Fundamentals of Materials Science Homework 10

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Homework Problems:

1. **Show that the minimum cation-to-anion radius ratio for a coordination number of 6 is 0.414. [Hint: use the NaCl crystal structure, and assume that anions and cations are just touching along cube edges and across the face diagonals.]**

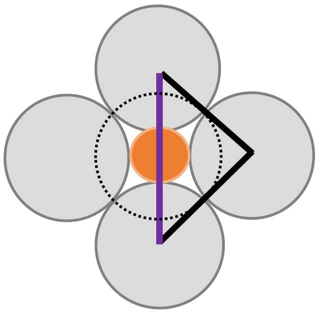
Solution:

The figure shows that:

$$2r_{Na^+} + 2r_{Cl^-} = \sqrt{2}a; a = 2r_{Cl^-}$$

$$\therefore 2r_{Na^+} + 2r_{Cl^-} = 2\sqrt{2}r_{Cl^-}$$

$$\therefore \frac{r_{Na^+}}{r_{Cl^-}} = \frac{2\sqrt{2}-2}{2} = 0.414$$



2. **On the basis of ionic charge and ionic radii given in the Table in your textbook or lecture note, predict crystal structures for the following materials:**
   (a) CaO, (b) MnS, (c) KBr, and (d) CsBr.
   Justify your selections.

Solution:

(a)CaO: $r_{Ca^{2+}} = 0.100nm; r_{O^{2-}} = 0.140nm$

$\therefore \frac{r_{Ca^{2+}}}{r_{O^{2-}}} = \frac{0.100nm}{0.140nm} = 0.714$; based on this ratio, coord#=6, structure=sodium chloride.

(b)MnS: $r_{Mn^{2+}} = 0.067nm; r_{S^{2-}} = 0.184nm$

$\therefore \frac{r_{Mn^{2+}}}{r_{S^{2-}}} = \frac{0.067nm}{0.184nm} = 0.364$; based on this ratio, coord#=4, structure=zinc blende.

(c)KBr: $r_{K^+} = 0.138nm; r_{Br^-} = 0.196nm$

$\therefore \frac{r_{K^+}}{r_{Br^-}} = \frac{0.138nm}{0.196nm} = 0.704$; based on this ratio, coord#=6, structure=sodium chloride.

(d)CsBr: $r_{Cs^+} = 0.170nm; r_{Br^-} = 0.196nm$

$\therefore \frac{r_{Cs^+}}{r_{Br^-}} = \frac{0.170nm}{0.196nm} = 0.867$; based on this ratio, coord#=8, structure=cesium chloride.

3. The unit cell for Al_2O_3 has hexagonal symmetry with lattice parameters *a* = 0.4759 nm and *c* =1.2989 nm. If the density of this material is 3.99 g/cm^3, calculate its atomic packing factor.

Solution:

Atomic weight of Al is 26.98g/mol ; Ionic radius of Al^{3+} is 0.053nm
Atomic weight of O is 16.00g/mol ; Ionic radius of O^{2-} is 0.140nm

$$\because \rho = \frac{nA}{VN_A} \therefore n = \frac{\rho V N_A}{A} = \frac{\rho V N_A}{(2A_{Al} + 3A_O)}$$

$$n = \frac{3.99g/cm^3 \times \frac{\sqrt{3}}{2} \times (0.4759nm)^2 \times 1.2989nm \times 6.02 \times 10^{23} atmos/mol}{2 \times 26.98g/mol + 3 \times 16.00g/mol} = 18$$

$$APF = \frac{nV_1}{V} = \frac{18 \times \left[\frac{4}{3}\pi \times (0.053nm)^3 + \frac{4}{3}\pi \times (0.140nm)^3\right]}{\frac{\sqrt{3}}{2} \times (0.4759nm)^2 \times 1.2989nm} = 0.84$$

4. Iron oxide (FeO) has the rock salt crystal structure and a density of 5.70 g/cm^3.
(a) Determine the unit cell edge length.
(b) How does this result compare with the edge length as determined from the radii in Table 4.4, assuming that the Fe^{2+} and O^{2-} ions just touch each other along the edges?

Solution:

(a).Atomic weight of Fe is 55.85g/mol ; Ionic radius of Fe^{2+} is 0.077nm
Atomic weight of O is 16.00g/mol ; Ionic radius of O^{2-} is 0.140nm

$$V = \frac{nA}{\rho N_A} = \frac{4 \times (55.85g/mol + 16.00g/mol)}{5.70g/cm^3 \times 6.02 \times 10^{23} atmos/mol} = 0.0837nm^3$$

$$a = \sqrt[3]{0.0837nm^3} = 0.437nm$$

(b). $a = 2r_{Fe^{2+}} + 2r_{O^{2-}} = 2\times 0.077nm + 2\times 0.140nm = 0.434nm$

5. **Compute the theoretical density of ZnS, given that the Zn-S distance and bond angle are 0.234 nm and 109.5°, respectively. How does this value compare with the measured density?**

Solution:

Atomic weight of Zn is 65.42g/mol
Atomic weight of S is 32.06g/mol

$$\frac{\sqrt{2}}{2}a = 2\times d\times \sin\left(\frac{180°-\theta}{2}\right) \therefore a = 2\sqrt{2}\times 0.234nm\times \sin 35.25° = 0.540nm$$

$$\therefore V = a^3 = (0.540nm)^3 = 0.157nm^3$$

$$\therefore \rho = \frac{nA}{VN_A} = \frac{4\times(65.42g/mol + 32.06g/mol)}{0.157nm^3\times 6.02\times 10^{23}atmos/mol} = 4.12g/mol$$

6. **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? Why?**
   b) **Will cations fill tetrahedral or octahedral positions? Why?**
   c) **What fraction of the positions will be occupied?**

Solution:

(a) The stacking sequence of close-packed planes of anions for the zinc blende cry stal structure will be the same as FCC (and not HCP) because the anion packing i s FCC.
(b) The cations will fill tetrahedral positions since the coordination number for cat ions is four.
(c) Only one-half of the tetrahedral positions will be occupied because there are t wo tetrahedral sites per anion, and yet only one cation per anion.

7. **Magnesium oxide has the rock salt crystal structure and a density of 3.58 g/cm^3.**
   a) **Determine the unit cell edge length.**
   b) **How does this result compare with the edge length as determined from the radii in your textbook or lecture note, assuming that the Mg^{2+} and O^{2-} ions just touch each other along the edges?**

Solution:

(a).Atomic weight of Mg is 24.31g/mol ; Ionic radius of Mg^{2+} is 0.072nm
Atomic weight of O is 16.00g/mol ; Ionic radius of O^{2-} is 0.140nm

$$V = \frac{nA}{\rho N_A} = \frac{4\times(24.31g/mol + 16.00g/mol)}{3.58g/cm^3 \times 6.02\times10^{23} atmos/mol} = 0.0748nm^3$$

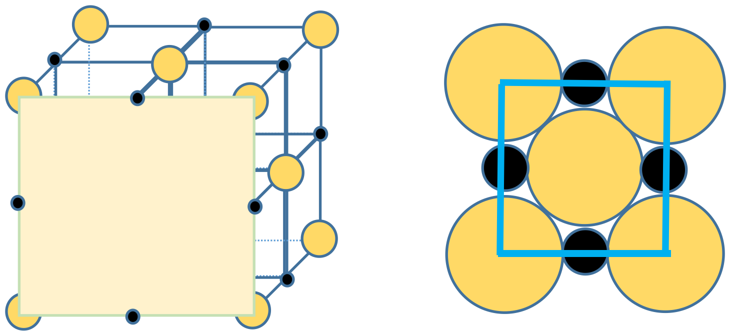
$$a = \sqrt[3]{0.0748nm^3} = 0.421nm$$

(b). $a = 2r_{Fe^{2+}} + 2r_{O^{2-}} = 2\times0.072nm + 2\times0.140nm = 0.424nm$

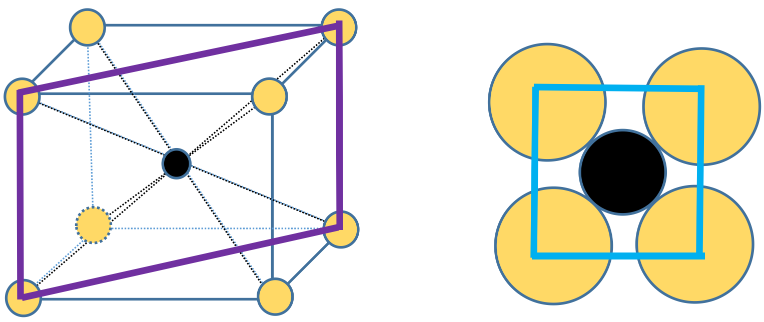
8. **For each of the following crystal structures, represent the indicated plane in the manner of Figure 4.20 and 4.21, showing both anions and cations:**
   a) (100) plane for the rock salt crystal structure,
   b) (110) plane for the cesium chloride crystal structure.

Solution:

(a)



(b)



9. **Nanowires are high aspect-ratio metal or semiconducting wires with diameters on the order of 1 to 100 nanometers and typical lengths of 1 to 100 microns. Nanowires likely will be used in the future to create high-density electronic circuits.**
   Nanowires can be fabricated from ZnO. ZnO has the wurtzite structure. The

wurtzite structure is a hexagonal lattice with four atoms per lattice point at Zn (0, 0, 0), Zn (2/3, 1/3, 1/2), O (0, 0, 3/8), and O (2/3, 1/3, 7/8).

a) How many atoms are there in the conventional unit cell?

b) If the atoms were located instead at Zn (0, 0, 0), Zn (1/3, 2/3, 1/2), O (0, 0, 3/8), and O (1/3, 2/3, 7/8), would the structure be different? Please explain.

c) For ZnO, the unit cell parameters are *a*=3.24 Å and *c*=5.19 Å. (Note: this is not the ideal HCP *c/a* ratio.) A typical ZnO nanowire is 20 nm in diameter and 5 μm long. Assume that the nanowires are cylindrical. Approximately how many atoms are there in a single ZnO nanowire?

Solution:

(a)Because there are 2 Zn atoms and 2 O atoms per unit cell,there are 10 atoms in the conventional unit cell.

(b)the structur will be same.

(c)???