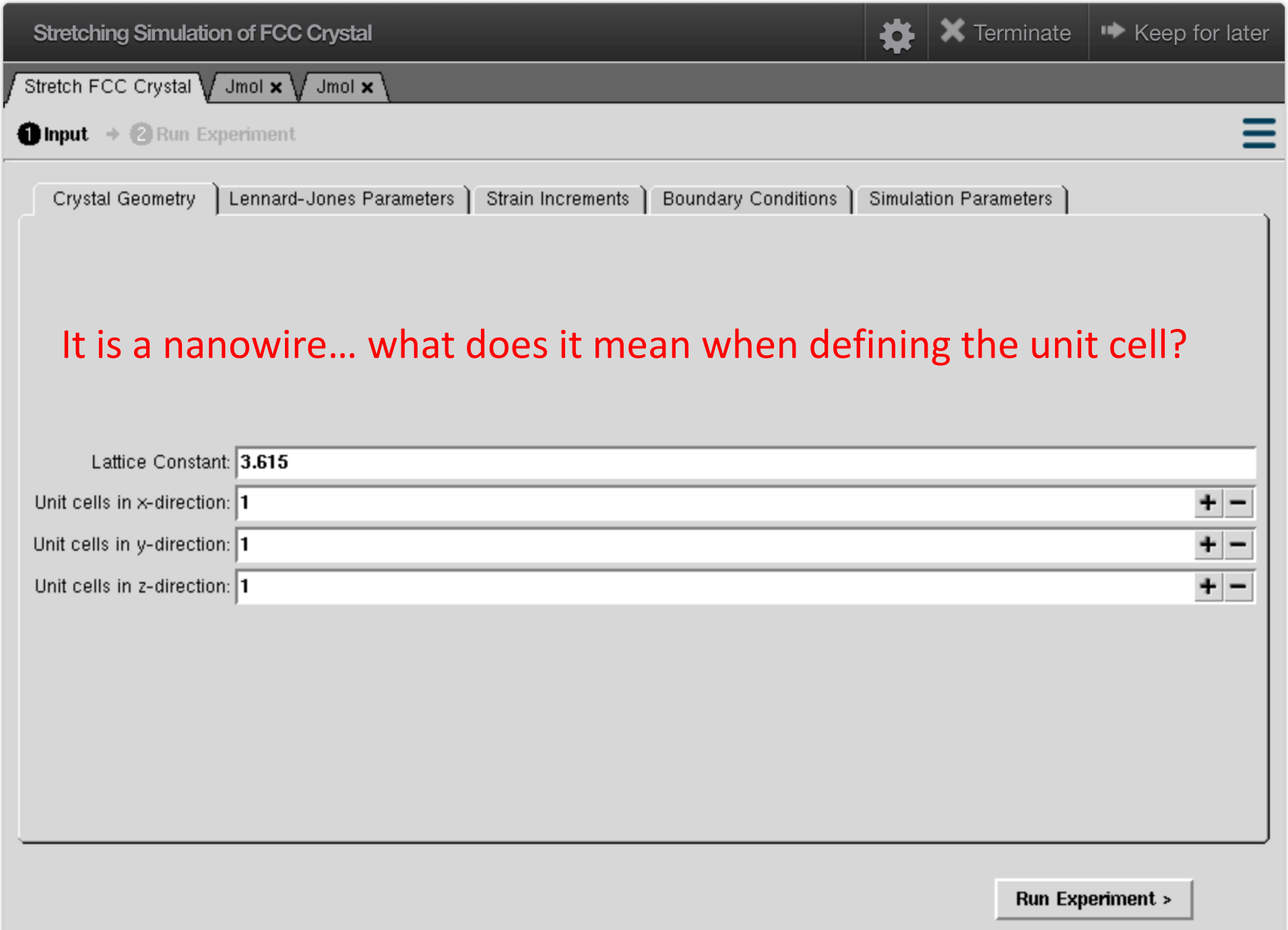
Category

Tools

Published on

03 Sep 2014


Stretching Simulation of FCC Crystal
Terminate
Keep for later
Stretch FCC Crystal
Jmol
Jmol
1 Input
2 Run Experiment
Crystal Geometry
Lennard-Jones Parameters
Strain Increments
Boundary Conditions
Simulation Parameters
It is a nanowire… what does it mean when defining the unit cell?
Lattice Constant: 3.615
Unit cells in x-direction: 1
Unit cells in y-direction: 1
Unit cells in z-direction: 1
Run Experiment »

Stretching Simulation of FCC Crystal

Terminate | Keep for later

Stretch FCC Crystal | Jmol × | Jmol ×

1 Input → 2 Run Experiment

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

Cutoff of potential: **5.38**

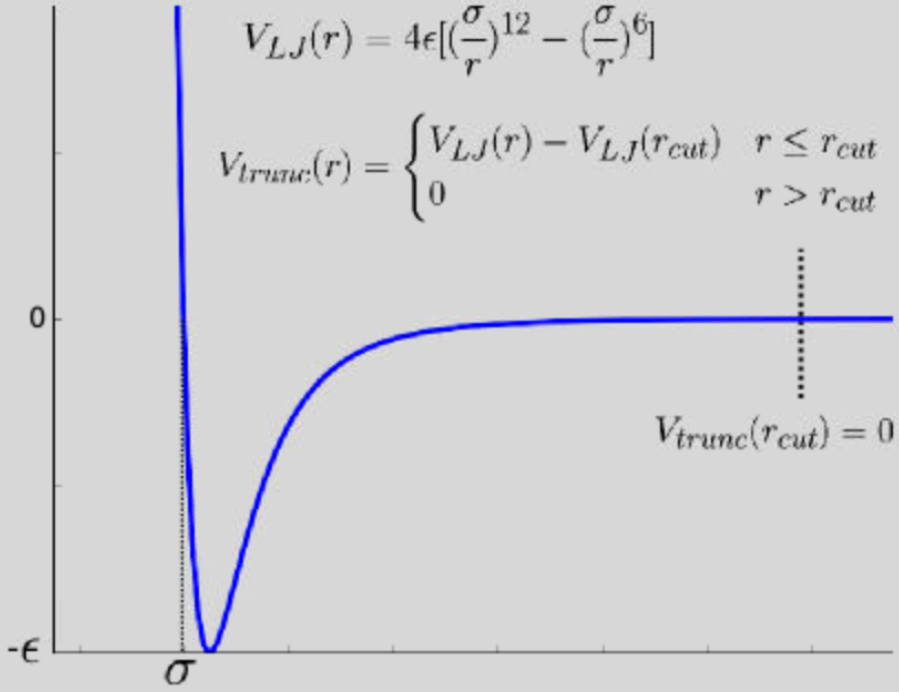
Epsilon:

Sigma:

From fitting!!

$$V_{LJ}(r) = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$$

$$V_{trunc}(r) = \begin{cases} V_{LJ}(r) - V_{LJ}(r_{cut}) & r \le r_{cut} \\ 0 & r > r_{cut} \end{cases}$$



Run Experiment >

Stretching Simulation of FCC Crystal

Terminate

Keep for later

1 Input → 2 Run Experiment

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

Strain increment interval: 100

Strain increments in the X direction:

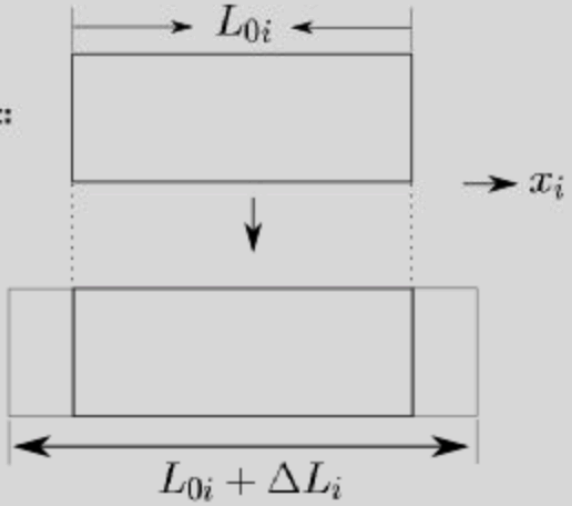
Strain increments in the Y direction:

Strain increments in the Z direction:

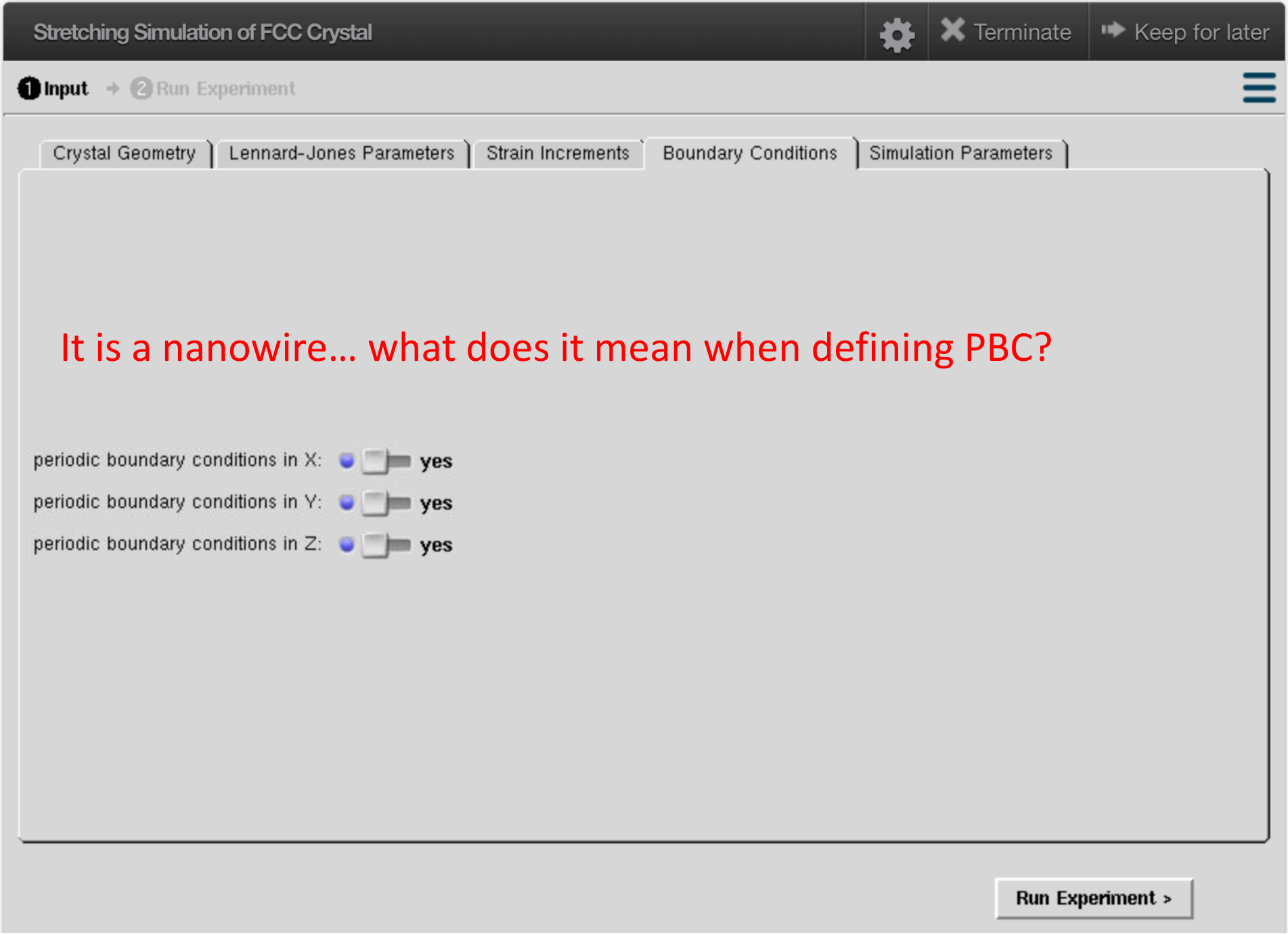
Do I apply strain in all directions?

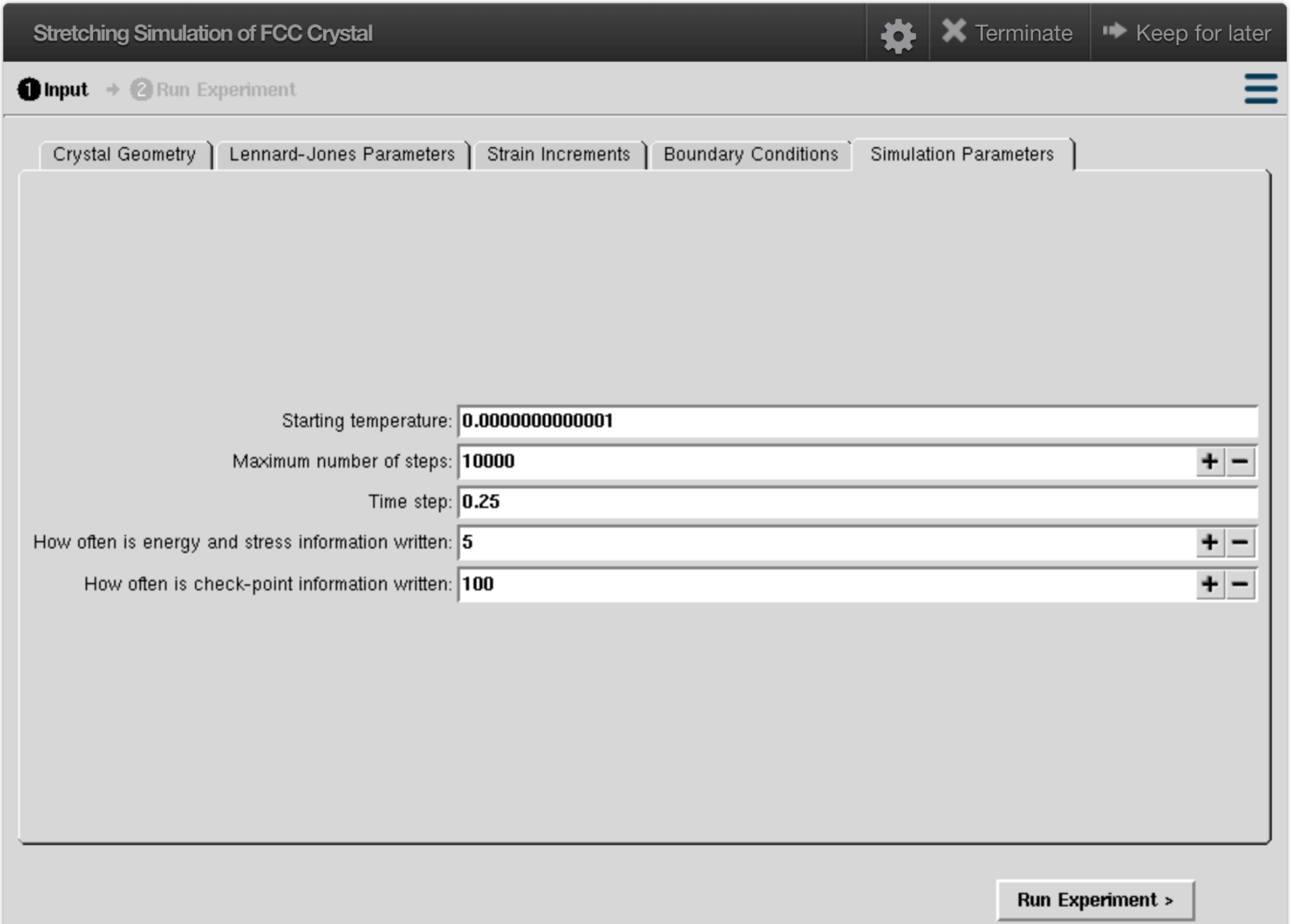
Strain Increment:

$$\epsilon = \frac{\Delta L_i}{L_{0i}}$$



Run Experiment >


Stretching Simulation of FCC Crystal
Terminate
Keep for later
1 Input
2 Run Experiment
Crystal Geometry
Lennard-Jones Parameters
Strain Increments
Boundary Conditions
Simulation Parameters
It is a nanowire… what does it mean when defining PBC?
periodic boundary conditions in X:
yes
periodic boundary conditions in Y:
yes
periodic boundary conditions in Z:
yes
Run Experiment ›


Stretching Simulation of FCC Crystal
Terminate
Keep for later
1 Input
2 Run Experiment
Crystal Geometry
Lennard-Jones Parameters
Strain Increments
Boundary Conditions
Simulation Parameters
Starting temperature:
0.0000000000001
Maximum number of steps:
10000
Time step:
0.25
How often is energy and stress information written:
5
How often is check-point information written:
100
Run Experiment »