MM 738 _ Physics of Materials

Assignment II

Tuesday 17 August 2021 **Due on 20 August 2021**

1. On the basis of ionic charge and ionic radii, predict the crystal structures for the following materials:
(a) CsI
(b) NiO
(c) KI, and
(d) NiS . Justify your selections

Ionic radii for several cations and anions (coordination number of 6)

Cation	*Ionic Radius* (*nm*)	*Anion*	*Ionic Radius* (*nm*)
Al^{3+}	0.053	Br^{-}	0.196
Ba^{2+}	0.136	Cl^{-}	0.181
Ca^{2+}	0.100	F^{-}	0.133
Cs^{+}	0.170	I^{-}	0.220
Fe^{2+}	0.077	O^{2-}	0.140
Fe^{3+}	0.069	S^{2-}	0.184
K^{+}	0.138		
Mg^{2+}	0.072		
Mn^{2+}	0.067		
Na^{+}	0.102		
Ni^{2+}	0.069		
Si^{4+}	0.040		
Ti^{4+}	0.061		

2. Compute the atomic packing factor for the Cesium chloride crystal structure in which $rC/rA = 0.732$.

3. Compute the theoretical density of diamond given that the C-C distance and bond angle are 0.154 nm and 109.5° respectively. How does this value compare with the measured density?

4. Cadmium sulfide (CdS) has a cubic unit cell, and from x-ray diffraction data it is known that the cell edge length is 0.582 nm. If the measured density is 4.82 g/cm^3, how many Cd^{2+} and S^{2-} ions are there per unit cell?

5. 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?

6. Explain why the properties of polycrystalline materials are most often isotropic.

7. In terms of bonding, explain why silicate materials have relatively low densities.