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Project 1

Problem 1:

1. a. Using the lmp-in.1a-relax file, I found the total energy of the FCC Pt to be -6.6474426 eV and the lattice constant is 3.920945 angstroms (need to ask about this)

b.

1. Using lmp-in.1b-relax and the Pt-Adams1989.eam parameter file which use EAM potential, I found the lattice constant to be 3.9200001 and the total energy to be -23.07999 eV. Using lmp-in.1b-single and the Pt-Adams1989.eam parameter file, I found the lattice constant to be 3.9200001 and the total energy to be -23.07999 eV.
2. The experimental lattice constant is 3.92 where as my calculated lattice constant using Leonard Jones potential was 3.92394 and for EAM potential it was 3.9209

Problem 2:

1. Using 3x3x3 supercell with lattice constant 3.92095

Energy of perfect bulk super cell= -179.480949

Energy of defect cell= -176.157228

Vacancy formation energy= 1.66186

E cohesive= Ecompound – sum of Eatom=

Ratio of Ev to

1. Using 3x3x3 supercell with lattice constant starting at 4

Energy of perfect bulk super cell= -179.480949

Energy of defect cell= -176.17945

Vacancy formation energy= 1.6396

1. Using relaxed file.

Using 3x3x3 supercell with lattice constant starting at 4

Energy of perfect bulk super cell= --623.15999

Energy of defect cell= -615.6251

Vacancy formation energy= 1.76489

Problem 3:

Two convergence parameters: the slab (the part with the atoms) and the vacuum thickness

Problem 4:

Lennard Jones potential is most suitable for materials such as noble gases or diatomic molecules. Lennard Jones potentials are useful in modelling/simulating interactions between simple atoms or molecules and non-directed interactions.

EAM potentials are best used for problems that need to model metallic bonding/ metallic systems.

Lennard Jones and EAM potential are not appropriate to use for covalent bonded atoms/molecules or to figure out the angle dependance of a molecule which is useful for figuring out the energy difference in organic molecules.

Problem 5: