Homework 3: Simulation of Copper – Introduction to LAMMPS

1) Lattice constant and cohesion energy of Cu

a) Use the input file "in.lj" to generate a 10x10x10 Cu FCC crystal, with a lattice a = 4.0 Å. Using the Lennard-Jones (LJ) potential parameterized for Cu, with a cutoff of 5 Å, perform a "box/relax" minimization to calculate the equilibrium lattice constant.
b) Calculate the cohesion energy (energy per atom at equilibrium). Gradually increase the cutoff and plot the cohesion energy and the computational time needed to perform the minimization with respect to the cutoff. Conclude and determine which cutoff should be used to obtain a reasonable accuracy while remaining computationally efficient. Keep this cutoff for the next questions.
c) Using the input file "in.eam", determine the equilibrium lattice constant and cohesion energy using the EAM potential.
d) Considering the experimental value of the lattice (a = 3.615 Å), can you evaluate which potential should be preferentially used?

2) Vacancy formation energy of Cu

The vacancy formation energy E_v is defined as the energetic cost to remove an atom from the crystal and put it into the bulk:

$$E_v = E_{n-1} - \frac{n-1}{n} E_{perfect}$$

where $E_{perfect}$ and E_{n-1} are the energies of the perfect supercell with n atoms and of the defect cell, respectively. Because $E_{perfect}$ scales with the number of atoms in the supercell, we can scale it with a multiplier $(n-1)/n$ so that we are comparing the energy of a defective cell with $n-1$ atoms to that of a perfect cell with $n-1$ atoms.

a) Starting directly from a lattice a = 3.615 Å, use the input file "in.defect" to calculate the vacancy formation energy using the LJ potential.
b) Recalculate the vacancy formation energy using the EAM potential.
c) Considering the experimental value of the vacancy formation energy (1.3 eV), conclude regarding which potential should preferentially be used.

3) Surface energy of Cu

The surface energy γ of a material is defined as the energy needed to create a surface S starting from a bulk material: $\gamma = (E_{cut} - E_{bulk})/S$

a) Starting directly from a lattice a = 3.615 Å, use the input file "in.surface" to calculate the surface energy using the EAM potential.
b) Compare the value that you find to that obtained by Foiles *et al.* (paper attached).

4) Mechanical properties of Cu

The elastic constant C_{11} of a material can be calculated through a uniaxial tensile (or compressive) test, as being the derivative of the stress with respect to the strain, or the second derivative of the energy with respect to the strain, normalized by the volume:

$$C_{11} = \frac{\partial \sigma_x}{\partial \varepsilon_x} = \frac{1}{V}\frac{\partial^2 E}{\partial \varepsilon_x^2}$$

a) Using the input file "in.elastic", simulate a uniaxial tensile test (with the EAM potential). Plot the strain-stress curve and the strain-energy curve. Based on these curves, calculate C_{11} with the two previously mentioned methods. Compare with the experimental value (found in Foiles *et al.*).
b) Modify the input file by increasing the maximum tensile strain imposed to the system, in order to ultimately observe the fracture of the material. Observe the fracture process using VMD. Plot the obtained strain-stress curve. Determine the intrinsic tensile strength of Cu, that is, the maximum stress that Cu can undergo before fracture.
c) Introduce one vacancy defect (remove one atom) from the previous system, and perform a fracture simulation again. Compare the obtained strain-stress curve and the value of strength to those obtained for the perfect system. Conclude.