

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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# Review from last week

- Interatomic potentials

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

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

# Let's solve it together

- QM calculations provide the 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?

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










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

# 2nd step: run stretchfcc lab

Simulation index (MIT tools for IM/S):

<http://star.mit.edu/molsim/nanohub/index.html>

**StarMolsim**

 Home  Biochem  CellBio  Genetics  Orf  Hydro  Molsim  Cluster  Hpc

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Tools

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## StarMolsim Tools on NanoHUB.org

The StarMolsim tools are hosted on [nanohub.org](http://nanohub.org). Below is a list of links to the StarMolsim tools migrated to nanohub.org:

- [stretchfcc](#) - simulates a continuous expansion of an FCC crystal while measuring the energy, stresses, etc
- [deformnanowire](#) - simulates tensile deformation of a copper nanowire
- [crackprop](#) - models supersonic crack propagation in a 2D triangular lattice
- [stretchmol](#) - stretching simulation of an alpha-helical protein domain
- [tad](#) - temperature-accelerated dynamics simulation
- [atomic scale modeling toolkit](#) - this set of simulation tools provides students with the fundamentals of computational problem-solving techniques that are used to understand and predict properties of nanoscale systems.

# Stretching Simulation of FCC Crystal

By Markus Buehler<sup>1</sup>, Justin Riley<sup>1</sup>, Joo-Hyoung Lee, [Jeffrey C Grossman](#)<sup>2</sup>

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](#))

📌 0 [wish\(es\)](#) ([New Wish](#))

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About

Usage

Citations

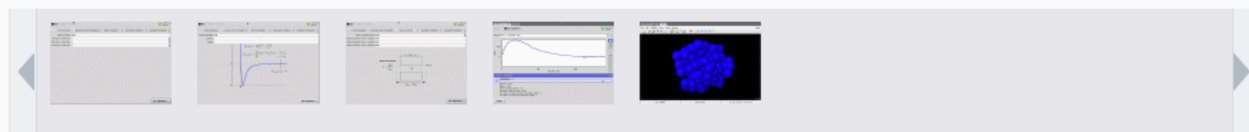
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Category

Tools

Published on

03 Sep 2014

Watch resource

When watching a resource, you will be notified of changes made. You may stop watching at any time.



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 &gt;





Stretch FCC Crystal

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1 Input → 2 Run Experiment

Crystal Geometry

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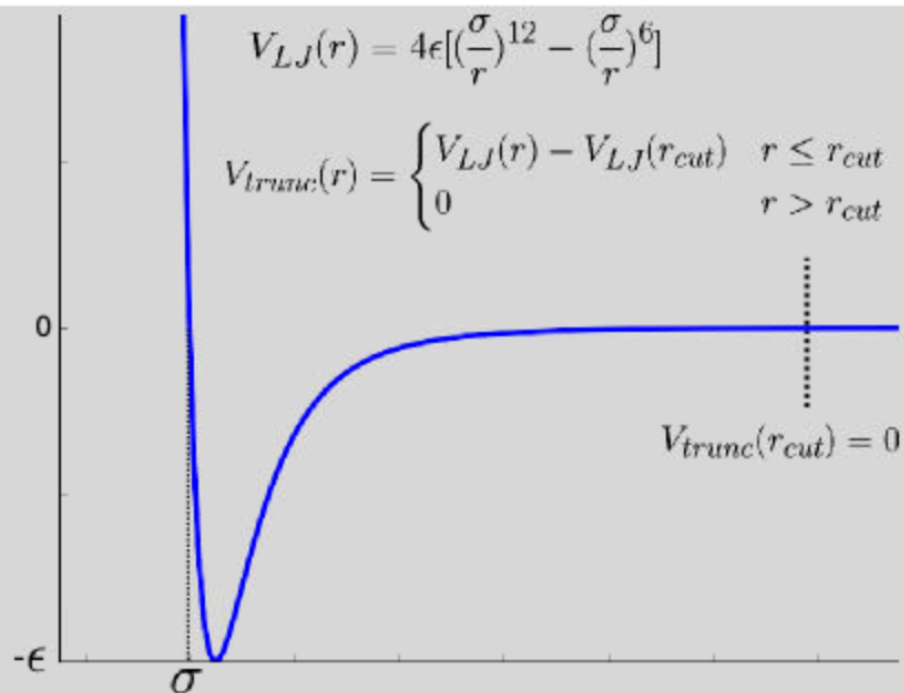
Simulation Parameters

Cutoff of potential: 5.38

Epsilon:

From fitting!!

Sigma:



Run Experiment &gt;



Crystal Geometry

Lennard-Jones Parameters

Strain Increments

Boundary Conditions

Simulation Parameters

Strain increment interval:

100

+

-

Strain increments in the X direction:

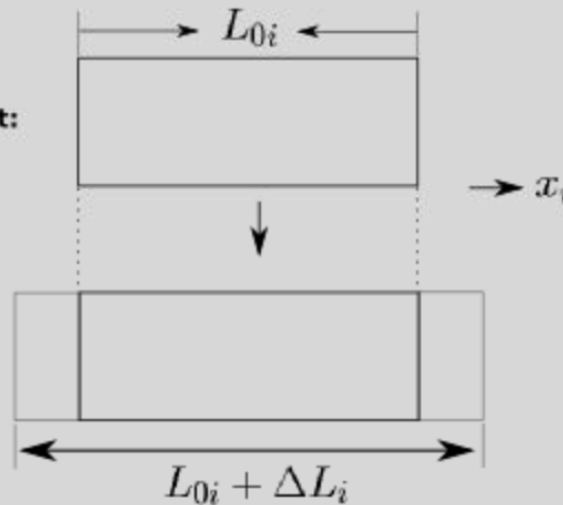
Strain increments in the Y direction:

Strain increments in the Z direction:

Do I apply strain in all directions?

**Strain Increment:**

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



Run Experiment &gt;



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 >](#)



Crystal Geometry

Lennard-Jones Parameters

Strain Increments

Boundary Conditions

Simulation Parameters

Starting temperature: 0.00000000000001

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 &gt;