PHYS 321 S 2022 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.

$$E_N = -\frac{A}{r} + \frac{B}{r^n} = -Ar^{-1} + Br^{-n}$$

To find $\underline{r_0}$:

$$\frac{dE_N}{dr} = (-1)(-A)r^{-2} - nBr^{-n-1} = 0$$

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

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

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

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

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

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

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

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1																	2 He -
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne -
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar -
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr -
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe -
55 Cs 0.7	56 Ba 0.9	57-71 La-Lu 1.1-1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn -
87 Fr 0.7	88 Ra 0.9	89-102 Ac-No 1.1-1.7															

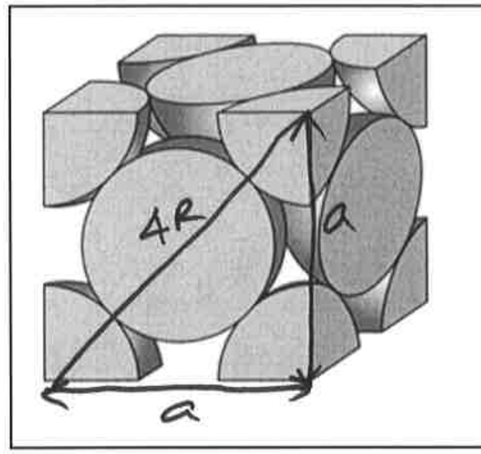
Mg = 1.2 Ga = 1.6

O = 3.5 As = 2.0

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

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

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: $a = 2R\sqrt{2}$

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

$2a^2 = 16R^2$

$a^2 = 8R^2$

$a = \sqrt{8}\,R = 2\sqrt{2}\,R$

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

2. Show that the atomic packing factor is 0.74 for FCC.

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

$$APF = \frac{16\pi}{3(2\sqrt{2})^3} = \underline{\underline{0.74}}$$

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

$\rho = \frac{M}{V} = 11.35 \frac{g}{cm^3}$ mass of a lead atom $= \frac{207.2}{6.022 \times 10^{23}} = 3.44 \times 10^{-22}\,g$

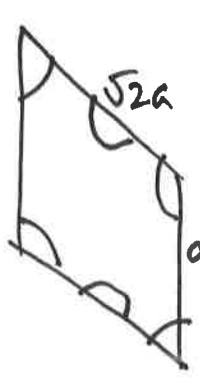
Volume of a unit cube $= \frac{M}{\rho} = \frac{4 \times 3.44 \times 10^{-22}}{11.35} = 1.212 \times 10^{-22}\,cm^3$

$a = (V)^{1/3} = (0.1212 \times 10^{-21})^{1/3} = 0.495 \times 10^{-7}\,cm$

$a = 0.495\,nm$

$R = \frac{a}{2\sqrt{2}} = \frac{0.495}{2\sqrt{2}} = \underline{\underline{0.175\,nm}}$

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



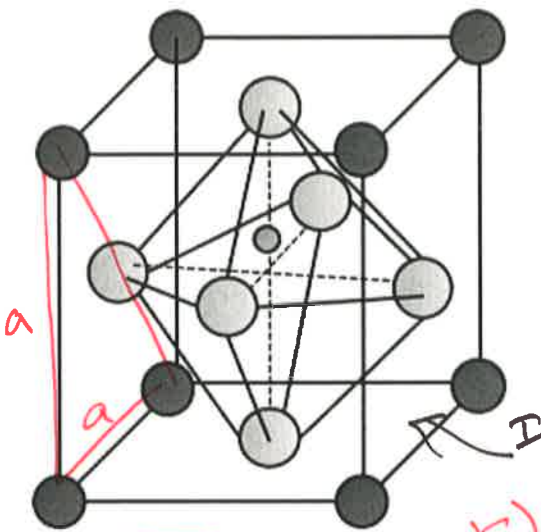
$$\text{planar density}_{(110)} = \frac{\#\text{ of atoms}}{\text{area of plane}}$$

$$= \frac{2}{a \cdot \sqrt{2}a} = \frac{2}{\sqrt{2}a^2} = \frac{2}{\sqrt{2} \cdot 4 \times 2R^2}$$

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

$$PD_{(110)} = 5.77\,nm^{-2}$$

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

Inside 1 Ca^{2+}, 3 O_2^-, 1 Ti^{4+}

$$\rho = \frac{m}{V} = \frac{[40.08 + 3\times16 + 47.87]}{6.022\times10^{23}\times[0.3394\times10^{-7}]^3}$$

$$\rho = 5.77\ \frac{g}{cm^3}$$

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

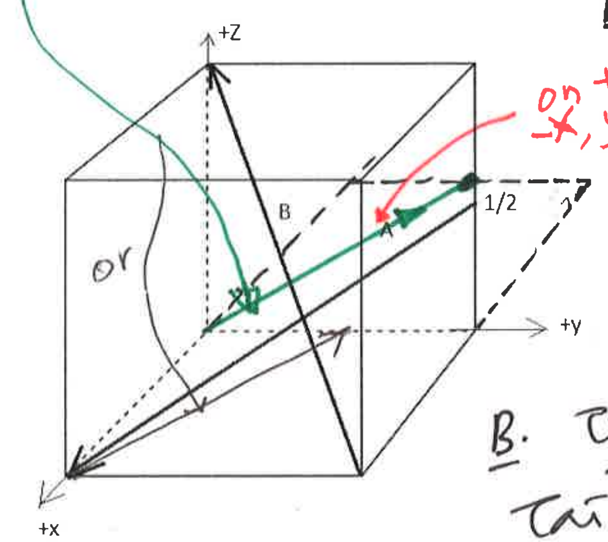
$$\sqrt{2}\,a = 2(0.100+0.140)$$

$$a = \sqrt{2}\times0.240$$

$$a = 0.3394\ nm$$

$$a = 0.3394\times10^{-7}\ cm$$

E. 1. What are the indices for the directions shown, A and B within a cubic unit cell?
2. Draw the direction [$\bar{2}$10].



on the -x, y Plane

A Tip: 1 0 0
Tail: 0 1 ½

1 −1 −½

2 −2 −1

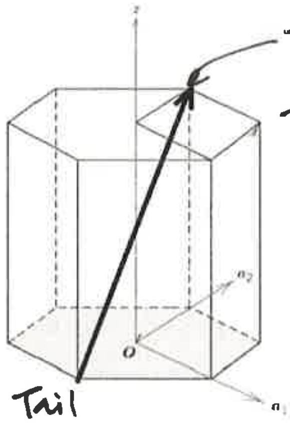
[2 $\bar{2}$ $\bar{1}$]

B. Tip: 0 0 1
Tail +1 1 0

−1 −1 1

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

F. 1. Determine the 3-axis indices and then convert them to 4-axis indices for the directions shown.



Tip: 0 1 1
Tail: 0 -1 0
0 2 1
[0 2 1]
u' = 0
v' = 2
w' = 1

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

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

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

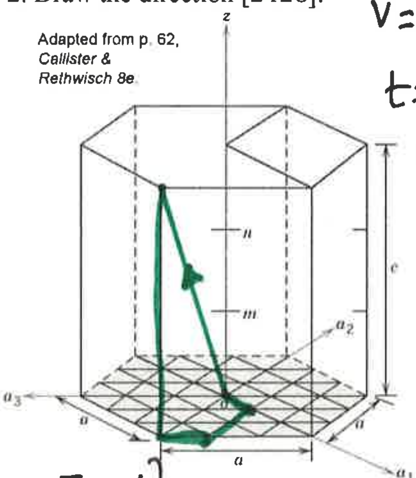
$$t = -(u + v)$$

$$w = w'$$

$u = \frac{1}{3}(2 \times 0 - 2) = -2/3$
$v = \frac{1}{3}(2 \times 2 - 0) = 4/3$
$t = -(-2/3 + \frac{4}{3}) = -2/3$
$w = w' = 1$
$[u\,v\,t\,w] = -2/3 \;\; \frac{4}{3} \;\; -\frac{2}{3} \;\; 1$
$[\bar{2}\,4\,\bar{2}\,3]$

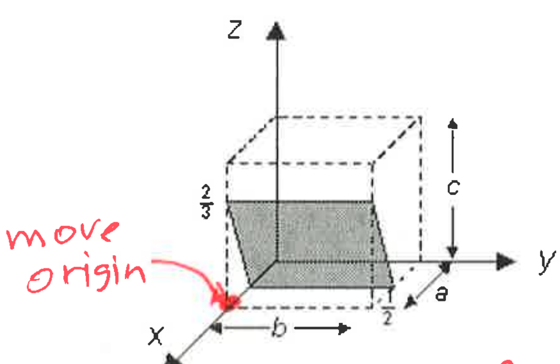
2. Draw the direction [2$\bar{4}$26].

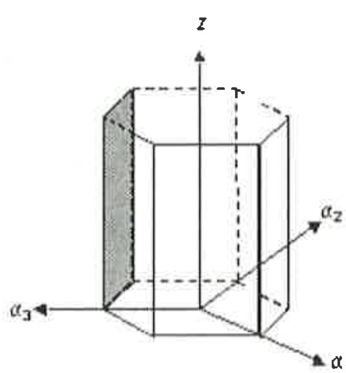
Adapted from p. 62, Callister & Rethwisch 8e.



$[2\bar{4}26]$
$\div 6$ $\frac{2}{6}$ $-\frac{4}{6}$ $\frac{2}{6}$ $\frac{6}{6}$
$1/3$ $-2/3$ $1/3$ 1

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





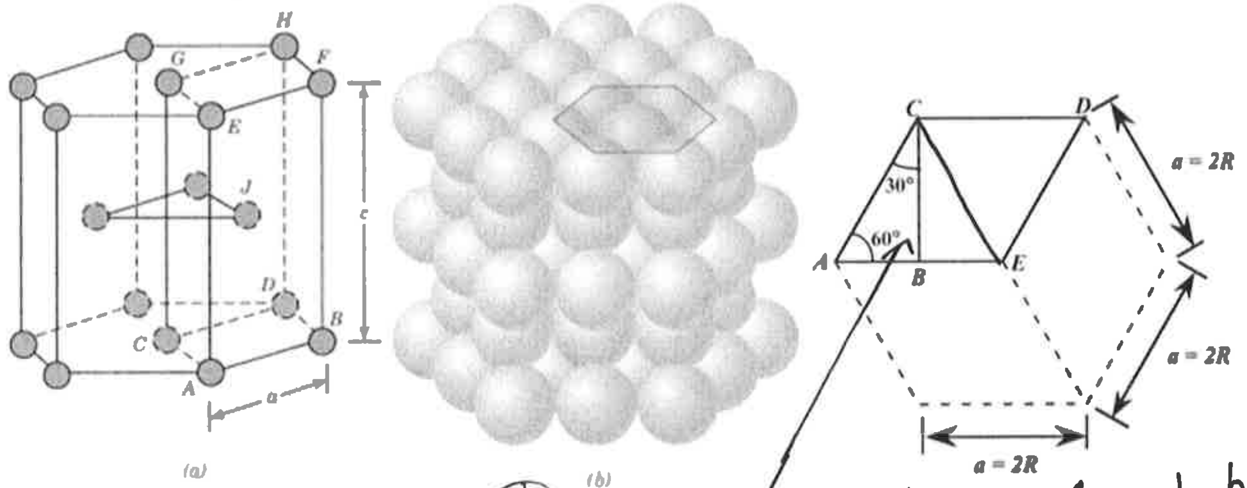
Intercepts: $-\frac{1}{2}$ ∞ $\frac{2}{3}$ — -1 ∞ 1 ∞
Reciprocal: -2 0 $3/2$ — -1 0 1 0
$(\bar{4}03)$ — $(\bar{1}010)$

H. <u>Hexagonal Closed Pack Structure</u>

1. Show that the base area of the unit cell for HCP is given by, $6\sqrt{3}R^2$.

2. Show that the atomic packing factor for HCP is 0.74.

3. Magnesium (atomic weight = 24.31) has an HCP unit cell for which the ratio of the lattice parameters *c/a* is 1.624. If the density of Mg is 1.74 g/cm³, determine the radius of the Mg atom.



(1) area of one triangle $= \frac{1}{2} bh$

$= \frac{1}{2} \times 2R \times 2R\sin 60^\circ$

$= 2R^2 \cdot \sqrt{3}/2 = \sqrt{3}R^2$

There are 6 of the above triangles in the base.

So, Base area $= 6\sqrt{3}R^2$

(2) Atomic Packing Factor $= \frac{V_{sph}}{V_{unitcell}}$

How many atoms in the unit cell? $= \frac{1}{6}\times 6 + \frac{1}{6}\times 6 + 2\times\frac{1}{2} + 3 = 6$

$$APF = \frac{6\times 4/3\pi R^3}{6\sqrt{3}R^2\times c} = \frac{6\times 4/3\pi R^3}{6\sqrt{3}R^2\times 1.624\times 2R} = \frac{4\pi}{3\sqrt{3}\times 1.624\times 2} = 0.74$$

(3) Unit cell volume $= V = \frac{m}{\rho} = \frac{6\times 24.31/(6.022\times 10^{23})}{1.74} = 0.139\times 10^{-21}\ cm^3$

$V = 6\sqrt{3}R^2\times c = 6\sqrt{3}R^2\times 1.624a = 6\sqrt{3}R^2\times 1.624\times 2R$

$V = 6\sqrt{3}\times 1.624\times 2R^3 = 0.139\times 10^{-21}$

$R^3 = \frac{0.139\times 10^{-21}}{6\sqrt{3}\times 1.624\times 2} =$

$R = \left(\frac{0.139\times 10^{-21}}{6\sqrt{3}\times 1.624\times 2}\right)^{1/3} = 0.160\times 10^{-7}\ cm$

$R = 0.160\ nm$