Homework #2

1. Suppose identical solid spheres are distributed through space in such a way that their centers are lie on the points of a lattice, and spheres on neighboring points just touch without overlapping. (Such an arrangement of spheres is called a close-packing arrangement.) Assuming that the spheres have unit density, show that the density of a set of close-packed spheres on each of the four structures (the "packing fraction") is:

- **fcc:** \( \frac{\sqrt{2}\pi}{6} = 0.74 \)
- **bcc:** \( \frac{\sqrt{3}\pi}{8} = 0.68 \)
- **sc:** \( \frac{\pi}{6} = 0.52 \)
- **diamond:** \( \frac{\sqrt{3}\pi}{16} = 0.34 \)

**Solution:**

For fcc structure, the nearest neighbor distance is \( a/\sqrt{2} \), thus \( R = a/(2\sqrt{2}) \). Here \( a \) is the lattice constant of the fcc lattice and \( R \) is the radius of the sphere. Since there are four lattice sites per fcc cubic cell, the density should be

\[
\left(4 \times \frac{4\pi R^3}{3}\right)/a^3 = \frac{16\pi}{3} \left(\frac{1}{2\sqrt{2}}\right)^3 = \frac{\pi}{\sqrt{2}} = \frac{\sqrt{2}\pi}{6} = 0.74 .
\]

For bcc structure, the nearest neighbor distance is \( \sqrt{3}a/2 \), thus \( R = \sqrt{3}a/4 \). Here \( a \) is the lattice constant of the bcc lattice and \( R \) is the radius of the sphere. Since there are two lattice sites per bcc cubic cell, the density should be

\[
\left(2 \times \frac{4\pi R^3}{3}\right)/a^3 = \frac{8\pi}{3} \left(\frac{\sqrt{3}}{4}\right)^3 = \frac{\sqrt{3}\pi}{8} = 0.68 .
\]

For sc structure, the nearest neighbor distance is \( a \), thus \( R = a/2 \). Here \( a \) is the lattice constant of the sc lattice and \( R \) is the radius of the sphere. Since there are one lattice sites per sc cubic cell, the density should be

\[
\left(1 \times \frac{4\pi R^3}{3}\right)/a^3 = \frac{4\pi}{3} \left(\frac{1}{2}\right)^3 = \frac{\pi}{6} = 0.52 .
\]

The diamond structure is two sets of fcc lattices shifted along the diagonal direction by a quarter of the diagonal distance. The nearest neighbor distance is \( \sqrt{3}a/4 \), thus \( R = \sqrt{3}a/8 \). Here \( a \) is the lattice constant of the fcc lattice and \( R \) is the radius of the sphere. Since there are 4+4=8 lattice sites within the fcc cubic cell for diamond structure, the density should be

\[
\left(8 \times \frac{4\pi R^3}{3}\right)/a^3 = \frac{32\pi}{3} \left(\frac{\sqrt{3}}{8}\right)^3 = \frac{\sqrt{3}\pi}{16} = 0.34 .
\]
2. (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 23K (the "martensitic" transformation). Assuming that the density remains fixed through this transition, find the lattice constant \( a \) of the hexagonal phase, given that \( a=4.23\text{Å} \) in the cubic phase and that \( c/a \) ratio is ideal in the hcp phase.

Solution:

(a) Let \( a_{\text{hcp}} \) be the hcp lattice constant, i.e., the edge length of the hexagon. Then

\[
\frac{c}{2} = \sqrt{\frac{2}{3}} a_{\text{hcp}} \cdot \frac{\sqrt{3} a_{\text{hcp}}}{2} = \frac{2}{3} a_{\text{hcp}} \cdot \sqrt{\frac{2}{3} a_{\text{hcp}}}.
\]

Thus

\[
\frac{c}{2} \cdot \frac{\sqrt{3} a_{\text{hcp}}}{2} = \frac{2}{3} a_{\text{hcp}} \cdot \sqrt{\frac{2}{3} a_{\text{hcp}}}
\]

(b) The volume of a hcp cell is \( \frac{3\sqrt{3}}{2} a_{\text{hcp}}^2 c = 3\sqrt{2} a_{\text{hcp}}^3 \). There are 6 atoms with each hcp cell. Thus the density is \( \rho = \frac{6w}{3\sqrt{2} a_{\text{hcp}}^3} = \frac{\sqrt{2} w}{a_{\text{hcp}}^3} \). Here \( w \) is the weight one sodium atom. For bcc sodium, there are 2 atoms within each bcc cubic cell. The density should be \( \rho = \frac{2w}{a_{\text{bcc}}} \). If the density doesn’t change during the hcp-bcc transition, there is \( \frac{\sqrt{2} w}{a_{\text{hcp}}^3} = \frac{2w}{a_{\text{bcc}}^3} \). Thus \( a_{\text{hcp}} = \frac{a_{\text{bcc}}}{\sqrt[3]{2}} = \frac{4.23\text{Å}}{1.122} = 3.77\text{Å} \).

3. Under what conditions, will the body centered tetragonal lattice become
(a) a bcc structure?
(b) an fcc structure?

Solution:
4. Figure out the indexes of the following lattice planes. (The arrows are the basic vectors of the lattice.)

Solution:
(a). \( \left( \frac{1}{2}, \frac{1}{4}, \frac{1}{3} \right) \) = (6, 3, 4)
(b). \( \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{4} \right) \) = (2, 4, 1)
(c). \( \left( \frac{1}{3}, \frac{1}{3}, \infty \right) \) = (1, 1, 0)

5. Make a drawing of the (110) plane of a bcc lattice. What's the distance between adjacent (110) planes if the lattice constant is \( a \)?

Solution:
The shaded is a (110) plane. The next (110) plane contains the site with red color. Thus the distance between the adjacent (110) plane (red line) is \( \frac{a}{\sqrt{2}} \).

6. Make a drawing of the (111) plane of an fcc lattice. What's the distance between adjacent (111) planes if the lattice constant is \( a \)?

Solution:

The shaded are two adjacent (111) planes. Their separation distance equals 1/3 of the diagonal distance, i.e., equals to \( \sqrt{3}a/3 \).