MATRL 100A: Structure and Properties I, Assignment 5

This assignment is due on Wednesday, November 15.

Chapter 12

1. Show that the minimum cation to anion radius ratio for a coordination number of 6 is 0.414. *Hint: think of the NaCl crystal structure but with the Cl ions just touching each other and just touching the cations.*

2. Sketch the (100), (110), (111), and (200) planes for $BaTiO_3$ (perovskite crystal structure).

3. Calculate the APF and theoretical density of CaF_2 (fluorite) given the following relevant information:

Ion	Radius (nm)	Atomic Mass (g/mol)
Ca^{2+}	0.100	40.078
F^{-}	0.133	18.988

4. Sapphire consists of an HCP-like arrangement of O^{2-} anions with the much smaller Al^{3+} cations filling in octahedral interstitial sites.

   (a) How many octahedral interstitial sites are there per oxygen anion?

   (b) What fraction of octahedral interstitial sites must be full of aluminum cations to satisfy charge balance?

   (c) Sketch two basal planes of O^{2-} anions on top of each other. Identify the octahedral interstitial sites and shade in the ones that are full of Al^{3+}.

   (d) Calculate the cation to anion radius ratio by looking up the radius of Al^{3+} and O^{2-}. What type of interstitial site would you expect aluminum to fill based on your result? Comment on why this prediction is incorrect in this case. *Hint: think about the assumptions of the hard sphere model.*

   (e) Pure Al_2O_3 sapphires are optically clear. However, natural sapphires can have a wide variety of colors due to impurities. Describe what kind of vacancies would form, and how many there would need to be per impurity ion of the following species: Ti^{4+} (blue coloration), Mg^{2+} (pink coloration), and Cr^{3+} (red coloration). Assume oxygen interstitials are too high energy to form.

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

6. The mole fraction of Schottky defects (N_s/N) in a hypothetical MO oxide ceramic was measured to be $2.8 * 10^{-27}$ at room temperature. How many Schottky pairs per ion would you expect to find at 1250°C.