In the Name of GOD

HW set 1 SSD - Fall 2016 – EE-SUT

Due date: 1395/07/25 Prof. M. Fardmanesh

1. (a) Calculate the lattice constant and free volume (not occupied by atoms) of a bcc unit cell with atomic radius of 0.125nm.

   (b) If the distance between two adjacent {110} planes in a bcc lattice is 0.203nm, calculate the atomic radius in nm.

2. (a) Calculate the packing fraction of fcc, bcc, sc, and diamond structures.

   (b) Let N_n be the number of nth nearest neighbors of a given bravais lattice point (e.g. in a simple cubic bravais lattice $N_1 = 6, N_2 = 12$, etc.). Let r_n be the distance to the nth nearest neighbor expressed as a multiple of the nearest neighbor distance (e.g. in a simple cubic bravais lattice $r_1 = 1, r_2 = \sqrt{2}$, etc.). Make a table of packing fraction, N_n, and r_n for n= 1,…,3 for the fcc, bcc, and sc bravais lattices.

3. Show that lattice planes with the greatest densities of points are the {111} planes in a face-centered cubic bravais lattice and the {110} planes in a body-centered cubic bravais lattice.

4. Silicon crystallizes in a diamond cubic crystal structure with a lattice constant of 0.54305 nm. How many Si atoms per cm^2 are there on (100), (110), and (111) planes?

5. Graphene is a 2D crystal with carbon atoms arranged in a honeycomb structure. Assuming that the unit cell is a hexagon of carbon atoms, how many atoms of carbon are there in each unit cell? Draw and calculate the basis vectors needed to reproduce the whole crystal in 2D space.

6. (a) Prove that the ideal *c/a* ratio for the hexagonal close-packed structure is $\sqrt{8/3} = 1.633$.

   (b) Sodium transforms from bcc to hcp at about 23**K** (the “martensitic” transformation). Assuming that the density remains fixed through this transition, find the lattice constant of *a* of the hexagonal phase, given that $a = 4.23\text{Å}$ in the cubic phase and that the *c/a* ratio is indistinguishable from its ideal value.