**CME 300 Properties of Materials**

Homework 1 September 23, 2011

Problems from R. E. Hummel Understanding Materials Science, History Properties Applications

Chapter 3: 3.1, 3.4, 3.6, 3.7, 3.8, 3.9, 3.11, 3.14, 3.16

Describe briefly the origin of the smelting of metal ore (Hummel chapter 1). (One paragraph)

Calister Problems

**3.30** Within a cubic unit cell, sketch the following directions:

**(a)** [101], **(e)** $[\bar{1}1\bar{1}]$,
**(b)** [211], **(f)** $[\bar{2}12]$,
**(c)** $[10\bar{2}]$, **(g)** $[3\bar{1}2]$,
**(d)** $[3\bar{1}3]$, **(h)** [301].

**3.17** Beryllium has an HCP unit cell for which the ratio of the lattice parameters $c/a$ is 1.568. If the radius of the Be atom is 0.1143 nm, **(a)** determine the unit cell volume, and **(b)** calculate the theoretical density of Be and compare it with the literature value.

**3.5** Show that the atomic packing factor for BCC is 0.68.

**3.6** Show that the atomic packing factor for HCP is 0.74.

***ONLY DO THE PROBLEMS ASSIGNED ABOVE FOR HUMMEL.***

## Problems

3.1. The set of {110} planes in an FCC unit cell passes through all corners of the cubic lattice and some face-centered atoms. The {110} set, however, misses the remaining face atoms. Write the Miller indices for a set of planes which is parallel to (110) but passes through all atoms of the FCC lattice.

3.2. List the Miller–Bravais indices of the six prism planes in a hexagonal lattice (show how you arrived at your result). What is the relationship to mutually opposite planes?

3.3. Show that the rhombohedral unit cell becomes an FCC or a BCC structure for specific angles $\alpha$. Calculate the values of these angles. Hint: Draw the lattice vectors of the *primitive* (non-cubic) unit cells of the FCC and BCC structures. The conventional (FCC, BCC) unit cells are *not* the smallest possible (primitive) unit cells.

3.4. Calculate the number of atoms for an HCP unit cell.

3.5. State the coordinates of the center atom in an HCP crystal structure ($a_1$, $a_2$, $c$) and show how one arrives at these values.

3.6. From the information given in Problem 3.5 above, show that the *c/a* ratio for the HCP structure is generally $\sqrt{8/3}$ if the atoms are assumed to be spherical. Compare this result with the experimental *c/a* ratios for Zn, Mg, and Zr.

3.7. State the slip plane and the slip direction in a hypothetical simple cubic lattice.

3.8. Show that a $\langle 111 \rangle$ direction lies in the (110) plane by sketching the appropriate direction and plane. Which one of the two (direction or plane) are close-packed assuming a BCC crystal structure? Discuss the implications for slip.

3.9. Determine (a) the coordination number, (b) the number of each ion per unit cell, and (c) the lattice constant (expressed in ionic radii) for the CsCl and the NaCl crystal structures.

3.10. Determine (a) the coordination number, (b) the number of each ion per unit cell, and (c) the lattice constant (expressed in ionic radii) for the zinc blende structure.

3.11. Calculate the packing factor for diamond cubic silicon.

3.12. Calculate the linear packing fraction of the [100] direction in (a) an FCC and (b) a BCC material assuming one atom per lattice point.

3.13. Calculate the planar packing fraction in the (111) plane in (a) the BCC and (b) the FCC structure.

3.14. Calculate the density of copper from its atomic mass. Compare your value with the density given in the Appendix. (The lattice parameter for Cu is $a = 3.6151$ Å.)

3.15. Sketch the $[1\bar{1}0]$ direction in the hexagonal crystal system. What is the four-digit index for this direction? Hint: The transformation equations between the 3-digit $[h'\ k'\ l']$ and the 4-digit $[h\ k\ i\ l]$ indices are:

$$h = \frac{1}{3}(2h' - k')$$

$$k = \frac{1}{3}(2k' - h')$$

$$i = -(h + k)$$

$$l = l'$$

3.16. Calculate the distance between two nearest face atoms of the conventional FCC unit cell.