Problem Set 6, Part II
IM/S Spring 2006
Due May 5, 2006

This homework assignment is focused on mechanical properties of crystalline materials. We will use molecular dynamics modeling to describe the elastic and fracture properties, applied to (i) a bulk system of copper, modeled using periodic boundary conditions, (ii) a cracked nanocrystal, and (iii) a nanowire of copper under extreme tensile loading.

We will be using the ITAP IMD molecular dynamics code – implemented via a web interface developed by Ivica Ceraj.

Please see:

http://www.itap.physik.uni- stuttgart.de/~imd/

for instructions and a manual – you don't have to run the code on the command line or create the input files "by hand".

Visualization: You may use the program "vmd" (download at http://www.ks.uiuc.edu/Research/vmd/) to visualize the resulting ".xyz" files (only necessary if you study the nanowire problem for extra credit). "vmd" is available free of charge.

The website also provides .png files that you can view immediately in your browser – this should be all you need to do the main part of this problem set.

Note: Please provide a clear write- up with graphs and captions that clearly describe your observations. Provide intermediate steps when you do derivations – they should be done clearly.

1. Unit cells and crystallographic orientations, MD units

The first step in understanding the relationship between atomistic structure and its elastic properties is to consider the crystal structure. Here we focus on single crystals of copper composed out of a repeating sequence of unit cells defining the crystal structure.

Copper has a FCC lattice constant of a = 3.615 Å.

Assume that all lengths in the atomistic model are given in Angstrom (1 Å = 1E-10 m).

1. Define and draw the atomic coordinates in Angstrom in proper unit cells for different crystallographic orientations of a FCC crystal of copper: [100][010][001] (cubical) orientation (see lecture notes).
2. Calculate the atomic volume and mass density of copper (defined as mass per volume), based on this atomic model of a perfect crystal.
3. Calculate the units of temperature and pressure (or equivalently stress) in terms of the reference units used in the code.
   Note that the reference length $l^* = 1\text{Å} = 1\text{E-}10$ m, the reference energy $E^* = 1$ eV and the reference mass $m^* = 1$ amu. All output in IMD is in these units.

2. Elastic properties of crystals modeled using a LJ pair potential

Pair potentials are one of the simplest potentials to describe the atomic interaction of crystalline materials. Here we derive a simple 12:6 Lennard-Jones pair potential for FCC copper to fit experimental values of elastic properties of copper.

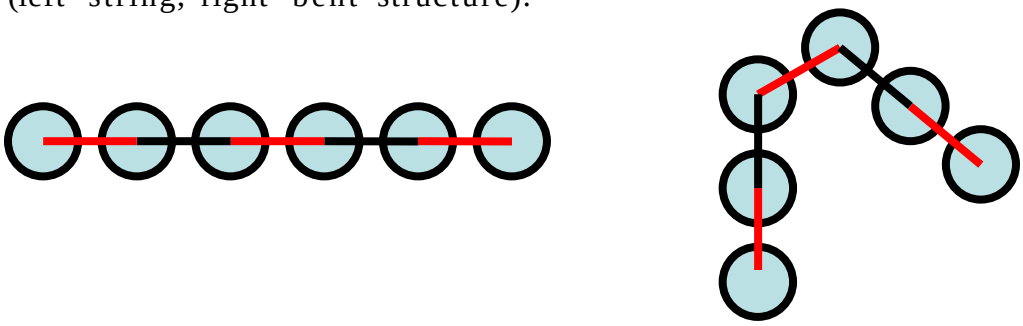
1. Assuming a 12:6 Lennard- Jones potential (see lecture notes), derive an expression for the equilibrium position between pairs of atoms (nearest neighbor interactions). Express the LJ length parameter σ as a function of the lattice parameter a.
2. Derive an expression for the minimum potential well of the LJ potential, corresponding to the cohesive energy stored in each bond.
3. Develop a Taylor series expansion of the LJ potential, considering up to second order terms, developed around the equilibrium distance between two atoms, denoted by r_0. Denote the second derivative of the potential by the parameter $\phi'' = k$.
4. The next step is to determine a set of parameters of the Lennard-Jones (LJ) potential that closely resemble experimental properties of copper. Determine numerical parameters for σ and ε based on experimental values for the lattice constant and bulk modulus of copper. Consider only nearest neighbor interactions. Compare the resulting values with the LJ copper potential reported by Cleri and coworkers [1].
   Discuss possible disagreement in light of the potential formulation and potential range.
   Hint: Take advantage of the following relations – valid for nearest neighbor interactions; shear modulus $\mu = r_0^2 / 2k$, Young's modulus is

$E = 8/3\mu$, and the bulk modulus where $\nu = 1/4$.
Write an expression for K as a function of relevant potential parameters, then determine the unknowns.

5. Using the web based code to calculate elastic properties, calculate the elastic properties of copper by plotting the stress tensor coefficients σ_{11}, σ_{22} and σ_{33} using (i) the LJ potential with the LJ parameters developed above (note: Consider only nearest neighbor interactions by choosing a proper cutoff radius, maybe 10..20% larger than the nearest neighbor distance $a/\sqrt{2}$) and (ii) using Cleri's potential (larger cutoff radius) [1]. Consider equitriaxial strain loading (corresponding to the bulk modulus K). Calculate the critical strain when the crystal becomes unstable, *i.e.* when the slope of the stress- strain plot approaches zero. (The plots from the program are actually the "pressure tensor" vs strain. The "pressure tensor" is the stress tensor times -1 .)

   Hint: Look at "engPlot.png" that plots the stress in the three spatial directions. Also, ask for more details if this question is confusing!

6. Assuming the LJ potential with nearest neighbor interactions, what is the energy difference between these two atomic configurations (left=string, right=bent structure):



   The red and black lines indicate an equal distance between atoms corresponding to the equilibrium separation. Discuss what implications this may have for modeling such a one- dimensional string of atoms.

3. Fracture and deformation of a copper nanowire using an EAM potential (extra credit)

Now we focus on fracture and deformation of a copper nanowires [2, 3]. Nanowires may play a critical role in future electronic devices, serving various needs including interconnects, waveguides or mechanical sensors. Due to the inherently small dimensions, classical, continuum descriptions are questionable and molecular modeling becomes the most reliable modeling tool to understand the mechanics of these materials.

Use the web based MD code that uses an EAM potential to model the atomic interactions.

1. Use the web based program to build and model tensile deformation of a copper nanowire. Choose dimensions of about 20 Å and 260 Å (8x8x60 unit cells). Model approximately 10,000 integration steps, or until you see significant deformation of the crystal. Use a displacement rate of 0.05 Å per 20 integration steps at the boundaries.
   Note: Apply the load in the z-direction, the axial direction of the nanowire.
2. Take snapshots of the system as it undergoes deformation and include them in your report for this problem set. Discuss the observed deformation mechanisms, in particular in light of earlier studies with a cracked crystal (qualitatively).
3. Plot the components of the stress tensor as the applied strain increases.
   Compare these with the results obtained earlier for the perfect crystal.
   How can the differences be explained?

Constants

$k_B = 1.3806503\text{E-}23$ J/K
1 eV = 1.60217646E-19 J
1 amu = 1.660538E-27 kg

References

1. Cleri, F., et al., *Atomic-scale mechanism of crack-tip plasticity: Dislocation nucleation and crack-tip shielding.* Phys. Rev. Lett, 1997. **79**: p. 1309-1312.
2. Heino, P., H. Häkkinen, and K. Kaski, *Molecular-dynamics study of mechanical properties of copper.* Europhysics Letters, 1998. **41**: p. 273-278.
3. Komanduri, R., N. Chandrasekaran, and L.M. Raff, *Molecular dynamics (MD) simulations of uniaxial tension of some single-crystal cubic metals at nanolevel.* Int. J. Mech. Sciences, 2001. **43**: p. 2237-2260.