Week 9 Discussion Answers

1) Answer the following questions related to diamond.

a) Describe the structure of diamond and determine its density given that the C-C bond distance is 1.54 Å.

FCC lattice with 1/2 tetrahedral sites occupied. All carbon. 8 carbons per unit cell.

$$C\text{-}C = 1.54\text{Å} = \frac{1}{4} a\sqrt{3}$$

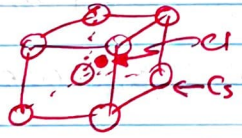
$$a = \frac{4(1.54)}{\sqrt{3}} = \boxed{3.56\text{ Å}}$$

Comes from C-C on the diagonal of cube since tetrahedral site occupied.

b) Draw a band structure of diamond.

2) If the unit edge-cell in CsCl is 4.1 Å, what is the Cs-Cl bond length?

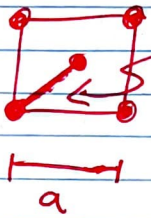
CsCl is simple cubic with Cl^- in center



Diagonal is $\sqrt{3}a \Rightarrow$ Cs-Cl is $\frac{\sqrt{3}}{2}a$

$$\boxed{CsCl \sim 3.55\text{ Å}}$$

b) If the Ag-Ag bond distance, is 2.54 Å, What is the length of the unit cell edge of silver? Assume FCC lattice.



$Ag\text{-}Ag \Rightarrow 2.54\text{ Å} = \frac{1}{2} a\sqrt{2}$

$\boxed{a \sim 3.59\text{ Å}}$

3) Solid Xenon is known to be very malleable and therefore used for matrix isolation experiments. Given that Xenon forms a close-packed structure with density 5.9 g/cm³, determine the ~~diameter~~ radius of a Xenon atom.

$\frac{5.9\text{ g}}{\text{cm}^3} = \frac{\text{mass}}{a^3}$

FCC ⇒ malleable

So, Xe ~~diameter~~ radius is $\frac{1}{2} a\sqrt{2}$

$a^3 = \frac{4\text{ atoms}}{\text{unit cell}} \times \frac{131.3\text{ g}}{\text{mol}} \times \frac{1\text{ mol}}{6.02\times10^{23}\text{ atoms}} \times \left(\frac{1\text{ Å}}{10^{-8}\text{ cm}}\right)^3$

$a = 5.29\text{ Å} \Rightarrow$ 3.74 Å is Xe ~~diameter~~ radius

4) Answer the following questions related to $RhBr_2$.

a) Describe the structure of $RhBr_2$ in terms of close-packing given that the radii of Rh^{2+} and Br^- are 160 pm & 50 pm respectively.

$\frac{r_+}{r_-} = \frac{160}{50} > 1 \Rightarrow \frac{r_-}{r_+} = 0.3125 \Rightarrow$ Tetrahedral for anion

1:2 compound ⇒ all tetrahedral sites occupied. Similar to fluorite.

So Rh^{2+} FCC with Br^- in all tetrahedral sites

b) Given that the average rhodium bromine bond length is 3.13 Å, determine the length of the unit cell of $RhBr_2$ in angstroms.

$a = \frac{4\,R(Rh\text{-}Br)}{\sqrt{3}}$ since,

$\frac{\sqrt{3}}{4}a$ gives the bond length

$\boxed{a = 7.23\ \text{Å}}$

c) Determine the density of $RhBr_2$ in g/cm^3.

$$\rho = \frac{1.66 \times 4 \times 262.7}{(7.23)^3} = \boxed{4.62\ \frac{g}{cm^3}}$$

5) a) Describe the structure of rock salt.
NaCl, all Octahedral sites filled with Cl^-
So, Cl^- in FCC lattice with Na^+ in all octahedral sites.

b) Describe the structure of zinc blende.
Anions in FCC lattice and cation in ½ tetrahedral holes.

c) Describe the structure of Cesium Chloride.
Anion in simple cubic and cubic hole filled with cation.

6) Consider NaCl.
a) Sodium atoms are larger than chlorine atoms; however as can be seen, sodium ions are smaller than Chloride ions. Why do you think this is?

$Na^+ \Rightarrow$ smaller ion, $Cl^- \Rightarrow$ larger. So sheilding plus nuclear charge $\Rightarrow Na^+ < Cl^-$ in regard to radii.

b) Identify whether the unit cell is cubic, BCC, or FCC.
FCC lattice of Cl.

c) How many Cl^- are in each unit cell?
$\frac{1}{8}(8) + \frac{1}{2}(6) = 1+3 = \boxed{4}$

d) How many Na^+ are present in each unit cell?
$\boxed{4}$
$\frac{1}{4}(12) + 1(1) = 3+1 = 4$

e) Are your answers consistent with the molecular formula?
Yes. $4:4 \Rightarrow 1:1$

Molecular formula is 1:1 - So all good?

7) Nickel has an FCC structure with density $8.90\ g/cm^3$.
a) Calculate the ~~nearest neighbor~~ nearest neighbor distance in crystalline nickel.

$$V = N_a a^3 = \frac{4(58.69\ g/mol)}{8.90\ g/cm^3}$$

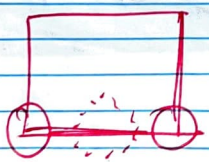
$$\Rightarrow a = 3.525 \times 10^{-8}\ cm$$

$$d = \frac{\sqrt{2}}{2} a = \boxed{2.49 \times 10^{-8}\ cm}$$

b) What is the atomic radii of nickel?
Across diagonal of the face.
$\frac{\sqrt{2}\,a}{4} = \boxed{1.25 \times 10^{-8}\ cm}$

c) What is the radius of the largest atom that could fit into the interstices of the nickel lattice?

Octahedral sites the largest



$\frac{a}{2} = R(Ni) + r \Rightarrow$

$\boxed{\frac{a}{2} - \frac{\sqrt{2}a}{4}}$ is largest radius.
$\approx \boxed{0.280 \times 10^{-8}\ cm}$