PHYS 321 F2019 Test #2 Name: Key

Braggs's Law	Inter-planar Spacing	Hydrogen Like Spectra ($R = 1.097 \times 10^7\ m^{-1}$)
$2d_{hkl}Sin\theta = n\lambda$	$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$	$\frac{1}{\lambda} = RZ^2\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

1. The 2Θ values in degrees for first order diffraction peaks are given below for a metal with cubic structure, using X-rays from Cu-K_α radiation (Z = 29): 36.3, 42.2, 61.6, 73.6.

(a) Determine the wavelength of the X-rays used.

$\frac{1}{\lambda} = RZ^2\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$\frac{1}{\lambda} = 1.097\times10^7 \times (29-1)^2\left(\frac{1}{1^2} - \frac{1}{2^2}\right) = 1.097\times10^7 \times 28^2 \times \frac{3}{4}$

$\frac{1}{\lambda} = 6.45\times10^9\ m^{-1} \Rightarrow \lambda = 1.55\times10^{-10}\ m = 0.155\ nm$

(b) Derive an expression for $\frac{Sin^2\theta}{h^2+k^2+l^2}$.

$2d_{hkl}Sin\theta = n\lambda$

$2\cdot\frac{a}{\sqrt{h^2+k^2+l^2}}\cdot Sin\theta = \lambda \Rightarrow \frac{4a^2\cdot Sin^2\theta}{(h^2+k^2+l^2)} = \lambda^2$

$\frac{Sin^2\theta}{(h^2+k^2+l^2)} = \frac{\lambda^2}{4a^2}$

(c) Complete the table below.

2θ (deg.)	θ	$Sin^2\theta$	Normalize	Clear Fractions	$h^2+k^2+l^2$	(hkl)	$\frac{Sin^2\theta}{h^2+k^2+l^2}$
36.3	18.15	0.09704	1	3	3	111	0.03235
42.2	21.1	0.1296	1.33	4	4	200	0.0324
61.6	30.8	0.2622	2.70	8	8	220	0.0328
73.6	36.8	0.3588	3.697	11	11	311	0.0326

(d) Determine the crystal structure. FCC, since (hkl) → odd or even Ave = 0.0325

(e) Determine the lattice constant.

(f) Determine the atomic radius.

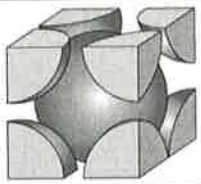
(e) $\frac{\lambda^2}{4a^2} = 0.0325 \Rightarrow a^2 = \frac{\lambda^2}{4\times0.0325} \Rightarrow a = \sqrt{\frac{0.155^2}{4\times0.0325}}$

$a = 0.430\ nm$

(f) $\sqrt{2}\,a = 4R$

$R = \frac{\sqrt{2}a}{4} = \frac{\sqrt{2}\times0.430}{4} = 0.152\ nm$

$R = 0.152\ nm$

$\rho_{ave} = \dfrac{100}{\dfrac{C_1}{\rho_1} + \dfrac{C_2}{\rho_2}}$	$A_{ave} = \dfrac{100}{\dfrac{C_1}{A_1} + \dfrac{C_2}{A_2}}$	

2. Calculate the unit cell edge length for an 85 wt% Fe-15 wt% V alloy. All of the vanadium is in solid solution, and, at room temperature the crystal structure for this alloy is BCC. The room-temperature density of Fe is 7.87 g/cm^3, and its atomic weight is 55.85 g/mol. The room-temperature density of V is 6.10 g/cm^3, and its atomic weight is 50.94 g/mol.

$$\rho_{ave} = \frac{100}{\frac{85}{7.87} + \frac{15}{6.10}} = 7.54\ g/cm^3$$

$$A_{ave} = \frac{100}{\frac{85}{55.85} + \frac{15}{50.94}} = 55.05\ g/mol$$

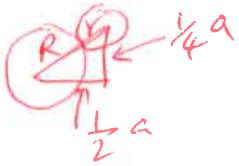
$$\rho = \frac{M}{V} \Rightarrow V = \frac{M}{\rho} = a^3 \Rightarrow a = \sqrt[3]{\frac{2 \times 55.05 / 6.022 \times 10^{23}}{7.54}} = \left(2.42 \times 10^{-23}\ cm^3\right)^{1/3}$$

$$a = 2.89 \times 10^{-8}\ cm$$

$$a = 0.289 \times 10^{-7}\ cm$$

$$a = 0.289\ nm$$

3. Compute the radius r of an impurity atom that just fits into a BCC tetrahedral interstitial site in terms of the atomic radius R of the host atom (without introducing lattice strains).



$$(R+r)^2 = \left(\frac{1}{2}a\right)^2 + \left(\frac{1}{4}a\right)^2$$

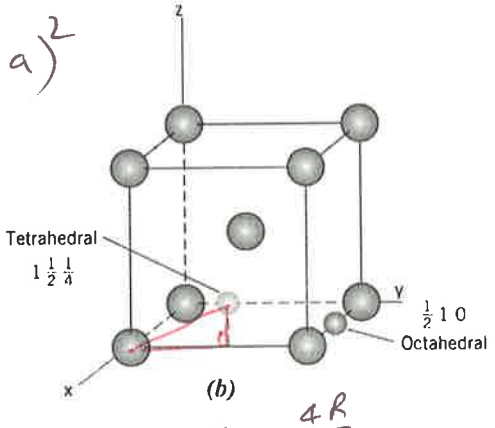
$$= \frac{a^2}{4} + \frac{a^2}{16}$$

$$(R+r)^2 = \frac{5a^2}{16}$$

$$(R+r)^2 = \frac{5}{16} \times \frac{16R^2}{3}$$

$$R + r = \sqrt{\frac{5}{3}} \cdot R = 1.291R$$

$$r = 0.291R$$



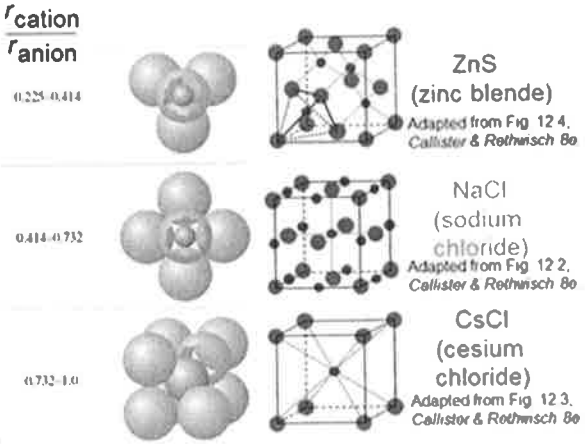
(b)

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

$$a^2 = \frac{16R^2}{3}$$

Table 12.3 Ionic Radii for Several Cations and Anions (for a 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		



4. On the basis of ionic charge and ionic radii given, predict crystal structures for the following materials: *(a) CaO* *(b) MnS* *(c) CsBr* *(d) MgO*

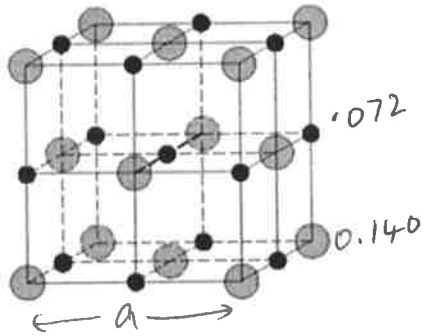
$\frac{r_c}{r_a} = \frac{0.1}{0.14} = 0.714$ NaCl structure

$\frac{r_c}{r_a} = \frac{0.067}{0.184} = 0.364$ ZnS structure

$\frac{r_c}{r_a} = \frac{0.170}{0.196} = 0.867$ CsCl structure

$\frac{r_c}{r_a} = \frac{0.072}{0.140} = 0.514$ NaCl structure

5. Determine the density and atomic packing factor of MgO: (atomic masses, Mg = 24.3 and O = 16.0)



$a = 2r + 2R = 2(0.072 + 0.140)$

$\rho = \frac{n}{V} = \frac{4(24.3+16)/6.02\times10^{23}}{[2(0.072+0.140)]^3 \times 10^{-21}}$ g/cm³

$\rho = 3.51$ g/cm³

$APF = \frac{4\left[\frac{4}{3}\pi(0.072^3) + \frac{4}{3}\pi(0.140^3)\right]}{[2(0.072+0.140)]^3} = \frac{0.05223}{0.0762} = 0.69$

APF = 0.69

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

6. The following electrical characteristics have been determined for both intrinsic and p-type extrinsic gallium antimonide (GaSb) at room temperature:

	$\sigma\ (\Omega\cdot m)^{-1}$	$n\ (m^{-3})$	$p\ (m^{-3})$
Intrinsic	8.9×10^4	8.7×10^{23}	8.7×10^{23}
Extrinsic (p-type)	2.3×10^5	7.6×10^{22}	1.0×10^{25}

Calculate electron and hole mobilities.

$8.9 \times 10^4 = 1.6 \times 10^{-19} (8.7 \times 10^{23})(\mu_e + \mu_h)$

$\frac{8.9 \times 10^4}{1.6 \times 10^{-19} \times 8.7 \times 10^{23}} = \mu_e + \mu_h = 0.6394$

$2.3 \times 10^5 = 1.0 \times 10^{25} \times 1.6 \times 10^{-19} \times \mu_h$

$\frac{2.3 \times 10^5}{1.6 \times 10^6} = \mu_h = 0.14$

$\mu_e = 0.49$

7. Germanium to which 5×10^{22} m^{-3} Sb atoms have been added is an extrinsic semiconductor at room temperature, and virtually all the Sb atoms may be thought of as being ionized (i.e., one charge carrier exists for each Sb atom).

↑ valence 5

(a) Is this material n-type or p-type?

(b) Calculate the electrical conductivity of this material, assuming electron and hole mobilities of 0.1 and 0.05 $m^2/V\text{-}s$, respectively.

$\sigma = n e \mu_e$, extrinsic, electrons are dominant carriers.

# of holes are negligible.

$\sigma = 5 \times 10^{22} \times 1.6 \times 10^{-19} \times 0.1$

$\sigma = 800\ (\Omega\cdot m)^{-1}$