NPRE 330 Hw 2

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The code for this homework can be found on GitHub at:
https://github.com/jspecht3/uiuc_classes/tree/main/npre330/hw2

1 Crystal Structure of Compounds I

To find the crystal structure for an AX compound, we first need to:

1. find the ionic radii of the cation and anion from Table 12.3,
2. then calculate the ratio of cation radius to anion radius,
3. find the coordination number corresponding to the ratio from Table 12.2,
4. use the coordination number to find the structure name and anion packing from table 12.4.

Doing the above steps for all given AX compounds: CaO, MnS, KBr, CsBr, 457generates the following results, which have been tabulated for ease of comparison.

Table 1: Question 1 Results

	Ionic Species		**Ionic Radii**			**Crystal Structure**		
	Cation	**Anion**	r_c **[nm]**	r_a **[nm]**	$r_c \div r_a$	**CN**	**Type**	**Anion Packing**
CaO	Ca	O	0.1	0.14	0.714	6	Rock Salt (NaCl)	FCC
MnS	Mn	S	0.067	0.184	0.364	4	Zinc Blende (Sphalerite)	FCC
KBr	K	Br	0.138	0.196	0.704	6	Rock Salt (NaCl)	FCC
CsBr	Cs	Br	0.17	0.196	0.867	8	Cesium Chloride	SC

The only argument that I can use to justify these selections is an appeal to authority as I used Callister for the references.

2 Crystal Structure of Compounds II

Below are the steps to find the atomic packing factor of Al_2O_3 given a = 0.4759 nm, c = 1.2989 nm, and $\rho = 3.99\ g/cm^3$.

1. Get the radii from Table 12.3: $r_{Al} = 0.053 \cdot 10^{-7}\ cm$ and $r_O = 0.140 \cdot 10^{-7}\ cm$.

2. Calculate the volume of a unit cell from the equation we derived in the first homework:

$$V_C = \frac{3^{3/2}a^2c}{2} = 7.643 \cdot 10^{-22}\ cm^3 \tag{1}$$

3. Get the atomic densities of Al and O from google: $M_{Al} = 29.98\ g/mol$ and $M_O = 16.00\ g/mol$.

4. Use Callister Eq. 12.1 to find the number of formula units, n' per unit cell.

$$\rho = \frac{n'\left(\Sigma A_c + \Sigma A_a\right)}{N_A V_C} \longrightarrow n' = \frac{\rho N_A V_C}{\Sigma A_c + \Sigma A_a} = 18.011\ molecules/cell \tag{2}$$

5. Find the volumes of Al and O assuming they are spheres.

$$V_{Al} = \frac{4}{3}\pi r_{Al}^3 = 6.235 \cdot 10^{-25}\ cm^3 \tag{3}$$

$$V_O = \frac{4}{3}\pi r_O^3 = 1.149 \cdot 10^{-25}\ cm^3 \tag{4}$$

6. Use Eq. 2, 3, and 4 to find the volume of atoms in a unit cell.

$$V_f = n'\left(2V_{Al} + 3V_O\right) = 6.435 \cdot 10^{-22}\ cm^3 \tag{5}$$

7. Take the ratio of Eq. 1 and 5 to find the atomic packing factor.

$$APF = \frac{V_f}{V_C} = 0.842 \tag{6}$$

3 Crystal Structure of Compounds III

3.a

To find the unit cell length of LiF, do the following steps.

1. Find the molar mass of Li^+ and F^-: $M_{Li} = 6.941\ g/mol$ and $M_F = 18.998\ g/mol$.

2. Sum the two molar masses to find the molar mass of LiF $= 25.939\ g/mol$

3. Start with a formula for density and solve for the edge length.

$$\rho = \frac{ZM_{LiF}}{a^3 N_A} \longrightarrow a = \left(\frac{ZM_{LiF}}{\rho N_A}\right)^{\frac{1}{3}} = 0.40467\ nm. \tag{7}$$

   Where Z is the number of molecules in the FCC, which is 4.

3.b

To find the density of BeF_2 assuming a fluorite crystal structure with $r_{F^-} = 0.133$ nm and $r_{Be^{2+}}$, do the following steps.

1. Assume in the unit cell, the diagonal from the corner to opposite corner, d, is 4 r_F + 4 r_{Be}.

$$d = 4r_{F^-} + 4r_{Be^{2+}} \tag{8}$$

2. Find the side length, a, corresponding to that diagonal. The side length, a, is half the diagonal as the cube diagonal is $\sqrt{2}$ times the square diagonal, which is $\sqrt{2}$ times the side length.

$$a = \frac{d}{2} = 3.56 \cdot 10^{-8}\ cm \tag{9}$$

3. Find the molar mass of BeF_2.

$$M_{BeF_2} = M_{Be} + 2M_F = 47.01\ g/mol \tag{10}$$

4. Use the formula for density in Eq. 7.

$$\rho = \frac{ZM_{BeF_2}}{a^3 N_A} = 6.921\ g/cc \tag{11}$$

This is 3.5 times higher than the actual density of 1.99 g/cm^3. The discrepancy is from the assumption that BeF_2 has a fluorite crystal structure, which is not true as it has a trigonal structure.

The packing fractions of BCC, which is the assumed fluorite structure, has an APF of 0.68 while the true BeF_2 structure, trigonal, has an APF of 0.52, which accounts for some discrepancy, but not the amount I have. The expected value for this problem would be 2.5 g/cm^3

4 X-ray Diffraction

4.a

To determine the index, we use the fact that the sum of the lattice parameters $h+k+l$ is even. We also assume the first peak corresponds to $n = 1$ and each subsequent peak increases n by 1. To determine the peak corresponding to the correct index, take $\sqrt{h^2+k^2+l^2}$ – the lower the norm, the lower the order.

Table 2: Indices for each Peak

Peak n:	**1**	**2**	**3**	**4**	**5**
2 θ [deg]	40	59	73	86	101
Indices (h k l)	(1 1 0)	(2 0 0)	(2 1 1)	(2 2 0)	(3 1 0)

4.b

To find the interplanar spacing, use Bragg's law and solve for d.

$$n\lambda = 2d\sin\theta \longrightarrow d = \frac{n\lambda}{2\sin\theta} \tag{12}$$

4.c

To find the radius of W, do the following steps.

Table 3: Interplanar spacing for each Peak

Peak n:	**1**	**2**	**3**	**4**	**5**
2 θ [deg]**:**	40	59	73	86	101
d [nm]	0.225	0.313	0.389	0.452	0.500

1. Take the interplanar distance and multiply it by the norm of the index to find the edge length of a BCC cell (Eq. 3.22).

$$a = \frac{d}{\sqrt{h^2 + k^2 + l^2}} \tag{13}$$

2. Use Eq. 3.4 to find the radius.

$$R = \frac{a\sqrt{3}}{4} \tag{14}$$

3. Normalize by n as each "unit cell" is really n unit cells joined together.

$$R_W = R/n \tag{15}$$

Table 4: Interplanar spacing for each Peak

Peak n:	**1**	**2**	**3**	**4**	**5**
2 θ [deg]**:**	40	59	73	86	101
a [nm]	0.319	0.626	0.952	1.279	1.580
$\mathbf{R}_W$ **[nm]**	0.138	0.136	0.137	0.138	0.137