**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:

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1. **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:**

1. **CaO: **

****; based on this ratio, coord#=6, structure=sodium chloride.

1. **MnS:**

****; based on this ratio, coord#=4, structure=zinc blende.

1. **KBr:**

****; based on this ratio, coord#=6, structure=sodium chloride.

1. **CsBr:**

****; based on this ratio, coord#=8, structure=cesium chloride.

1. **The unit cell for Al2O3 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/cm3, calculate its atomic packing factor.**

**Solution:**

Atomic weight of Al is 26.98g/mol ; Ionic radius of Al3+ is 0.053nm

Atomic weight of O is 16.00g/mol ; Ionic radius of O2- is 0.140nm

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1. **Iron oxide (FeO) has the rock salt crystal structure and a density of 5.70 g/cm3.**

**(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 Fe2+ and O2– ions just touch each other along the edges?**

**Solution:**

(a).Atomic weight of Fe is 55.85g/mol ; Ionic radius of Fe2+ is 0.077nm

Atomic weight of O is 16.00g/mol ; Ionic radius of O2- is 0.140nm





(b).

1. **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

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1. **The zinc blende crystal structure is one that may be generated from close-packed planes of anions.**
   1. **Will the stacking sequence for this structure be FCC or HCP? Why?**
   2. **Will cations fill tetrahedral or octahedral positions? Why?**
   3. **What fraction of the positions will be occupied?**

**Solution:**

**(a)**The stacking sequence of close-packed planes of anions for the zinc blende crystal structure will be the same as FCC (and not HCP) because the anion packing is FCC.

**(b)**The cations will fill tetrahedral positions since the coordination number for cations is four.

**(c)**Only one-half of the tetrahedral positions will be occupied because there are two tetrahedral sites per anion, and yet only one cation per anion.

1. **Magnesium oxide has the rock salt crystal structure and a density of 3.58 g/cm3.**
   1. **Determine the unit cell edge length.**
   2. **How does this result compare with the edge length as determined from the radii in your textbook or lecture note, assuming that the Mg2+ and O2- ions just touch each other along the edges?**

**Solution:**

(a).Atomic weight of Mg is 24.31g/mol ; Ionic radius of Mg2+ is 0.072nm

Atomic weight of O is 16.00g/mol ; Ionic radius of O2- is 0.140nm





(b).

1. **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:**
   1. **(100) plane for the rock salt crystal structure,**
   2. **(110) plane for the cesium chloride crystal structure.**

**Solution:**

**(a)**

**(b)**

1. **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).**

* 1. **How many atoms are there in the conventional unit cell?**
  2. **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.**
  3. **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 m long. Assume that the nanowires are cylindrical. Approximately how many atoms are there in a single ZnO nanowire?**

**Solution:**

1. Because there are 2 Zn atoms and 2 O atoms per unit cell,there are 10 atoms in the conventional unit cell.
2. the structur will be same.
3. ???