MATRL 100A: Structure and Properties I, Problem Set 5

This problem set is due in lecture on **Wednesday, Nov 14th** in hard copy. Write neatly, show your work clearly, and include units in all answers. While you are free to discuss this problem set with your classmates, the product that you turn in must be your own work. Do not copy or paraphrase each other's work.

Chapter 12

1. On the basis of ionic charge and ionic radii given below (1), predict crystal structures for the following materials. Justify your selections.
   (a) CsI
   (b) NiO
   (c) KI
   (d) NiS

Cation	*Ionic Radius (nm)*	*Anion*	*Ionic Radius (nm)*
Al^{3+}	0.053	Br^{-}	0.196
Ba^{2+}	0.136	Cl^{-}	0.181
Ca^{2+}	0.100	F^{-}	0.133
Cs^{+}	0.170	I^{-}	0.220
Fe^{2+}	0.077	O^{2-}	0.140
Fe^{3+}	0.069	S^{2-}	0.184
K^{+}	0.138		
Mg^{2+}	0.072		
Mn^{2+}	0.067		
Na^{+}	0.102		
Ni^{2+}	0.069		
Si^{4+}	0.040		
Ti^{4+}	0.061		

Figure 1: Ionic radii for several cations and anions (for a coordination number of 6)

2. Compute the atomic packing factor for the cesium chloride crystal structure in which $r_C/r_A = 0.732$.
3. The zinc blende crystal structure is one that may be generated from close-packed planes of anions.
   (a) Will the stacking sequence for this structure be FCC or HCP?
   (b) What is the coordination number of the cations?
   (c) Will cations fill tetrahedral or octahedral positions? Why?
   (d) What fraction of the positions will be occupied?
4. Compute the theoretical density of diamond given that the C–C distance and bond angle are 0.154 nm and 109.5°, respectively. How does this value compare with the measured density?
5. Cadmium sulfide (CdS) has a cubic unit cell, and from x-ray diffraction data it is known that the cell edge length is 0.582 nm. If the measured density is 4.82 g/cm^3, how many Cd^{2+} and S^{2-} ions are there per unit cell?

6. For each of the following crystal structures, represent the indicated plane in the manner of Figure 2b, showing both anions and cations. Only the plane view is necessary.

   (a) (100) plane for the rock salt crystal structure

   (b) (110) plane for the cesium chloride crystal structure

   (c) (111) plane for the zinc blende crystal structure

   (d) (110) plane for the perovskite crystal structure

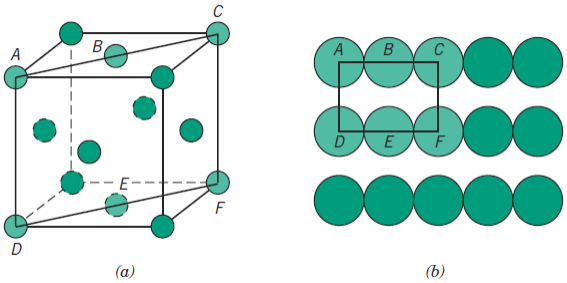

Figure 2: (a) Reduced-sphere FCC unit cell with the (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.

7. Would you expect Frenkel defects for anions to exist in ionic ceramics in relatively large concentrations? Why or why not?

8. Using the following data (3) that relate to the formation of Schottky defects in some oxide ceramic (having the chemical formula MO), determine the following:

   (a) The energy for defect formation (in eV)

   (b) The equilibrium number of Schottky defects per cubic meter at 1000°C

   (c) The identity of the oxide (i.e., what is the metal M?)

T (°C)	ρ (g/cm^3)	N_s (m^{-3})
750	5.50	9.21×10^{19}
1000	5.44	?
1250	5.37	5.0×10^{22}

Figure 3: Data for Problem 11

9. (a) Suppose that NaF is added as an impurity to MgF_2. If the Na^+ substitutes for Mg^{2+}, which element would you expect to form vacancies? How many vacancies are created for every Na^+ added?

   (b) Suppose that MgO is added as an impurity to $MgCl_2$. If the O^{2-} substitutes for Cl^-, which element would you expect to form vacancies? How many vacancies are created for every O^{2-} added?