

MS 115a, Problem Set #2

assigned 10/11/07

due 10/17/07

- The atomic packing factor for a crystal structure is defined as the ratio of volume occupied by the atoms in the unit to the total volume of the unit cell. Show that the atomic packing factor
 - for the cubic close-packed (CCP) structure is 0.74
 - for the ideal hexagonal close-packed (HCP) structure is 0.74
 - for the body-centered cubic packed structure is 0.68
- 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).
 Specify the coordinates of
 - the four tetrahedral sites in the HCP structure
 - the two octahedral sites in the HCP structure
 - the eight tetrahedral sites in the CCP structure
 - the four octahedral sites in the CCP structure
- Calculate the radius of an iridium atom given that Ir has a cubic-close packed crystal structure, a density of 22.4 g/cm^3 , and an atomic weight of 192.2 g/mol .
- Zirconium has an HCP crystal structure and a density of 6.51 g/cm^3 .
 - What is the volume of its unit cell in cubic meters?
 - If the c/a ratio is 1.593, compute the values of c and a .
- 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</i> (g/mol)	<i>Density</i> (g/cm ³)	<i>Atomic Radius</i> (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

6. Show that the minimum cation-to-anion radius ratio for a coordination number of 6 is 0.414.
7. Which of the cations listed below would you predict to form iodides having the cesium chloride crystal structure? Justify your choices. The ionic radius of I is 2.2 Å.

Cation	Al ³⁺	Ba ²⁺	Ca ²⁺	Cs ⁺	Fe ²⁺	Fe ³⁺	K ⁺	Mg ²⁺	Mn ²⁺	Na ⁺	Ni ²⁺	Si ⁴⁺	Ti ⁴⁺
<i>R</i> (Å)	0.53	1.36	1.00	1.70	0.77	0.69	1.38	0.72	0.67	1.02	0.69	0.40	0.61

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) The measured density is 3.99 g/cm³. How do you explain the slight discrepancy between your calculated value and the measured one?
- (c) Compute the atomic packing factor for CsCl in its normal structure
- (d) Compute the atomic packing factor for a hypothetical form of CsCl assuming it adopts the rock salt (NaCl) structure type.
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 terms of bonding, explain why silicate materials have relatively low densities.
11. 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.