ECE 340 Homework I Spring 2003

Due: Wednesday, January 29, 2003
(30 points)

1. *How many atoms are found inside a unit cell of a simple cubic (sc), body-centered cubic (bcc), face-centered cubic (fcc), diamond structure, and zinc-blende structure crystal? Find the maximum fractions of the unit cell volume that can be filled by hard sphere in the sc, bcc, fcc and diamond lattices. If all unit cells have the same lattice constants, i.e. the unit cell dimension, which structure among sc, bcc, fcc, diamond and zincbelnde has the largest atomic density (atoms/cm^3)? Which of them has the highest packing density, i.e. highest volume fraction being occupied by hard spheres? (12 points)*

Solutions:
Each corner atom is shared by 8 other unit cell, therefore, each corner atom can be counted as 1/8 atom. Similarly, each face atom is counted as ½ atom. Atoms that are completely inside the unit cell are counted as whole atoms. Zinc-blende lattice is very similar to diamond structure.

	Corner atoms	Face atoms	Inside Atoms	Sum
Simple cubic	8	0	0	1
Body-centered cubic	8	0	1	2
Face-centered cubic	8	6	0	4
Diamond Structure	8	6	4	8
Zinc Blende	8	6	4	8

Assuming lattice constant is a:

For SC: $$VolumeFraction = \frac{1\times\frac{4}{3}p\left(\frac{a}{2}\right)^3}{a^3} \approx 52\%$$

For BCC $$VolumeFraction = \frac{2\times\frac{4}{3}p\left(\frac{\sqrt{3}a}{4}\right)^3}{a^3} \approx 68\%$$

For FCC $$VolumeFraction = \frac{4\times\frac{4}{3}p\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3} \approx 74\%$$

For Diamond $$VolumeFraction = \frac{8\times\frac{4}{3}p\left(\frac{\sqrt{3}a}{8}\right)^3}{a^3} \approx 34\%$$

If all unit cells have same lattice constant, then the diamond and zinc-blende lattice has largest atomic density since there are 8 atoms/lattice in diamond, which is the largest.

As calculated above, the FCC has highest packing density.

2. Beginning with a sketch of a fcc lattice, add atoms at (1/4, 1/4, 1/4) from each fcc atom to obtain the diamond lattice. Show that only four added atoms in Fig. 1-8a appear in the diamond unit cell. (8 points)

3. The atomic radii of In and Sb atoms are approximately 1.44 Å and 1.36Å, respectively. Using the hard-sphere approximation, find the lattice constant of InSb, which is of zincblende structure. Calculate the areal density of atoms (number of atoms/cm^2) on the (100) and (110) planes. (10 points)

Solutions:
Assuming lattice constant is a,

Distance between neighboring atoms in zincblende is $\frac{\sqrt{3}}{4}a$.

$1.44 + 1.36 = \frac{\sqrt{3}a}{4}$, $\quad a = 6.47$ Å

For area density, each corner atom is counted as 1/4 atom. Each edge atom is counted as ½ atom. Inside atom is counted as a whole atom.
On (100) plane, there are two whole atoms, therefore,

$$AreaDensity = \frac{2}{a^2} = \frac{2}{\left(6.47\times10^{-8}\right)^2} = 4.78\times10^{14} atoms/cm^2$$

On (110) plane, it's a little difficult to visualize which atoms are on the plane. If you have difficulties, carefully study the graph you drew in problem 2. There are 4 atoms in the plane:

$$AreaDensity = \frac{4}{\sqrt{2}a^2} = \frac{4}{\sqrt{2}\left(6.47\times10^{-8}\right)^2} = 6.76\times10^{14} atoms/cm^2$$