Lab sheet – 2

Cell relaxation of crystal structures of three elements: Alumium, Copper and Iron.

1. Run the sample calculation and record the following:
Total energy of unit cell in eV.
Cohesive energy of Al.
Lattice constant of Al.
Which force field file did you use for Al?

2. What will be the final energy (in eV) and lattice parameter of Al, if one changes the initial lattice constant to 4.5 Angstrom. Rerun the calculations and obtain the above results.
Are the results same or different from Que 1? Explain your answer.

3. Describe the following commands in LAMMPS, with all the options that are allowed in the input:
a. lattice
b. boundary
c. compute

4. Can Al exist in bcc structure?
What all parameters would you change in the input file to get the hypothetical bcc Al structure.
What are the relaxed total energies of the two structures (bcc and fcc) Al?

5. Run the calculation for fcc Cu, as in Que 1, and record the following:
The parameters you changed in the LAMMPS input file.
Total energy of unit cell in eV.
Cohesive energy of Cu.
Lattice constant of Cu.
Which force field file did you use for Cu?

6. Run the cell-relax calculation for bcc Fe and record the following:
The parameters you changed in the LAMMPS input file.
Total energy of unit cell in eV.
Cohesive energy of Fe.
Lattice constant of Fe.
Which force field file did you use for Fe?