# WORKSHEET
# PRACTICAL-2

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COURSE: MED201

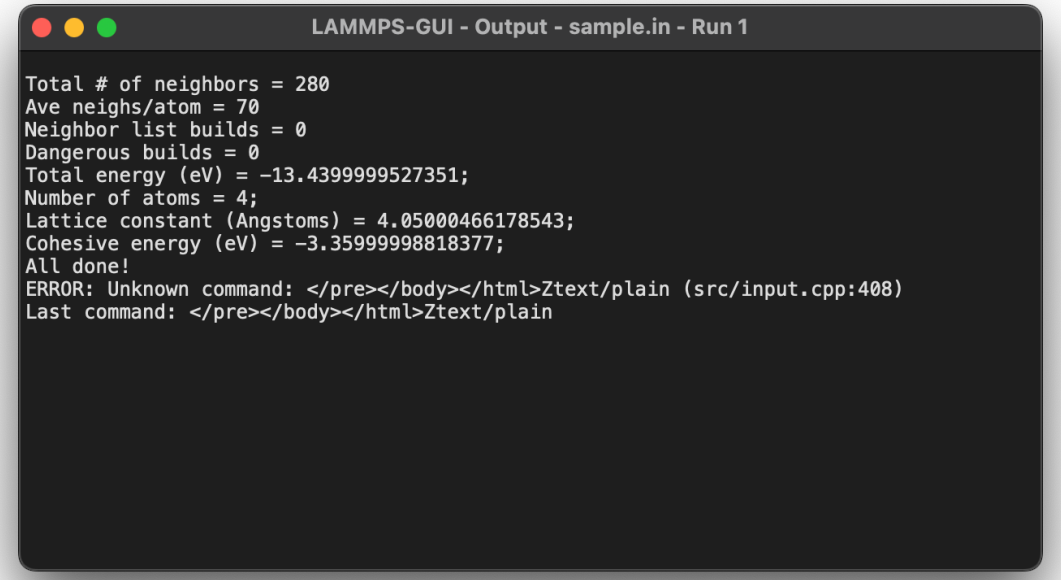
BATCH: PA

STREAM: BTech CSE

## QUESTION 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?

## ANSWER 1

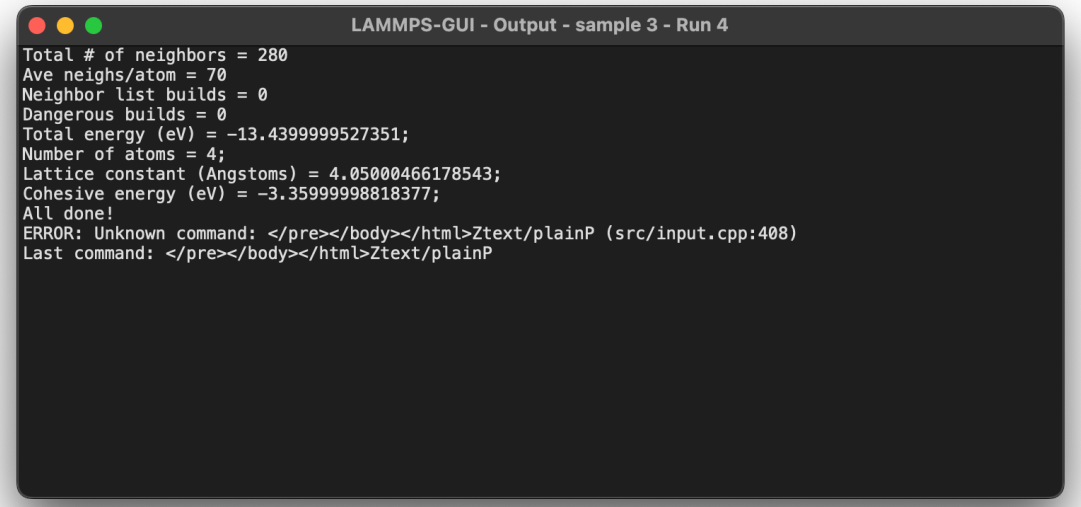



| | |
|---|---|
| Total energy of unit cell in eV | : -13. 4399999527351 |
| Cohesive energy of Al in eV | : -3.35999998818377 |
| Lattice constant of Al in Angstroms | : 4.05000466178543 |
| Which force field file did you use for Al? | : Al99.eam.alloy |

## QUESTION 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 Question 1? Explain your answer.

## ANSWER 2




Upon modifying the face-centered cubic (fcc) structure to 4.5 Angstrom, the energy calculations remained unchanged from the previous configuration, indicating the system had already achieved its energy minimum state. This is typical in crystal systems, where an optimal lattice parameter exists at equilibrium to minimize the total energy. Small variations around this equilibrium value often remain within the local energy minimum, resulting in negligible energy differences.

## QUESTION 3

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

## ANSWER 3

### a. Lattice

The lattice command in LAMMPS is used to define the atomic lattice for a simulation. It sets the arrangement, orientation and spacing of atoms in a periodic pattern.

OPTIONS:
style = none or sc or bcc or fcc or hcp or diamond or sq or sq2 or hex or custom
scale = scale factor between lattice and simulation box

keyword - origin or orient or spacing or a1 or a2 or a3 or basis or triclinic/general

### b. Boundary

The boundary command sets the boundary conditions for each dimension in the simulation box.

OPTIONS:
x,y,z = p or s or f or m, one or two letters

**c. Compute**

The compute command in LAMMPS is used to calculate properties on a per-atom, per-group or global basis. It is versatile, supporting a wide range of computations.

OPTIONS:
ID = user-assigned name for the computation
group-ID = ID of the group of atoms to perform the computation on
style = one of a list of possible style names (specifies the type of computation)
args = arguments used by a particular style

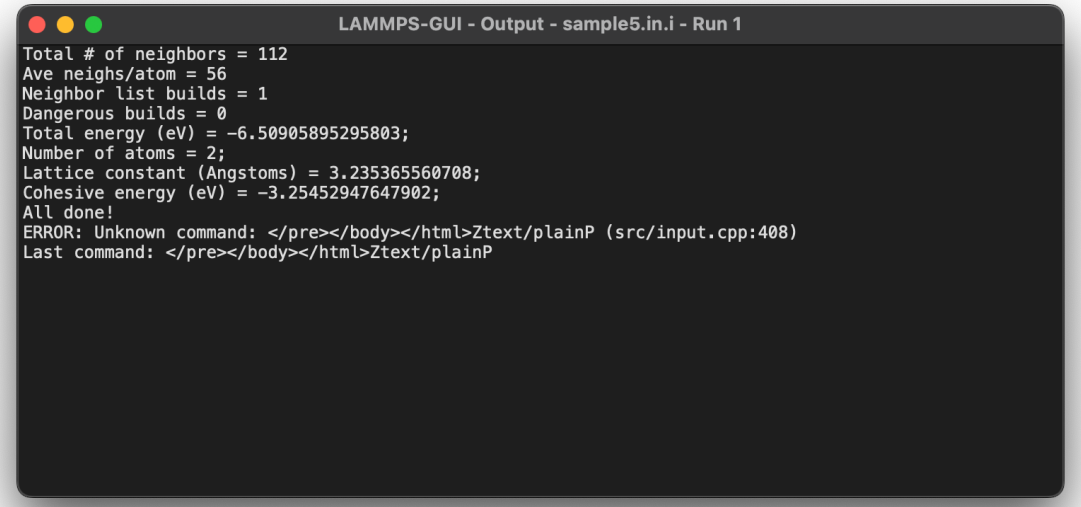
## QUESTION 4

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?

## ANSWER 4

Aluminium (Al) can **theoretically exist** in a body-centered cubic (BCC) structure, but this is hypothetical since aluminium naturally crystallizes in a face-centered cubic (FCC) structure.

In the sample.in file, change “fcc” to “bcc” and then run the file.




As we can see the total energy of Al in bcc is –6.509 but as we know this result is only for 2 atoms, so to compare it to fcc we have to multiply the bcc result by 2.
Therefore, the new Total energy for bcc will be –13.018.

But, the Total energy for fcc is –13.439.

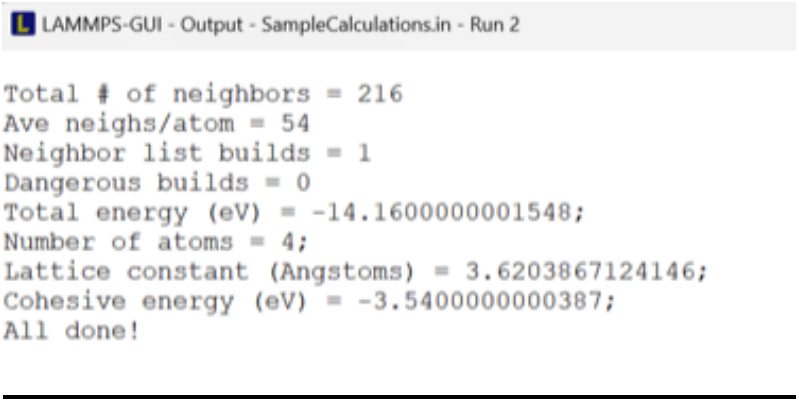
The relaxed total energy for BCC aluminium is higher than that of FCC aluminium.

This difference in energy demonstrates why Al prefers an FCC structure.
FCC is the stable phase for Al. Al exists naturally in FCC structure.

## QUESTION 5

Run the calculation for fcc Cu, as in Question 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?

## ANSWER 5

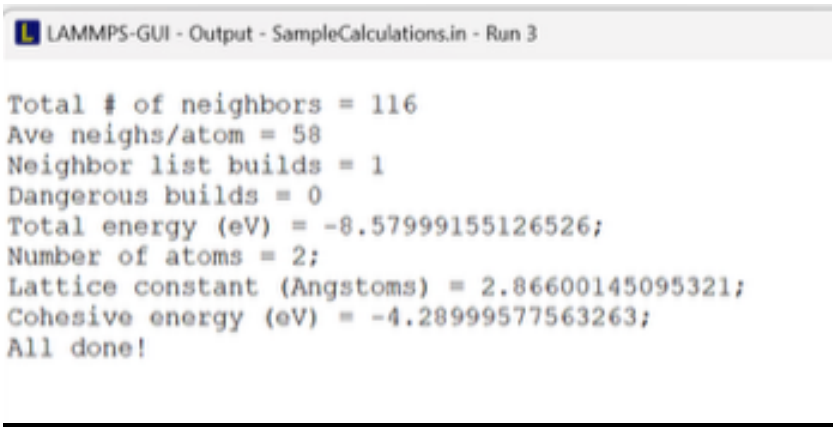



Parameters changed in input file: : pair style and pair coefficient
Total energy of unit cell in eV : -14.600000001548
Cohesive energy of Cu in eV : -3.5400000000387
Lattice constant of Cu in Angstroms : 3.6203867124146
Which force field file did you use for Cu? : Cu.meam

## QUESTION 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 eVs.
Cohesive energy of Fe.
Lattice constant of Fe.
Which force field file did you use for Fe?

## ANSWER 6




| | |
|---|---|
| Parameters changed in input file: | : pair style and pair coefficient and fcc to bcc |
| Total energy of unit cell in eV | : -8.57999155126526 |
| Cohesive energy of Fe in eV | : -4.28999577563263 |
| Lattice constant of Fe in Angstroms | : 2.86600145095321 |
| Which force field file did you use for Fe? | : Fe.meam |