

MS 115a, Problem Set #2

assigned 10/10/12

due 10/17/12

1. There are four atoms in the unit cell of a cubic close-packed metal. The atomic (or fractional) coordinates of these atoms can be written as

0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$; and $\frac{1}{2}$, 0 $\frac{1}{2}$

where none of the positions in this set of coordinates is related by simple unit cell translation (*i.e.*, you can't add 1 to one of the coordinates and get one of the others).

In this same manner, specify the coordinates of

- (a) the four tetrahedral sites in the HCP structure
 - (b) the two octahedral sites in the HCP structure
 - (c) the eight tetrahedral sites in the CCP structure
 - (d) the four octahedral sites in the CCP structure
2. Calculate the radius of an aluminium atom given that Al has a cubic close-packed crystal structure, a density of 2.70 g/cm^3 , and an atomic weight of 26.98 g/mol .
3. Yttrium has an HCP crystal structure, a density of 4.472 g/cm^3 , and the c/a ratio is 1.572.
- (a) What is the volume of its unit cell in cubic meters?
 - (b) What are the magnitudes of the unit cell parameters c and a ?
4. Below are listed the atomic weight, density, and atomic radius for three hypothetical metals. For each determine whether its crystal structure is CCP, BCC-packed, or simple cubic packed and then justify your determination. A simple cubic packed structure has atoms at the corners of the unit cell (only) with atoms touching along the unit cell edge.

<i>Metal</i>	<i>Atomic Weight (g/mol)</i>	<i>Density (g/cm³)</i>	<i>Atomic Radius (nm)</i>
A	55.80	7.82	0.114
B	83.08	8.01	0.144
C	93.46	11.5	0.129

5. Show that the minimum cation-to-anion radius ratio for a cation coordination number of 3 is 0.155.
6. Show that the minimum cation-to-anion radius ratio for cation coordinate number of 4 is 0.225.
7. Why is octahedral coordination adopted by purely ionic compounds over trigonal prismatic given that both correspond to a coordination number of 6?

8. (a) The ionic radii of Cs and Cl are 1.70 and 1.81 Å, respectively. Compute the expected density of CsCl (for the normal CsCl structure).
- (b) Compute the atomic packing factor (volume of atoms in one unit cell/total volume of one unit cell, assuming atoms are hard spheres) for CsCl in its normal structure.
- (c) Compute the atomic packing factor for a hypothetical form of CsCl assuming it adopts the rock salt (NaCl) structure type. Does the difference from the result in (b) tell you anything about why CsCl adopts the structure that it does?
9. A hypothetical AX type of ceramic material is known to have density of 2.65 g/cm³ and a unit cell of cubic symmetry with a cell edge length of 4.3 Å. The atomic weights of the A and X elements are 86.6 and 40.3 g/mol, respectively. On the basis of this information, which of the following crystal structures is (are) possible for this material: rock salt, cesium chloride, or zinc blende? Justify your choice(s)
10. In a purely ionic compound, should the larger ions take on a CCP array or an HCP array? Hint: examine the distances between interstitial sites.
11. When considering the location of impurity atoms in metals, a general criterion is that the impurity atom must be *small* enough to fit into the interstitial site. When considering the location of cations of ionic compounds in which anions are in a close-packed array, a general criterion is that the cation must be *large* enough for the interstitial site. Explain why the two situations are treated differently.
12. Show that for the ideal perovskite structure, one expects the following to hold

$$\frac{(R_O + R_A)}{\sqrt{2}(R_O + R_B)} = 1$$

the term on the left is known as the ‘Goldschmidt tolerance factor’ and is given the symbol t . It typically ranges from 0.88 to 1.02. When $t \neq 1$, the structure becomes distorted in some from the ideal cubic form, and such distortions are often responsible for usual properties.