PHYS 321 S 2016 Test #1 Name: KEY

A. The net potential energy between two adjacent ions, E_N, may be represented by:

$$E_N = -\frac{A}{r} + \frac{B}{r^n}$$

Calculate the equilibrium inter-ionic spacing, r_0 and the bonding energy E_0 in terms of the parameters A, B, and n.

$$E_N = -\frac{A}{r} + \frac{B}{r^n}$$

$$E_N = -Ar^{-1} + Br^{-n}$$

$$\frac{dE_N}{dr} = Ar^{-2} - Bnr^{-n-1} = 0$$

$$Ar_0^{-2} - Bnr_0^{-(n+1)} = 0$$

$$\frac{A}{r_0^2} = Bn \cdot r_0^{-(n+1)}$$

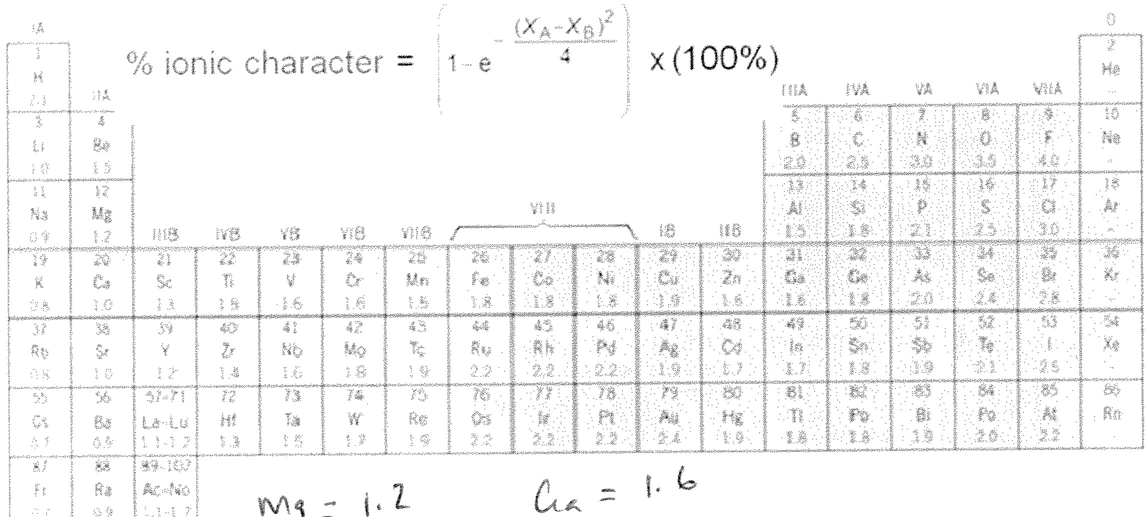
$$\frac{A}{nB} = r_0^{2-n-1} = r_0^{1-n}$$

$$\boxed{r_0 = \left(\frac{A}{nB}\right)^{\frac{1}{1-n}}}$$

$$\boxed{E_0 = \frac{-A}{\left(\frac{A}{nB}\right)^{\frac{1}{1-n}}} + \frac{B}{\left(\frac{A}{nB}\right)^{\frac{n}{1-n}}}}$$

B. Compute the percent ionic character of the inter-atomic bonds for the following compounds: MgO and GaAs. The electronegativity values are given below.

$$\%\text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\%)$$



Mg = 1.2 Ga = 1.6

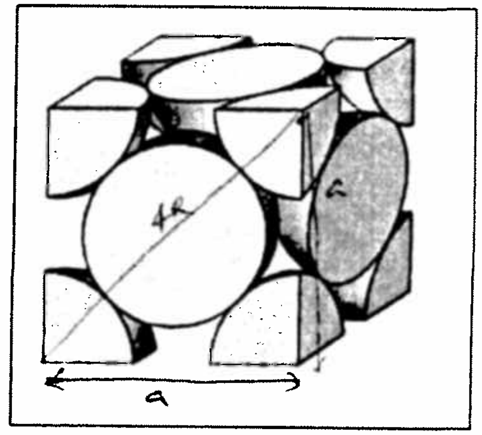
O = 3.5 As = 2.0

$$\text{MgO } \%\text{IC}: = \left(1 - e^{-\frac{(1.2-3.5)^2}{4}}\right) \times 100\% = 73.35 \simeq 73\%$$

$$\text{GaAs } \%\text{IC} = \left(1 - e^{-\frac{(1.6-2.0)^2}{4}}\right) \times 100\% = 3.9\%$$

C. The unit cell for the face-centered cubic crystal structure is shown below.

1. Show that the cube edge length, a and the atomic radius, R are related by: $a = 2R\sqrt{2}$



$a^2 + a^2 = (4R)^2$

$2a^2 = 16R^2$

$a^2 = 8R^2$

$a = \sqrt{8}\,R = \sqrt{4\times2}\cdot R$

$\boxed{a = 2\sqrt{2}\,R}$

2. Show that the atomic packing factor is 0.74 for FCC. ← 4 atom/unit cube.

$$APF = \frac{\text{Volume of atoms}}{\text{Volume of the cube}} = \frac{4\times\frac{4}{3}\pi R^3}{a^3} = \frac{\frac{16}{3}\pi R^3}{(2\sqrt{2}R)^3} = \frac{16\pi}{3(2\sqrt{2})^3}$$

$$= 0.74$$

3a. Calculate the atomic radius of a lead atom, given that Pb has a FCC crystal structure, a density of 11.35 g/cm³, and an atomic weight of 207.2 g/mol.

$\rho = \frac{M}{V} = 11.35\ g/cm^3$ Mass of a lead atom $= \frac{207.2\ g}{6.022\times10^{23}} = 3.44\times10^{-22}\ g$

Volume of a unit cube $= V = \frac{M}{\rho} = \frac{4\times3.44\times10^{-22}}{11.35}\ cm^3 = 1.212\times10^{-22}\ cm$

$a = (V)^{1/3} = 4.95\times10^{-8}\ cm$

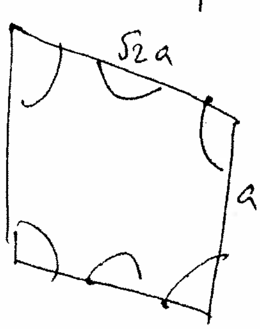
$R = \frac{a}{2\sqrt{2}} = 1.75\times10^{-8}\ cm = \underline{0.175\ nm}$

3b. Calculate the planar density for (110) planes in lead.

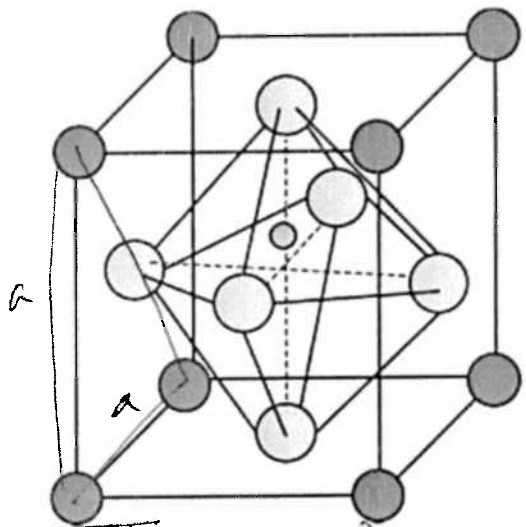
$$\text{planar density} = \frac{\#\text{ of atoms}}{\text{area of plane}} = \frac{2}{a\cdot\sqrt{2}a} = \frac{2}{\sqrt{2}\cdot a^2} = \frac{2}{\sqrt{2}\cdot 8R^2}$$

$$= \frac{1}{4\sqrt{2}\,R^2} = \frac{1}{4\sqrt{2}\,(0.175\ nm)^2}$$

$$= 5.77\ nm^{-2}$$



D. Determine the density of $CaTiO_2$. Ionic radius: Ca = 0.100 nm, O = 0.140 nm, and Ti = 0.068 nm. Atomic masses: Ca = 40.08, O = 16, Ti = 47.87



	m	r
Ca^{2+}	40.08	0.100
O^{2-}	16	0.140
Ti^{4+}	47.87	0.068

$$\rho = \frac{m}{V} = \frac{\left[(40.08 + 3\times 16 + 47.87)/6.022\times10^{23}\right] g}{(0.3394\times10^{-7})^3\ cm^3}$$

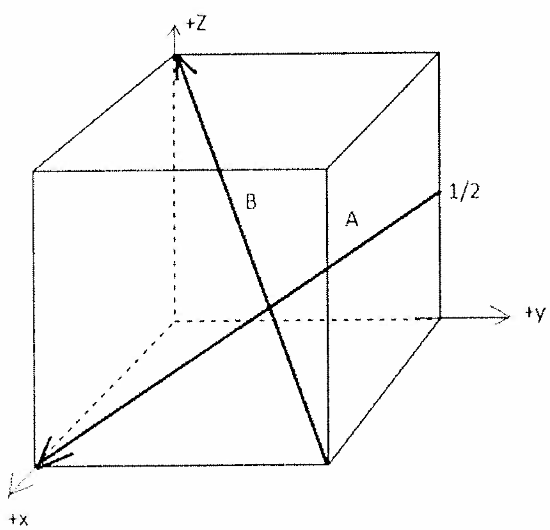
$$\sqrt{a^2+a^2} = 2(r_{Ca}+r_o)$$

$$\sqrt{2}\,a = 2(0.100+0.140)$$

$$a = 0.3394\ nm$$

$$\boxed{\rho = 5.77\ g/cm^3}$$

E. What are the indices for the directions shown, A and B within a cubic unit cell?



A: Tip: 1 0 0
Tail: − 0 1 $\frac{1}{2}$

1 −1 $-\frac{1}{2}$

2 −2 −1

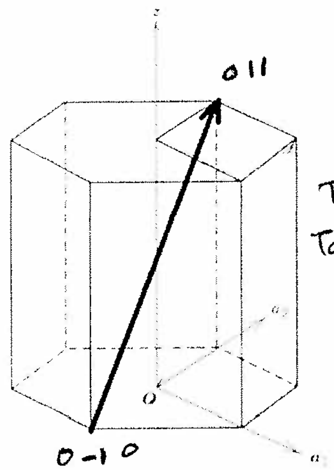
$[2\bar{2}\bar{1}]$

B. Tip: 0 0 1
Tail: − 1 1 0

−1 −1 1

$[\bar{1}\bar{1}1]$

F. Determine the 3-axis indices and then convert them to 4-axis indices for the directions shown.



$$[u'v'w'] \rightarrow [uvtw]$$

$$u = \frac{1}{3}(2u'-v')$$

$$v = \frac{1}{3}(2v'-u')$$

$$t = -(u+v)$$

$$w = w'$$

Tip 011
Tail − 0-10

0 +2 1

[021]

$u' = 0$
$v' = 2$
$w' = 1$

$u = \frac{1}{3}(2\times 0 - 2) = -\frac{2}{3}$

$v = \frac{1}{3}(4 - 0) = \frac{4}{3}$

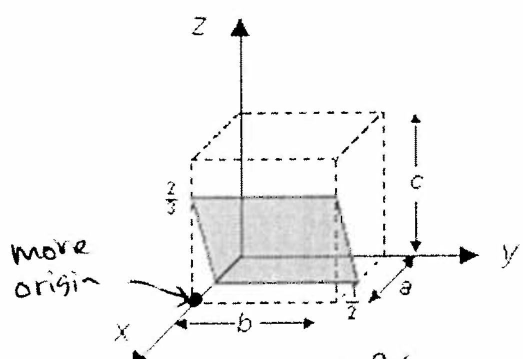
$t = -(u+v) = -(-\frac{2}{3}+\frac{4}{3}) = -\frac{2}{3}$

$w = w' = 1$

$[u\,v\,t\,w] = -\frac{2}{3}\ \frac{4}{3}\ -\frac{2}{3}\ 1$

$[\bar{2}\ 4\ \bar{2}\ 3]$

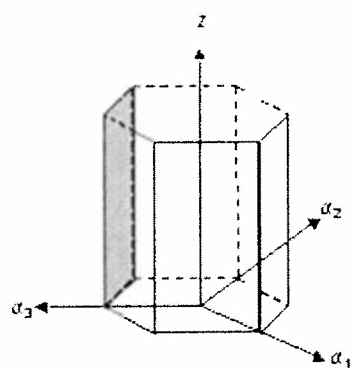
G. What are the Miller indices for the planes shown below?



$-\frac{1}{2}\ \infty\ \frac{2}{3}$

$-2\ 0\ \frac{3}{2}$

$(\bar{4}\ 0\ 3)$



$-1\ \infty\ 1\ \infty$

$-1\ 0\ 1\ 0$

$(\bar{1}\ 0\ 1\ 0)$

H. X-ray Diffraction:

Bragg=s law: $2d_{hkl}Sin\theta = n\lambda$ $\qquad$ $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$.

Additional Conditions: BCC: $h+k+l$=even $\qquad$ FCC: h,k,l either odd or even

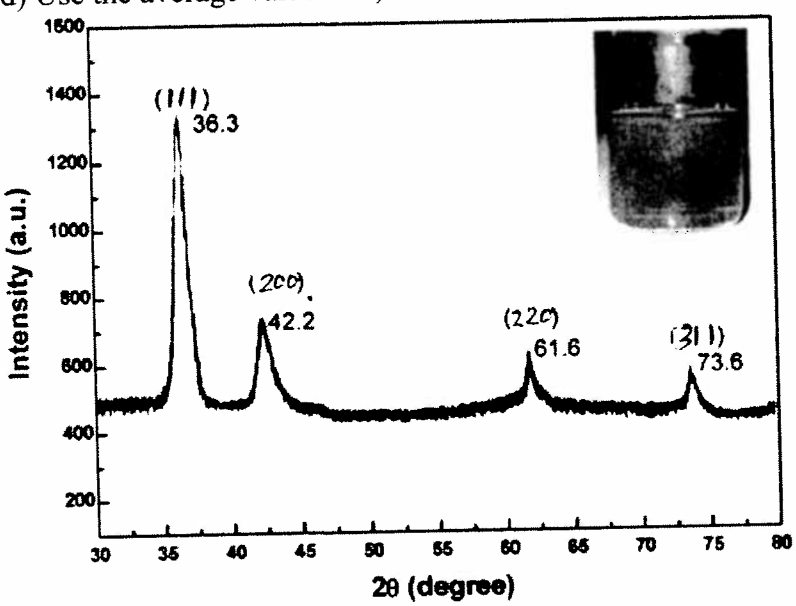
1. Figure below shows the first four peaks of the first order x-ray diffraction pattern for Cu_2O nanoparticles, which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

(a) Index (i.e., give h, k, and l indices) for each of these peaks, inside the parenthesis.

(b) Determine the interplanar spacing for each of the peaks.

(c) For each peak, determine the lattice constant, *a*.

(d) Use the average value of a, to calculate the diffraction angle for the next peak. (222)



$d_{hkl} = \dfrac{\lambda}{2\sin\theta} = \dfrac{0.1542}{2\sin\theta}$

$d_{111} = \dfrac{0.1542}{2\sin(\frac{36.3}{2})} = 0.2475\text{ nm} \longrightarrow a_{111} = d_{111}\cdot\sqrt{1^2+1^2+1^2}$

$= 0.2475\times\sqrt{3} = 0.4287$ n.

$d_{200} = \dfrac{0.1542}{2\sin(\frac{42.2}{2})} = \longrightarrow a_{200} = d_{200}\times\sqrt{2^2} = 0.4283$ nm

$a_{220} = \dfrac{0.1542}{2\sin(\frac{61.6}{2})}\times\sqrt{2^2+2^2+0} = 0.4259$ nm

$a_{311} = \dfrac{0.1542}{2\sin(\frac{73.6}{2})}\times\sqrt{3^2+1^2+1^2} = 0.4269$ nm

$a_{ave} = 0.4274$

(d) $d_{222} = \dfrac{0.42745}{\sqrt{2^2+2^2+2^2}}$

$d_{222} = 0.1234$ nm

$\sin\theta = \dfrac{\lambda}{2d_{222}} = \dfrac{0.1542}{2\times0.1234} = 0.6248$

$\theta = 38.67$

$\boxed{2\theta = 77.3^{\circ}}$