PHYS 446 Fall 2007 Homework Assignment 1 Due Sept 21
(5 problems)

1. a) Using Table 1.2 from Omar (below), calculate the densities of the following solids: Al, Fe, Zn, and Si. b) The density of NaCl is 2.16×10^3 kg/m^3. Calculate the unit cell parameter (the length of the edge of a cubic cell).

Table 1.2
Structures and Cell Dimensions of Some Elements and Compounds

Element or compound	Structure	a, Å	c, Å
Al	fcc	4.04	
Be	hcp	2.27	3.59
Ca	fcc	5.56	
C	Diamond	3.56	
Cr	bcc	2.88	
Co	hcp	2.51	4.07
Cu	fcc	3.61	
Ge	Diamond	5.65	
Au	fcc	4.07	
Fe	bcc	2.86	
Pt	fcc	3.92	
Si	Diamond	5.43	
Ag	fcc	4.08	
Na	bcc	4.28	
Zn	hcp	2.66	4.94
LiH	Sodium chloride	4.08	
NaCl	Sodium chloride	5.63	
AgBr	Sodium chloride	5.77	
MnO	Sodium chloride	4.43	
CsCl	Cesium chloride	4.11	
TlBr	Cesium chloride	3.97	
CuZn (β-brass)	Cesium chloride	2.94	
CuF	Zincblende	4.26	
AgI	Zincblende	6.47	
ZnS	Zincblende	5.41	
CdS	Zincblende	5.82	

2. Find the ratio *c/a* in ideal hexagonal close-packed (hcp) structure, where atomic spheres touch each other.

3. The *packing ratio* is defined as a fraction of the total volume of the unit cell that is filled by atoms. Determine the maximum values of the packing ratio for equal spheres located at the points of simple cubic, body-centered cubic, face-centered cubic, and hcp structures.

4. Determine, which planes in fcc and bcc structures have the highest density of atoms. Calculate this density for Cu and Fe, using the data from the Table 1.2 above.

5. In a quantitative theory of bonding in ionic crystals developed by Born and Meyer the potential energy of the system is taken to be

$$U(R) = -N\frac{\alpha e^2}{4\pi\varepsilon_0 R} + N\frac{A}{R^n}$$

where N is the number of positive-negative ion pairs, A and n are constants determined from experiment. The first term represents attractive Coulomb potential, where α, known as Madelung constant, depends only on the crystal structure of the solid.

a) Find the expression for the equilibrium interatomic distance as a function of A, n and α.

b) Determine the expression for the binding energy at equilibrium.

c) Calculate the constant n for NaCl, using the data from the Table 1.2 above and the fact that the measured binding energy is 7.95 eV per molecule (pair of ions). The Madelung constant for NaCl is 1.75.