**Molecular Statics Lab 2 – LAMMPS**

1. Completed LAMMPS tutorial 1

Total energy (eV) = -13.4399999527351;

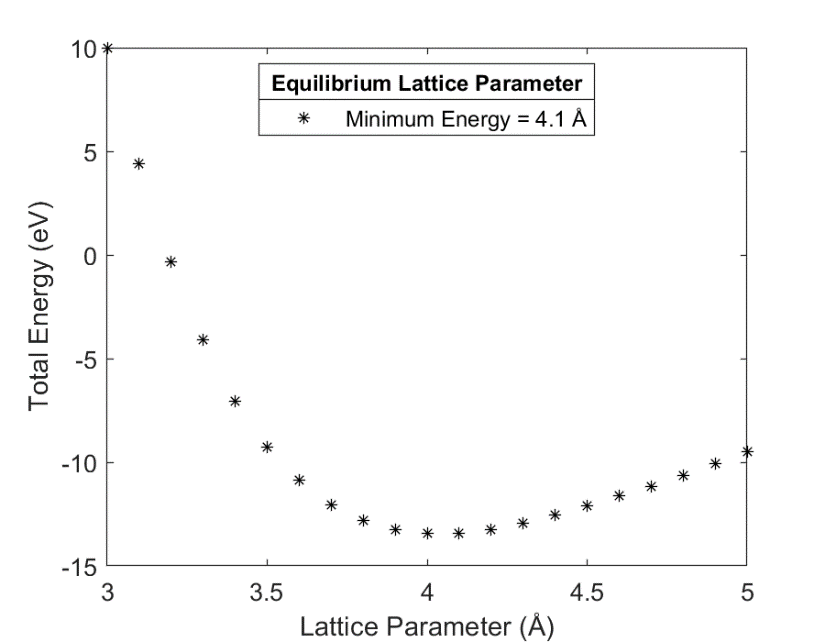
Number of atoms = 4;

Lattice constant (Angstoms) = 4.05000466178543;

Cohesive energy (eV) = -3.35999998818377;

print "All done!"

2. Completed LAMMPS tutorial 2. Below is the plot for total energy versus the lattice parameter from 3.0 to 5.0 Angstroms with increments of 0.1 Angstroms. The equilibrium lattice parameter is 4.1 Angstroms which is closest to the 4.05 calculated previously.



3. EAM potential used from recommended….

i) Lattice constant and cohesive energy for FCC Cu using energy minimization using EAM and LJ.

EAM: Lattice constant (Angstoms) = 3.63908745701191;

Cohesive energy (eV) = -3.2831162091543;

LJ: Lattice constant (Angstoms) = 3.53350974280472;

Cohesive energy (eV) = -4.47765319575385;

ii) Plotted below is the cohesive energy for the EAM and LJ potentials versus various lattice parameters. The lattice parameters calculated previously using energy minimization are also plotted along their respective curves. The EAM potential slightly overpredicts the experimental lattice parameter of 3.615 Å but is closer than that calculated by the LJ potential.

Chart, line chart

Description automatically generated

4. test