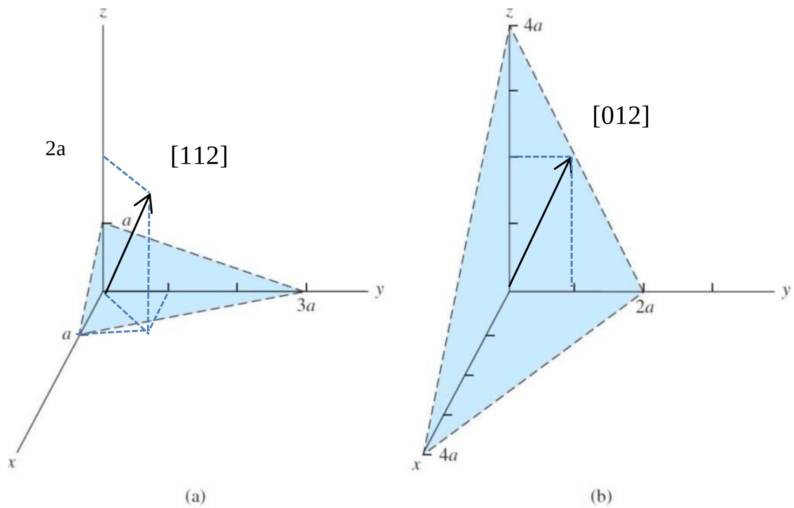
ECE 3030 Spring 2025 Homework 1 Solutions

1. (a) $\left(\frac{1}{1}, \frac{1}{3}, \frac{1}{1}\right) \Rightarrow (313)$

   (b) $\left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right) \Rightarrow (121)$



2. The linear density, **LD**, is the ratio of $\mathbf{L_c}$ and $\mathbf{L_l}$ where L_c is the portion of line covered by atoms and L_l is the total line length. For the [110] direction in BCC, $\mathbf{L_c} = 2\mathbf{R}$, whereas $\mathbf{L_l} = \frac{4\mathbf{R}\sqrt{2}}{\sqrt{3}}$ (since the body diagonal = 4R = a √3, a = 4R/√3, and L_l along (110) = √2 a). Therefore

   $$LD = \frac{L_c}{L_l} = \frac{2R}{\frac{4R\sqrt{2}}{\sqrt{3}}} = 0.61$$

For the [111] direction in BCC, $\mathbf{L_c} = \mathbf{L_l} = 4\mathbf{R}$; therefore $L_D = \frac{4R}{4R} = 1.0$

3. Planar density, **PD**, is defined as $PD = \frac{A_c}{A_p}$

where $\mathbf{A_p}$ is the total plane area within the unit cell and $\mathbf{A_c}$ is the circle plane area within this same plane. For the (100) plane in BCC, in terms of the atomic radius, **R**, and the unit cell edge length **a**

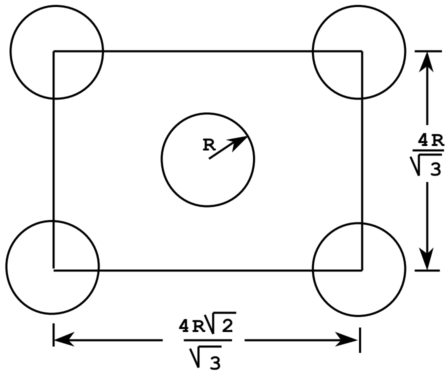
$$A_p = a^2 = \left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$$

Also, upon examination of that portion of the (100) plane within a single unit cell, that there resides a single equivalent atom--one-fourth from each of the four corner atoms. Therefore,

$$A_c = \pi R^2$$

Hence, $PD = \pi R^2/(16R^2/3) = 0.59$

That portion of a (110) plane that passes through a BCC unit cell forms a rectangle as shown below.



In terms of the atomic radius **R**, the length of the rectangle base is $4\mathbf{R}\sqrt{2}/\sqrt{3}$, whereas the height is $\mathbf{a} = \frac{4\mathbf{R}}{\sqrt{3}}$. Therefore, the area of this rectangle, which is just $\mathbf{A_p}$ is

$$A_p = \left(\frac{4R\sqrt{2}}{\sqrt{3}}\right)\left(\frac{4R}{\sqrt{3}}\right) = \frac{16R^2\sqrt{2}}{3}$$

Now for the number equivalent atoms within this plane. One-fourth of each corner atom and the entirety of the center atom belong to the unit cell. Therefore, there is an equivalent of 2 atoms within the unit cell. Hence $A_c = 2(\pi R^2)$

And PD = $2\pi R^2/(16R^2\sqrt{2}/3) = 0.83$

4. Find the number of atoms/unit cell and the nearest neighbor distance for sc, bcc, and fcc lattices.
   sc: atoms/unit cell = 8·1/8 = 1; nearest neighbor distance = a
   bcc: atoms/unit cell = (8·1/8) + 1 = 2; nearest neighbor distance = a√3/2
   fcc: atoms/unit cell = (8·1/8) + 6·½ = 4; nearest neighbor distance = a√2/2

5. (a) Simple cubic: a = 2r = 3.9 Å
   (b) fcc: a = 4r/√2 = 5.515 Å
   (c) bcc: a = 4r/√3 = 4.503 Å
   (d) diamond: a = 2 (4r/√3) = 9.007 Å

6. (a) a = 5.65 Å. 1/4 of the body diagonal (√3 a) = √3 a/4
   so 2r = √3 a/4 and a = 8r/√3.

   Then $r = \frac{a\sqrt{3}}{8} = \frac{(5.65)\sqrt{3}}{8}$ = 1.223 Å

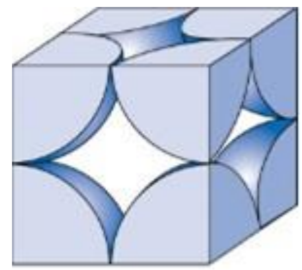
   Center of one Ge atom to center of nearest neighbor = 2r = 2.45 Å.

   (b) Number density N $= \frac{8}{\left(5.65\times10^{-8}\right)^3}$ = 4.44×10^{22} cm^{-3} since 2 x 4 = 8 atoms/unit cell in diamond lattice (two interpenetrating fcc lattices)

(c) Mass density $= \rho = \dfrac{N(At.Wt.)}{N_A} = \dfrac{(4.44\times10^{22})(72.61)}{6.02\times10^{23}} \rightarrow \rho = 5.35$ grams/cm^3.

7. Density of silicon atoms = 4 electrons per atom x 4 atoms/FCC lattice x 2 FCC lattices/unit cell divided by unit cell volume V= a^3. Lattice constant a = 5.43 x10^{-8} cm so V = 5 x 10^{22} cm^{-3} and 4 valence electrons per atom, so density of valence electrons = 2 x 10^{23} cm^{-3}.

8. Here is a crystalline substance with the unit cell structure shown, an atomic weight of 35.2g/mol, and a density of 3.65 g/cm^3. Solve for the atomic radius.



$\rho = (n/V_c)A/N_A$ Simple cubic so 2R = a

#atoms/unit cell = 1/8 x 8 = 1

Vc = a^3 = ($nA/\rho N_A$ = 1 atom x 35.2 g/mol / (3.65 g/cm^3 x 6.02 x 10^{23} atoms/mole)

a^3= 1.602 x 10^{-23} cm^3

a =2.52 x 10^{-8} cm = 2.52 Å

a = 2R so R = 1.26 Å

9. Lattice constants of AlSb, AlAs, and InP are 6.14 Å, 5.66 Å, and 5.87 Å, respectively from Appendix. Using Vegard's Law,

6.14Å·x + 5.45 Å·(1-x) = 5.87 Å → x = 0.44

$AlSb_{0.44}As_{0.56}$ lattice matches InP and has Eg=1.9 eV from Fig. 1-13.