Assignment 2 Solutions

1. Silicon has the diamond structure (8 atoms per unit cell), a cell parameter at room temperature of a = 5.4309 °A, and a density of 2330 kg m^{-3}. Use this information to estimate the Avogadro number. The atomic mass of Si is 28.086.

   N_a = # of atoms / mol
   a = 5.4309 x 10^{-10} m
   ρ = 2330 kg / m^3
   m_a = 28.086 g / mol = .028086 kg / mol
   8 atoms / unit cell

   8 x 28.086 x 10^{-3} / 2330 / (5.4309 x 10^{-10})^3 = **6.0202^{23} atoms / mol**

2. The cell parameter of bcc Fe is a = 2.8665 °A. What would the cell parameter be if the structure were fcc instead of bcc (Hint: The atomic radius of Fe could be expected to remain the same.)

   bcc = 3 atoms touch along body diagonal
   4r = √3 x a a = 2.8665 x 10^{-10} m
   r = 1.241 x 10^{-10} m
   fcc = 3 atoms touch along face diagonal
   4r = √2 x a
   a = 3.510 x 10^{-10} m

3. The cell parameter of NaCl is a = 5.63 °A. What is its density ? What would the density be if 5% of the Na atoms in NaCl are missing ? Remember that there are 4 Na and 4 Cl atoms in the unit cell.

   $m_{a\,(Na)}$ = 22.99 g/mol
   $m_{a\,(Cl)}$ = 35.45 g/mol
   a = 5.63 x 10^{-10} m

   22.99 / 6.02 x 10^{23} = 3.80 x 10^{-23} g / atom
   x 4 = 1.52 x 10^{-22} g / unit cell
   x 3.8 = 1.45 x 10^{-22} g / unit cell (5% Na deficiency)
   35.45 / 6.02 x 10^{23} = 5.89 x 10^{-23} g / atom
   x 4 = 2.36 x 10^{-22} g / unit cell
   ρ_1 = (1.52 x 10^{-22} + 2.36 x 10^{-22}) / (5.63 x 10^{-10})^3 = **2174 kg / m^3**
   ρ_2 = (1.45 x 10^{-22} + 2.36 x 10^{-22}) / (5.63 x 10^{-10})^3 = **2135 kg / m^3**

4. Calculate the bond lengths (the shortest distance of contact) between cations and anions in the following compounds with the NaCl structure. Also calculate the nearest distance between pairs of cations.

   (a) LiF (a = 4.02 °A) (b) LiCl (a = 5.14 °A) (c) LiBr (a = 5.50 °A) and (d) LiI (a = 6.00 °A).

All share NaCl structure, therefore d (bond length) = a / 2 & s_{nc} (separation between cation pairs) = $\sqrt{2}$ a / 2

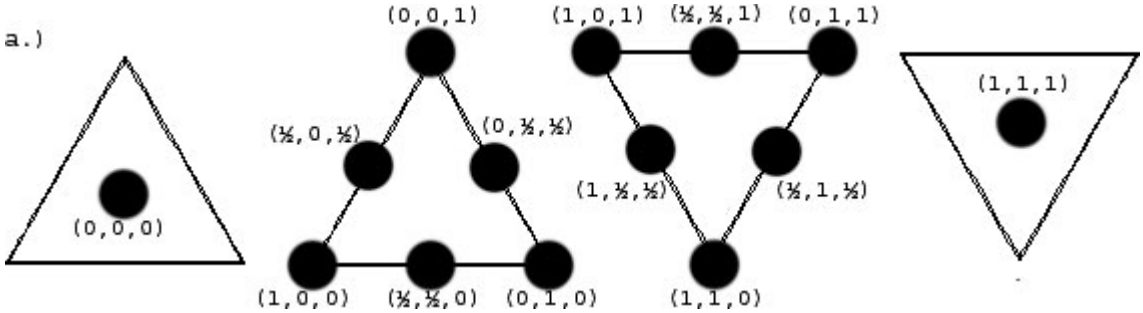
a.) d = 2.01 x 10^{-10} m , s_{nc} = 2.84 x 10^{-10} m
b.) d = 2.57 x 10^{-10} m , s_{nc} = 3.63 x 10^{-10} m
c.) d = 2.75 x 10^{-10} m , s_{nc} = 3.89 x 10^{-10} m
d.) d = 3.00 x 10^{-10} m , s_{nc} = 4.24 x 10^{-10} m

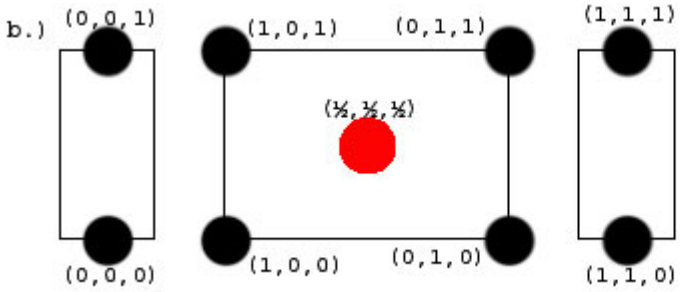
5. We have been projecting structures by considering sections along the z axis. But we could easily consider other projections:

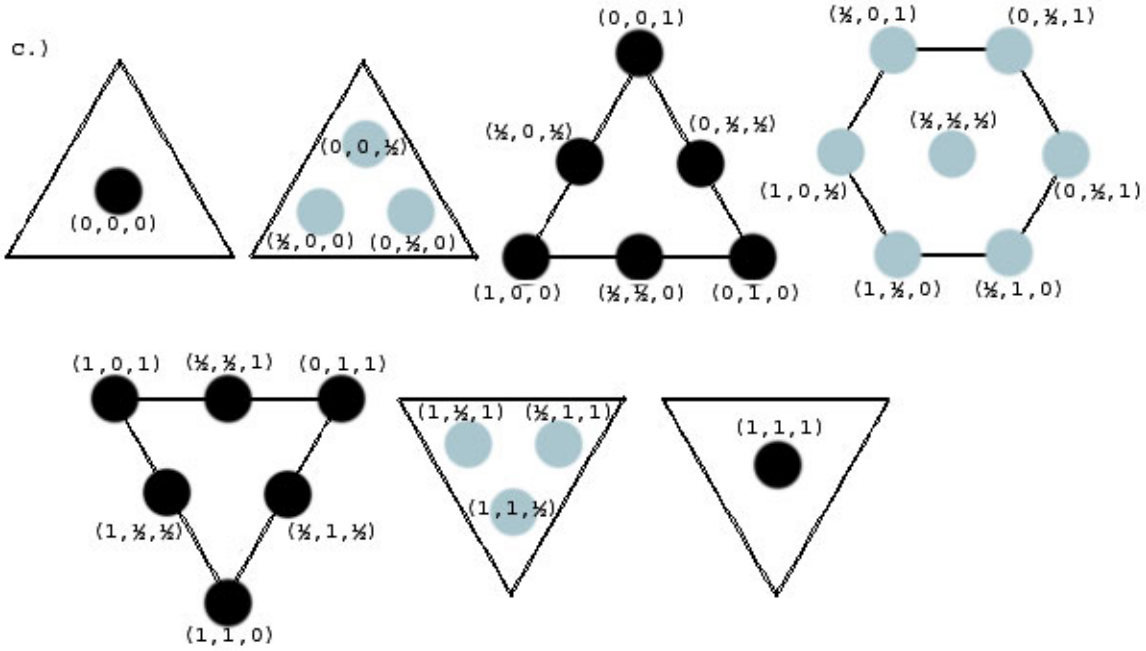
(a) Sketch sections of a single fcc unit cell along the body diagonal [the line connecting the cartesian points (0,0,0) and (1,1,1); the sections are perpendicular to this line].

(b) Sketch sections of the CsCl cell along a face diagonal [Sections perpendicular to the line joining (0,0,0) and (1,1,0).]

(c) Sketch sections of the NaCl cell along a body diagonal







6. Show using side-by-side projections that the zinc blende structure and the diamond structure are closely related. What can you say about the structures of the following compounds, all of which have the same number of valence electrons per atom as Si: AlP, GaAs and InSb ?

   The projections are in your class notes (part 2 of the Crystals, Packings, etc. notes.) The structure of compounds which have the same number of valence electrons as silicon per atom will tend to take on the diamond structure, with the atoms of each element in the compound taking up every other lattice site. (in other words adopt the Zinc Blende structure.)

7. Calculate the packing efficiency for the diamond structure. Note that it is very small. Suggest why some elements and compounds might adopt this structure, rather than a structure with higher packing efficiency.

   $8r = \sqrt{3}*a$ *from looking at the body diagonal
   $V_s = (4/3)\,\pi\, r^3$
   $= (4\pi/3)*(\sqrt{3}*a/8)^3$
   $= .34a^3$

   Elements & compounds which adopt this structure tend to be covalent solids and therefore have directional bonds which do not lend themselves to the tighter packing of fcc, bcc, etc. The system is not similar to packing hard spheres, it is the packing of tetrahedrals.