PHYS 321 F2017 Test #1 KEY

A. Uranium metal can be produced by the reaction of uranium tetrafluoride (UF_4) with magnesium (Mg) in a sealed reactor heated to 700°C. The by-product is magnesium fluoride (MgF_2). To ensure that all the magnesium is consumed in the reaction, the reactor is charged with excess UF_4, specifically 10% more than the stoichiometric requirement of the reaction. To produce 222 kg of U, how much UF_4 and Mg must be introduced into the reactor? Express your answers in kg.

$$UF_4 + 2Mg \longrightarrow 2MgF_2 + U$$

$$222{,}000\text{ g U}\left(\frac{1\text{ mol U}}{238.0289\text{ g}}\right) = 932.66\text{ mol U to be made}$$

U / UF_4 is 1:1 $\longrightarrow$ 932.66 mol UF_4

U / Mg is 1:2 $\longrightarrow 2 \times 932.66 = 1865.32$ mol Mg $\frac{24.3\text{ g}}{1\text{ mol Mg}} = 45327.3$ g Mg

45.3273 kg Mg

$$932.66\text{ mol }UF_4 \times (.1 + 1) = 1025.93\text{ mol }UF_4\text{ used}$$

$$1025.93\text{ mol }UF_4\ \frac{[238.0289 + 4(19)]\text{ g}}{1\text{ mol }UF_4} = 321{,}980\text{ g} = \boxed{321.98\text{ kg }UF_4}$$

B. Compute the percent ionic character of the inter-atomic bonds for the following compounds: TiO_2 and CdS. The electronegativity values are given below.

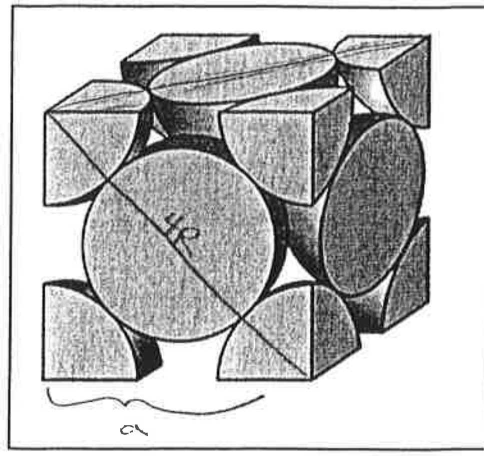
$$\%\text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\%)$$

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	18	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															

TiO_2: $\%IC = \left(1 - e^{\wedge}\left[\frac{(3.5 - 1.5)^2}{-4}\right]\right) \times (100\%) = 63.2\%$ IC for TiO_2

CdS: $\%IC = \left(1 - e^{\wedge}\left[-\frac{(2.5 - 1.7)^2}{4}\right]\right) \times (100\%) = 14.7856\%$ IC for CdS

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

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

$2a^2 = 16R^2$

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

$a^2 = 8R^2$

$a = 2R\sqrt{2}$ ✓

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

$APF = \frac{\text{vol. atom}}{\text{vol. cell}} = \frac{4\cdot(4/3\pi R^3)}{a^3} = \frac{4(\frac{4}{3}\pi \times (.3535a)^3)}{a^3}$ $\quad R = \frac{a}{2\sqrt{2}} = .3535a$

$= 4(4/3\pi \times .3535^3) = .74$ ✓

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.

$\rho = 11.35 \frac{g}{cm^3} = \frac{nA}{V_c \cdot N_A}$

$11.35\ g/cm^3 = \frac{4\ atoms/cell\ (207.2\ g/mol)}{6.022 \times 10^{23} \frac{atoms}{mol} \times V_c}$ ✓

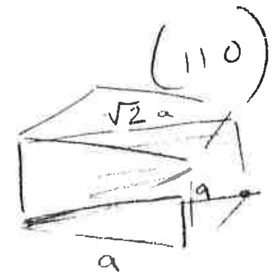
$V_c = 1.2 \times 10^{-22}\ cm^3$

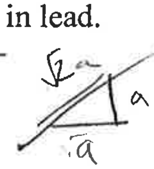
$V_c = a^3 = (2R\sqrt{2})^3$

$1.2 \times 10^{-22}\ cm^3 = (2R\sqrt{2})^3$ ✓

$R = 1.74 \times 10^{-8}\ cm$

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





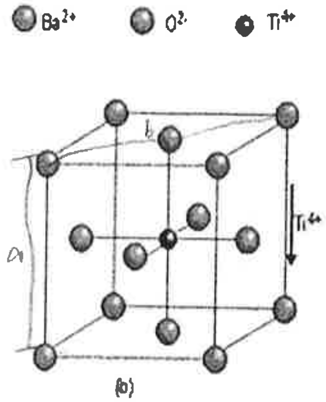
$L.D. = \frac{atoms}{length} = \frac{2}{\sqrt{2}a} = \frac{2}{\sqrt{2}\cdot 2R\sqrt{2}} = \frac{2}{\sqrt{2}\cdot 2(1.74 \times 10^{-8}\ cm)\sqrt{2}}$

$= 2.87 \times 10^{7}\ \frac{atoms}{cm}$

$PD = \frac{atoms}{area} = \frac{2}{a \times \sqrt{2}a} = \frac{2}{2R\sqrt{2} \times \sqrt{2}(2R\sqrt{2})} = \frac{2}{2(1.74 \times 10^{-8})\sqrt{2} \times \sqrt{2}(2 \cdot 1.74 \times 10^{-8} \cdot \sqrt{2})}$

$= 5.839 \times 10^{14}\ \frac{atoms}{cm^2}$

D. Determine the density of $BaTiO_3$, which forms a perovskite crystal structure, shown below:



	Ionic Radius (nm)	Atomic mass (g/mol)
Ba (Corner)	0.136	137.3
O (Face center)	0.140	16
Ti (Middle)	0.145	47.87

1 Ba atom   1 Ti atom

3 O atoms

$2R_{Ti} + 2R_O = b$

$2a^2 = b^2$

$\sqrt{2a^2} = \sqrt{(2R_{Ti}+2R_O)^2}$

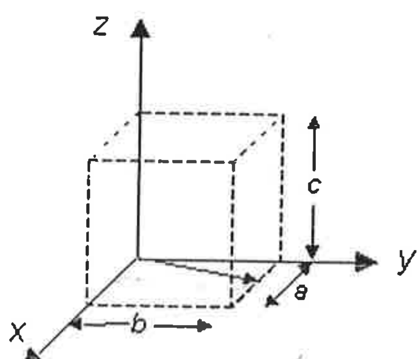
$\sqrt{2}\,a = 2R_{Ba} + 2R_O$

$a = \frac{2R_{Ba}+2R_O}{\sqrt{2}}$

$$\rho = \frac{1\cdot 137.3\frac{g}{mol} + 1\cdot 47.87\frac{g}{mol} + 3\cdot 16\frac{g}{mol}}{\left(\frac{2R_{Ba}+2R_O}{\sqrt{2}}\right)^3 \left(6.022E23\frac{1}{mol}\right)} = 6.51E\text{-}21\frac{g}{nm^3}$$

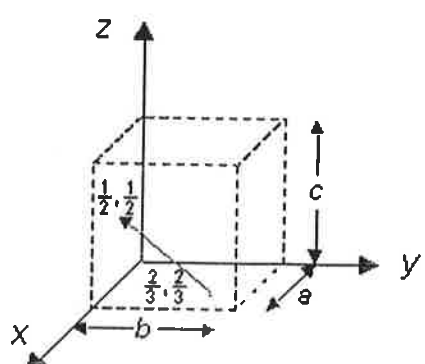
$$6.51E\text{-}21\frac{g}{nm^3}\left(\frac{1\,nm}{E\text{-}7\,cm}\right)^3 = \boxed{6.51\frac{g}{cm^3}}$$

E. What are the indices for the directions represented by the vector that has been drawn within a unit cell?



$\frac{1}{2}, 1, 0$

[1 2 0]

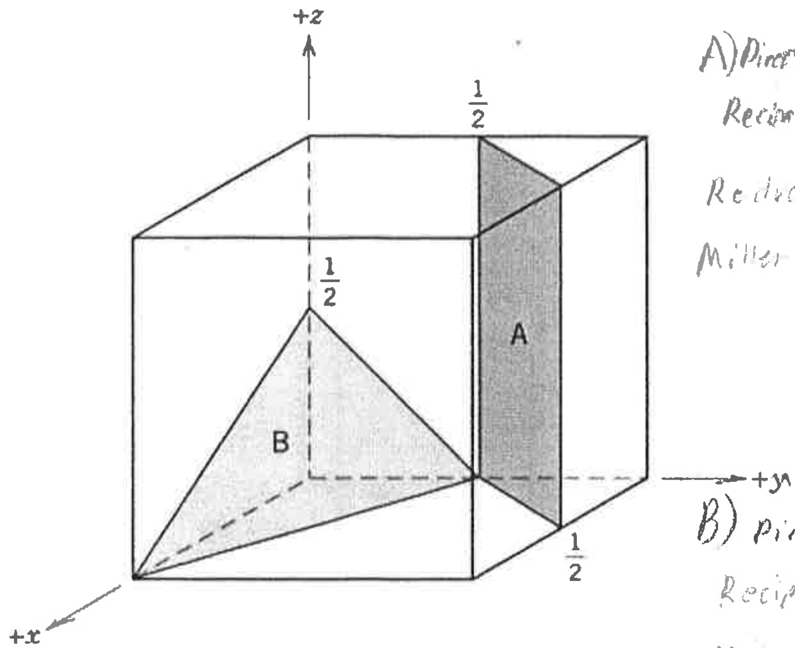


$\frac{3}{6}\;\; 0\;\; \frac{1}{2}$

$-\;\frac{4}{6}\;\; \frac{2}{3}\;\; 0$

$-\frac{1}{6}\;\; -\frac{2}{3}\;\; \frac{1}{2} \;\cdot 6 = [\bar{1}\,\bar{4}\,3]$

F. Determine the Miller indices for the planes shown in the following unit cell:



A) Directions $\frac{1}{2}$ $-\frac{1}{2}$ ∞

Reciprocal 2 -2 0

Reduce by ÷ 2

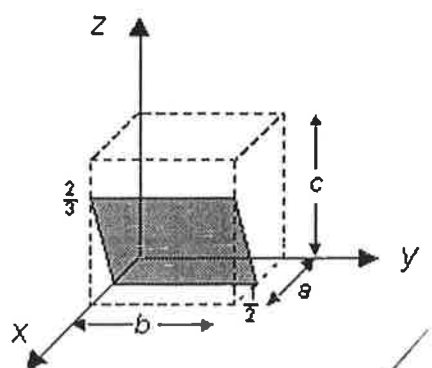
Miller Is = $(1\bar{1}0)$

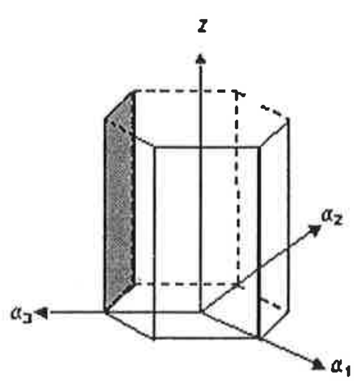
B) Directions = 1 $\frac{1}{2}$ $\frac{1}{2}$

Reciprocal = 1 2 2

Miller Is = (122)

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





Directions = $-\frac{1}{2}$ ∞ $\frac{2}{3}$

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

Reduce by × 2

Miller Is = $(\bar{4}03)$

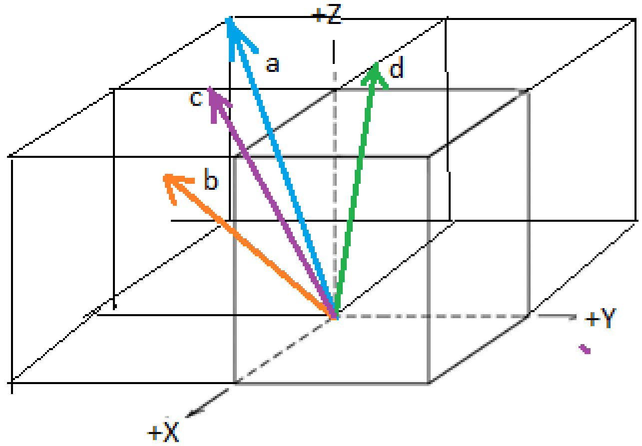
-1 ∞ 1 ∞

-1 0 1 0

$(\bar{1}010)$

H. *Within a cubic unit cell, sketch the following directions:*

(a) $[\bar{1}\bar{1}1]$, *(b)* $[\bar{1}\bar{2}1]$, *(c)* $[0\bar{1}2]$, *(d)* $[\bar{1}03]$.



I. *Sketch the* $[1\bar{2}\bar{2}3]$ *direction in a hexagonal unit cell.*