3.021 Pset 2

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1 Problem 1

(a) Using the Lennard-Jones Potential equation and the unit cell of an FCC Crystal:

$$\Phi\left(r_{ij}\right) = 4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

An expression for the equilibrium position r_0 between pairs of atoms can be expressed as the following:

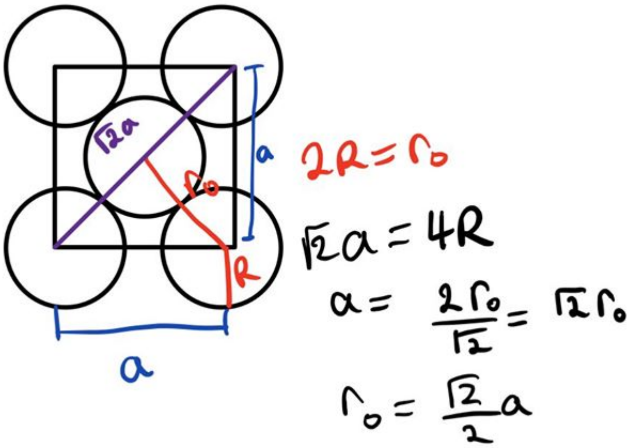
$\sqrt{2}a$
r_0
R
a
a
$2R = r_0$
$\sqrt{2}a = 4R$
$a = \frac{2r_0}{\sqrt{2}} = \sqrt{2}r_0$
$r_0 = \frac{\sqrt{2}}{2}a$

Figure 1: Diagram of FCC Unit Cell to calculate r_0

$$r_0 = \frac{\sqrt{2}}{2}a_0 \tag{2}$$

By taking the derivative of the potential and setting it equal to 0, the length parameter σ can be written as:

$$\sigma = \frac{r_0}{2^{1/6}} = \frac{\sqrt{2}}{2 * 2^{1/6}}a_0 \tag{3}$$

(b) The second derivative of the potential is the following:

$$\Phi_r^{"} = k = 4\epsilon\left(\frac{156\sigma^{12}}{r_0^{14}} - \frac{42\sigma^{6}}{r_0^{8}}\right) \tag{4}$$

(c) By using the values for copper $a_0 = 3.64A$ and $K = 140.0GPa$ as well as the expression for K as shown:

$$K = \frac{E}{\left(3\left(1-2\nu\right)\right)} \tag{5}$$

Where E is the Young's Modulus and equals:

$$E = \frac{8}{3}\mu \tag{6}$$

Where μ is the Shear Modulus which equals:

$$\mu = r_o^2 \frac{k}{2V} \tag{7}$$

Where r_o is the nearest neighbor distance, V is the volume of the unit cell, where:

$$V = \frac{a_0^3}{4} \tag{8}$$

and ν is the Poisson Ratio which is assumed to be 0.25. We calculated the parameters $\epsilon = 0.1646eV$ and $\sigma = 2.29306A$.

(d) Comparing parameters: Cleri used $\epsilon = 0.167eV$, $\sigma = 2.314A$, $a_0 = 1.56\sigma = 3.609A$ [1]. These parameters differed slightly from ours because Cleri utilized a simulation accounting for between fourth and fifth nearest neighbors, while our calculations were only for the first nearest neighbors. Despite this, our numbers are very similar, thus we will consider them to be a good estimate of the fcc lattice interactions for our calculations.

(e) MD simulation:

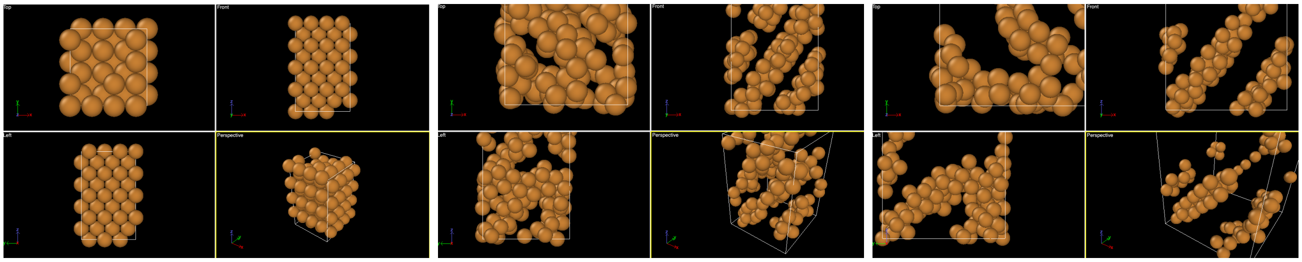

Figure 2: Images of our simulation of Copper, using an LJ 12:6 potential with a σ of 2.293A, and an ϵ of 0.1646 eV.

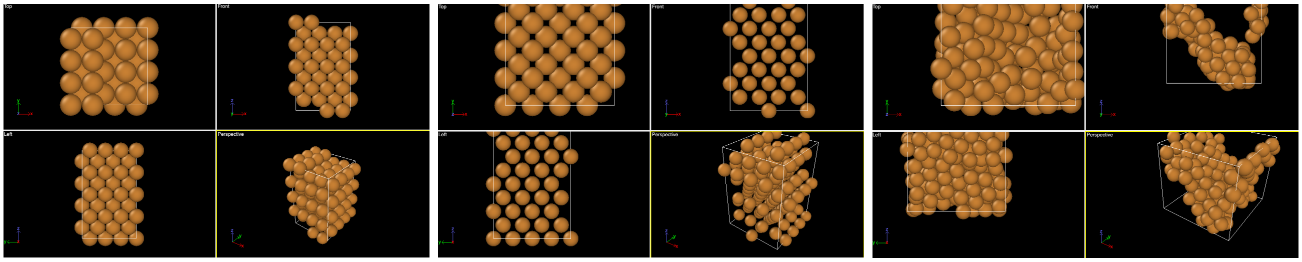

Figure 3: Images of simulation of Copper, using an LJ 12:6 potential with a σ of 2.314A, and an ϵ of 0.167 eV.

(f) The critical strain was calculated by plotting the stress-strain curve then determining at what strain the slope becomes zero.

- Cleri potential critical strain: 9.1 percent
- Our potential critical strain: 10.2 percent

2 Problem 2

In this problem the folowing assumptions were made:

- The substrate would be taken into account

[1] Cleri paper citation

- only square matrices could be used
- If the cell fell onto the substrate, it could move in different lengths than moving from pillar to pillar
- If the cell went on the pillar it would grow on it
- If the cell ran into another cell, it would continue growing (Implementing a push method would be something for a future work)

The code was split into the following sequences:

1. Make the board using a m (number of rows) by n (number of columns) matrix
2. Fill the matrix with 1s (pillars) or 0s (empty substrate) according to the size of matrix and the pillar spacing (1,2, or 4 μm)
3. A while loop would then pick a random number, which along with the position of the cell growth epicenter, whether or not the epicenter was on the substrate or on the pillar (WIP), the size of the matrix, and the pillar spacing would be passed to a move function called **mover**
4. **mover** would check if the random number fell within the cutoffs to move left, right, up, or down, and then return the possible coordinates of the next move (A possible state B)
5. An energy checking function called en_{fun} would check if the new position, B, was energetically favorable by using the Metropolis Hastings Equation:

   $$\rho = exp\left(\frac{-\Delta E}{k_B * T}\right) \tag{9}$$

   Where k_B is the Boltzmann Constant in eV/K, T is the temperature in K (assumed to be 298K), and ΔE is the energy for making the move which was assumed to be based on a harmonic model:

   $$\Delta E = \frac{1}{2}kp^2 \tag{10}$$

   Where k is a spring parameter and p is the pillar spacing. k was varied based on whether or not the cell was going from pillar to pillar (favorable at low p), pillar to substrate (favorable at higher p, around 4 microns), and substrate to pillar (always unlikely). en_{fun} would return the ρ using the ΔE calculated based on the necessary state, and the returned probability would be binned properly. For example in the pillar to pillar case, for p = 1, would be around 0.99, 0.98 for p = 2, and 0.04 for p = 4. The equations used to calculate k, which was what tuned the parameters are in the following equations:

   $$k_{pp} = 10^{-6} * 10^{p} \tag{11}$$
   $$k_{ps} = 10^{-p} \tag{12}$$
   $$k_{sp} = 10^{-1} \tag{13}$$
   $$\tag{14}$$

   Where k_{pp} is the k used from pillar to pillar, k_{ps} is the k used from pillar to substrate, and k_{sp} is the k used from substrate to pillar.
6. Another random roll would be generated, and the probabilities from en_{fun} would be used to determine if the cell grew to that place or not. This would be continued until the number of trials had finished
7. The matrix was then printed to the console for debugging, and the matrix was passed to a ROOT 2D Histogram which was converted to a heatmap using **h1→Draw"COLZ"**, a command native to ROOT.
8. To generate the figures, 100000 trials were used for the 1 micron spacing trial, 5000 for 2 micron spacing, and 4000 for the 4 micron spacing. Trials are the number of times the while loop repeated.

To improve the code I would have included the ability for the cell to push what it had already grown forward, this would have made dendrite veins grow in the 2 micron setting. I would have also improved the energy function to more accurately reflect the experiment.

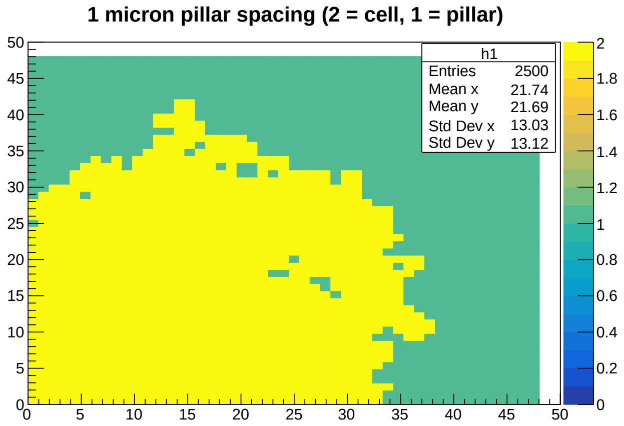

Figure 4: Picture with 1 micron Pillar Spacing and 100000 Trials

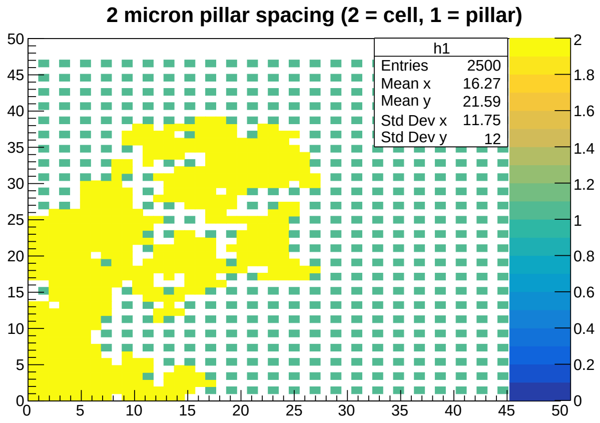

Figure 5: Picture with 2 micron spacing and 5000 Trials

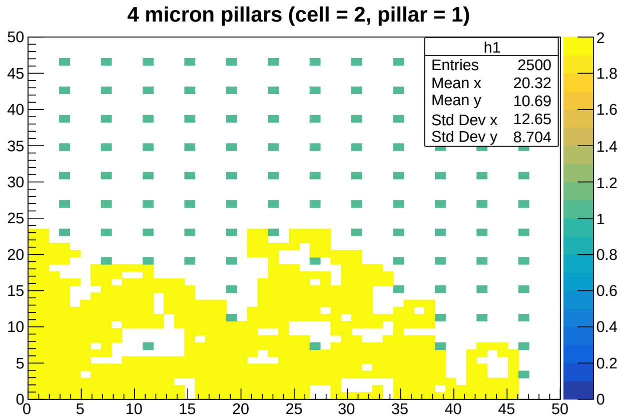

Figure 6: Picture with 4 micron spacing and 4000 Trials

2.1 Running the Code

To run the code, the following must be done - go to **Link to Pre-requisites**:

1. Type - ”git clone http://github.com/root-project/root.git”

2. ”cd root mkdir builddir”
3. ”cd builddir”
4. ”cmake ../”
5. ”cmake –build . − -jN” where N is the number of cores available on your computer
6. Source the Environment variable in your bashrc ”source /path/to/install/dir/bin/thisroot.sh”
7. start root with ”root”
8. Alternatively on OSX MacPort can be used to install ROOT with ”sudo port install root”
9. Change into the directory with prob2.C and run ”root prob2.C++”
10. to change the pillar spacing go to line 132 and change ”int p = N;” where N is 1,2, or 4.

3 Problem 3 (Extra credit)

Completed parts a-c for fun. Here is a link to a Colab notebook where the code for making an xyz file of a chain of atoms. The xyz file can be downloaded and visualized in VMD!
https://colab.research.google.com/drive/1Jrex6TmFys7MTbPnJwV62R$_{a}in4pLya-$

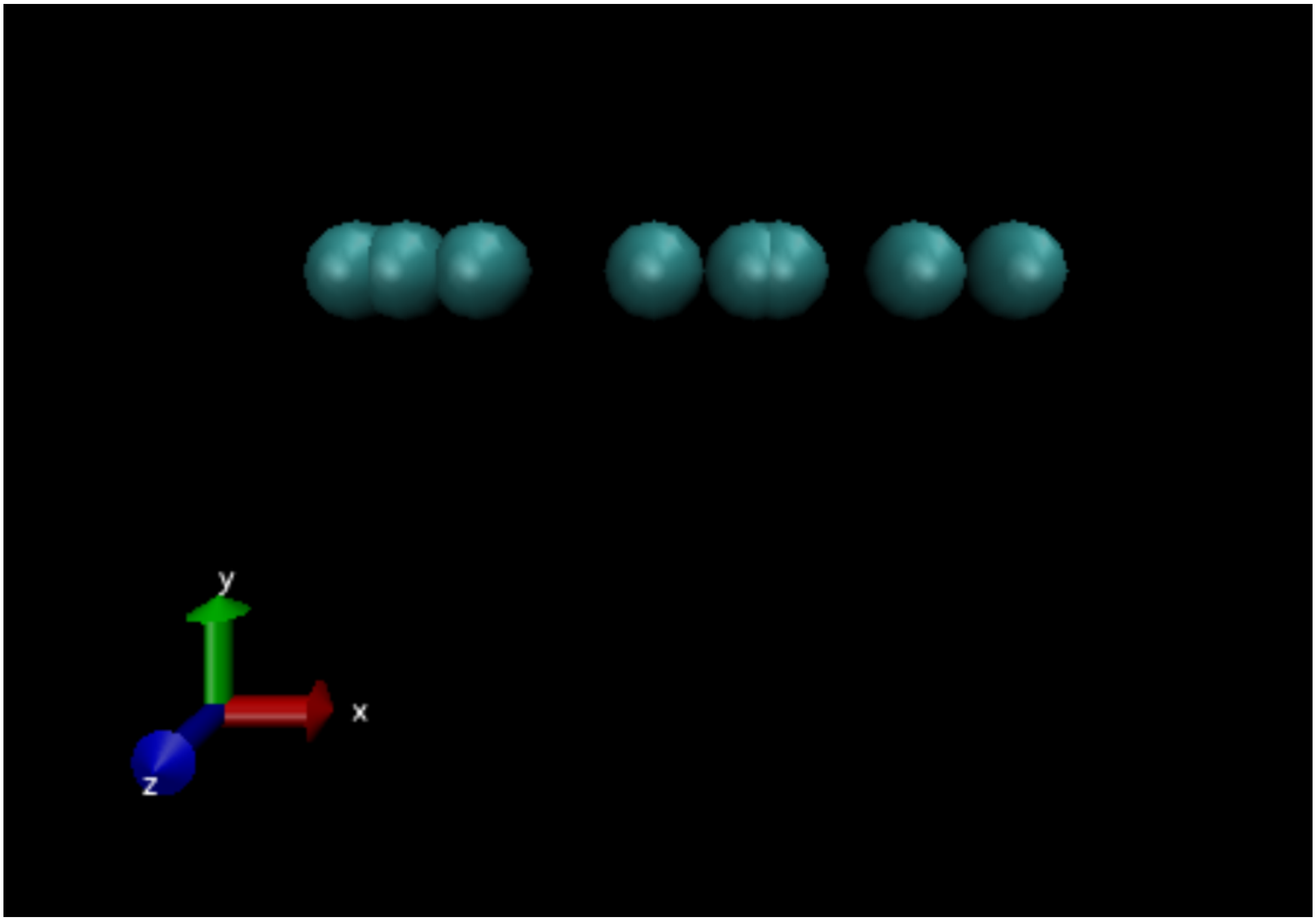

Figure 7: Capture of atom chain simulated in VMD