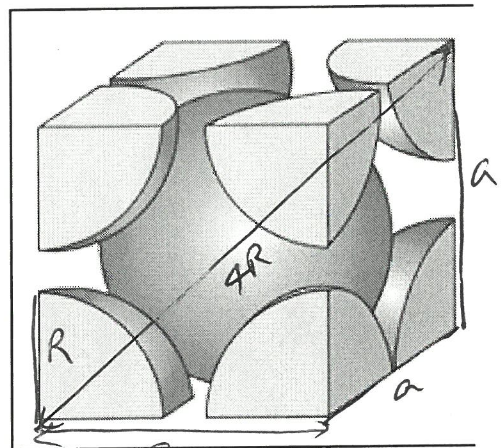
PHYS 321 S2025 Test #1 Name: Answer Key

I. Body Centered Cubic Structure

1. How many atoms are inside the cubic unit cell of BCC?

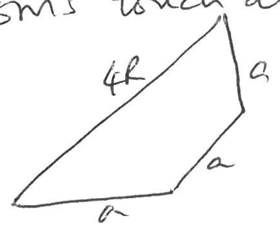
2



2. Show the cube edge length, a and the atomic radius, R in the figure.

3. Show that the cube edge length, a and the atomic radius, R are related by: $a = \frac{4}{\sqrt{3}}R$

Atoms touch along the diagonal, which is 4R



$$4R = \sqrt{a^2 + a^2 + a^2}$$

$$4R = \sqrt{3a^2}$$

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

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

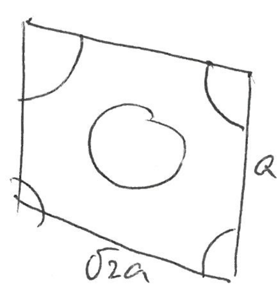
4. Calculate the density of iron, Fe, which has a BCC crystal structure. Its atomic radius = 0.126 nm and atomic weight = 55.845 g/mol. (Avogadro's number = 6.022×10^{23})

$$\rho = \frac{m}{V} = \frac{2 \times 55.845 / 6.022 \times 10^{23}}{\left(\frac{4}{\sqrt{3}} \times 0.126 \times 10^{-7}\right)^3} = \frac{2 \times 55.845}{6.022 \times 10^{23} \times \left(\frac{4}{\sqrt{3}} \times 0.126 \times 10^{-7}\right)^3}$$

$$\boxed{\rho = 7.53 \ g/cm^3}$$

5. Calculate the planar density for (110) planes in iron.

Planar density $= \frac{\#\text{atoms}}{\text{area}} = \frac{2}{\text{area}}$



$$= \frac{2}{\sqrt{2} a^2}$$

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

$$= \frac{3\sqrt{2}}{16 R^2} = \frac{3\sqrt{2}}{16 \times 0.126^2} = 16.7 \ nm^{-2}$$

$$= 16.7 \times 10^{18} \ m^{-2}$$

$$= 1.67 \times 10^{19} \ m^{-2}$$

$$PD_{110, Fe} = 1.67 \times 10^{15} \ cm^{-2}$$

II. Hafnium has six naturally occurring isotopes: 0.16% of ^{174}Hf, with an atomic weight of 173.940 amu; 5.26% of ^{176}Hf, with an atomic weight of 175.941 amu; 18.60% of ^{177}Hf, with an atomic weight of 176.943 amu; 27.28% of ^{178}Hf, with an atomic weight of 177.944 amu; 13.62% of ^{179}Hf, with an atomic weight of 178.946 amu;. and 35.08% of ^{180}Hf, with an atomic weight of 179.947 amu. Calculate the average atomic weight of Hf.

$$\frac{0.16}{100}\times 173.94+\frac{5.26}{100}\times 175.941+\frac{18.6}{100}\times 176.943+\frac{27.28}{100}\times 177.944$$
$$+\frac{13.62}{100}\times 178.946+\frac{35.08}{100}\times 179.947$$

$$\boxed{\bar{A}_{Hf}=178.485\text{ amu}}$$

III. Net potential energy E_N between two adjacent ions is sometimes represented by the expression

$$E_N=-\frac{C}{r}+D\exp\left(-\frac{r}{\rho}\right)\text{..........(I)}$$

in which r is the interionic separation and C, D, and ρ are constants whose values depend on the specific material.

(a) Derive an expression for the bonding energy E_0 in terms of the equilibrium interionic separation r_0 and the constants D and ρ using the following procedure:

1. Differentiate E_N with respect to r and set the resulting expression equal to zero.
2. Solve for C in terms of D, ρ, and r_0.
3. Determine the expression for E_0 by substitution for C in Equation (I).

(b) Derive another expression for E_0 in terms of r_0, C, and ρ.

$$\frac{dE_N}{dr}=\frac{C}{r^2}-\frac{D}{\rho}e^{-r/\rho}.$$

$$\frac{C}{r_0^2}-\frac{D}{\rho}e^{-r_0/\rho}=0\rightarrow C=\frac{Dr_0^2}{\rho}e^{-r_0/\rho}$$

$$D=\frac{C\rho e^{r_0/\rho}}{r_0^2}$$

$$E_0=-\frac{Dr_0^2}{\rho r_0}\cdot e^{-r_0/\rho}+De^{-r_0/\rho}$$

$$\boxed{E_0=De^{-r_0/\rho}\left(1-\frac{r_0}{\rho}\right)}$$

$$E_0=-\frac{C}{r_0}+\frac{C\rho}{r_0^2}e^{r_0/\rho}\cdot e^{-r_0/\rho}$$

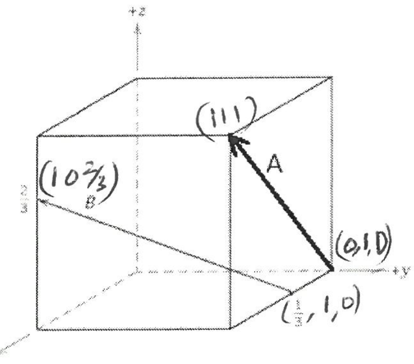
$$\boxed{E_0=\frac{C}{r_0}\left(\frac{\rho}{r_0}-1\right)}$$

IV. Determine the indices for the directions shown (A and B) in the cubic unit cell.

A: 1 1 1
− 0 1 0
1 0 1

A: [1 0 1]

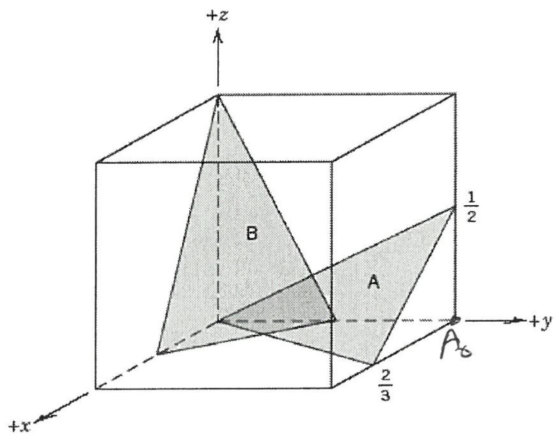
B: 1 0 2/3
1/3 1 0
2/3 −1 2/3
2 −3 2
[2 $\bar{3}$ 2]



V. Determine the Miller indices for the planes (B and A) shown in the following unit cell:

B Intercept $\frac{1}{2}$ $\frac{1}{2}$ 1
(2 2 1)

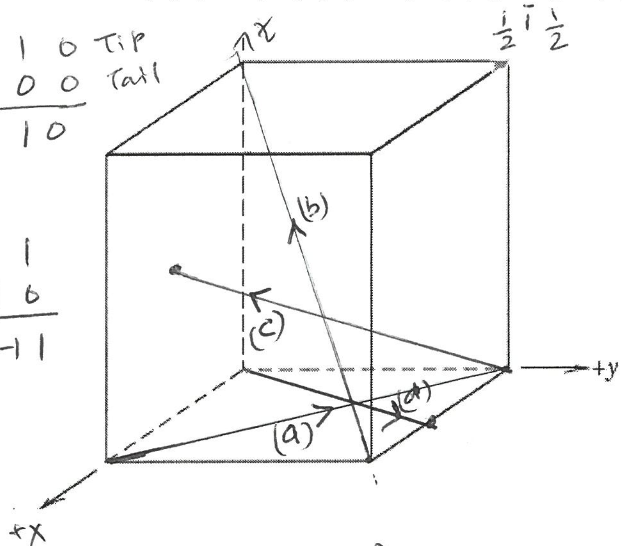
A Intercept $\frac{2}{3}$ −1 $\frac{1}{2}$
$\frac{3}{2}$ −1 2
3 −2 4
(3 $\bar{2}$ 4)



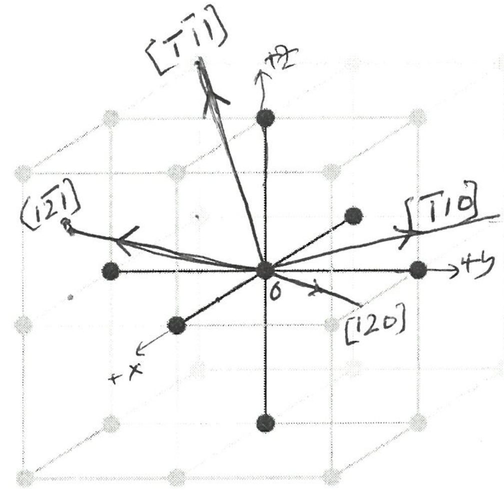
VI. In one of the cubic cell pictures, choose an origin and XYZ axes and sketch the following directions: (*a*) [$\bar{1}$10] (*b*) [$\bar{1}\bar{1}$1] (*c*) [1$\bar{2}$1] (*d*) [120]

(a) 0 1 0 Tip
1 0 0 Tail
−1 1 0

(b) 0 0 1
1 1 0
−1 −1 1



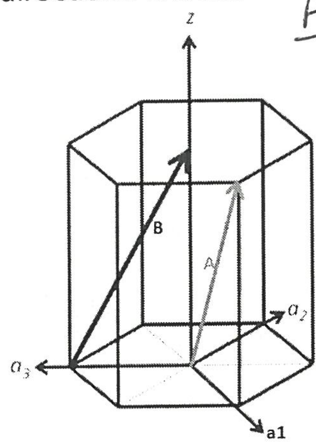
OR



(c) ½ 0 ½
0 1 0
1 −2 1
$\frac{1}{2}$ −1 $\frac{1}{2}$

(d) ½ 1 0
0 0 0
$\frac{1}{2}$ 1 0

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



A: 101
$u'v'w'$

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

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

$t = -(\frac{2}{3} - \frac{1}{3}) = -\frac{1}{3}$

$w = w' = 1$

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

$[2\bar{1}\bar{1}3]$

B: 001
$-1\,-1\,0$
$1\;1\;1$
$u'\;v'\;w'$

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

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

$t = -(\frac{1}{3} + \frac{1}{3}) = -\frac{2}{3}$

$w = w' = 1$

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

$[11\bar{2}3]$

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

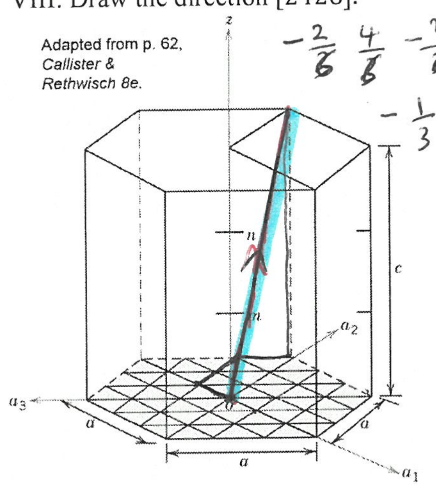
$$u = \frac{1}{3}(2u' - v')$$

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

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

$$w = w'$$

VIII. Draw the direction $[\bar{2}4\bar{2}6]$.

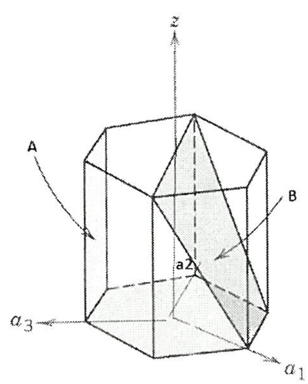


Adapted from p. 62, *Callister & Rethwisch 8e.*

$-\frac{2}{6} \quad \frac{4}{6} \quad -\frac{2}{6} \quad \frac{6}{6}$

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

VIII. Determine the 4-index miller indices for the planes A & B shown below.



A: $a_1 \quad a_2 \quad a_3 \quad z$

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

$-1 \quad 0 \quad 1 \quad 0$

$(\bar{1}010)$

B: $1 \quad \infty \quad -1 \quad 1$

$1 \quad 0 \quad -1 \quad 1$

$(10\bar{1}1)$