Solution of Tute Sheet #5

1. $R = 1.278\ \mathring{A} = 1.278 \times 10^{-10}\ m = 1.278 \times 10^{-8}\ cm$

$A_{Cu} = 63.54\ gm/mole$

Unit cell diamension $= 0.3615nm$

$(4r)^2 = (0.3615nm)^2 + (0.3615nm)^2$

$\therefore r = 0.1278$

$\Rightarrow \rho = \frac{n A_{Cu}}{V N_A}$

For FCC $n = 4$

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

$= 16\sqrt{2}R^3$

We know that in FCC structure there are 4 atoms/cell

Atomic weight $= 63.54\ g/mol$

$\rho = \frac{4 \times 63.54}{16\sqrt{2} R^3 \times (6.023 \times 10^{23})}$

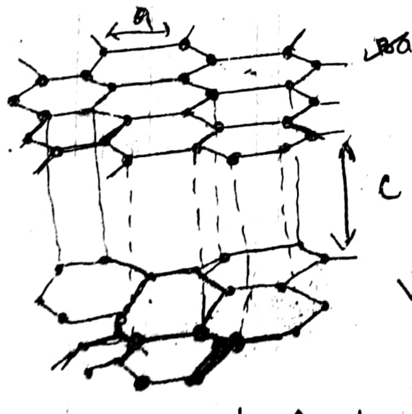
$= \frac{4 \times 63.54}{16\sqrt{2} \times (1.278 \times 10^{-8})^3 \times 6.023 \times 10^{23}}$

$= 8.935\ g/cm^3$ Ans.

$h^2 = a^2 - \frac{a^2}{4}$

$\frac{1}{6} \times 12 = 2$

2) Graphite Structure,



Layered structure of Graphite

Base plane is made up of 6 equilateral traingle

$\Delta = \frac{1}{2} \times$ Base $\times$ height

$\frac{1}{2} \times a \times \frac{\sqrt{3}}{2} a = \frac{\sqrt{3}}{4} a^2$

Area of 6 equilateral $\Delta = 6 \times \frac{\sqrt{3}}{4} a^2 = \frac{3\sqrt{3}}{2}$

Vol. of unit cell $=$ Base $\times$ height

$= \frac{3\sqrt{3} a^2}{2} \times c$

No of atom/unit cell

Effective no. of Carbon atoms $= 2$

Volume of hexagonal unit cell $= 6 \times \frac{1}{2} a^2 \sin\theta \times c$

$= 6 \times \frac{\sqrt{3}}{4} \times a^2 c$

P.F. .. 0.18, 0.16

where $a = 1.42\ \mathring{A} = 1.42 \times 10^{-10}\ m = 1.42 \times 10^{-8}\ cm$

$c = 3.44\ \mathring{A} = 3.44 \times 10^{-10}\ m = 3.44 \times 10^{-8}\ cm$

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$\rho = \dfrac{n A_c}{V \times N_A}$

$= \dfrac{2 \times 12\ g/mole}{6 \times \frac{\sqrt{3}}{4} a^2 c \times 6.023 \times 10^{23}}$

$= \dfrac{2 \times 12}{6 \times \frac{\sqrt{3}}{4} \times (1.42)^2 \times 3.44 \times 6.023 \times 10^{23}}$

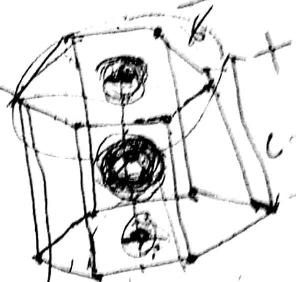
$= \dfrac{2 \times 12}{6 \times \frac{\sqrt{3}}{4} \times (1.42 \times 10^{-8})^2 \times 3.44 \times 10^{-8} \times 6.023 \times 10^{23}} = 2.211\ gm/cm$

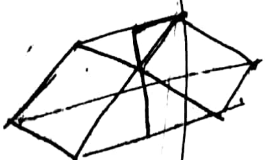
3) Given height of unit cell i.e. $c = 4.94\ \text{Å}$

$= 4.94 \times 10^{-8}\ cm$

At. wt. of Zn i.e. $A_{Zn} = 65.37\ gm/mole$

For HCP $n = 6$





Volume $(V) = 6 \times \frac{\sqrt{3}}{4} a^2 c$

$= 6 \times \frac{\sqrt{3}}{4} a^2 \times 4.94$

$= 6 \times \frac{\sqrt{3}}{4} \left(\frac{\sqrt{3}}{\sqrt{8}} c\right)^2 \times 4.94$

$\because \frac{c}{a} = \sqrt{\frac{8}{3}}$

$a = \sqrt{\frac{3}{8}}\, c$

$\therefore \rho = \dfrac{n \times A_{Zn}}{V \times N_A}$

$= \dfrac{6 \times 65.37}{6 \times \frac{\sqrt{3}}{4} \left(\frac{\sqrt{3}}{\sqrt{8}} \times 4.94\right)^2 \times 4.94 \times 6.023 \times 10^{23}}$

$= \dfrac{6 \times 65.37 \times 4 \times 8}{6 \times \sqrt{3} \times 3 \times (4.94)^3 \times (10^{-8})^3 \times 6.023 \times 10^{23}}$

$= 5.55\ gm/cm^3$

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) $a_{BCC} = 3.32 \mathring{A}$

Volume per atom for BCC i.e.,

$$V_{BCC} = \frac{a^3}{2} = 18.3 \mathring{A}^3 \rightarrow \text{wrong}$$

Now, $a_{HCP} = 2.956 \mathring{A}$

$c = 4.683 \mathring{A}$

$6 \times \frac{\sqrt{3}}{4} a^2 c$

Volume per atom for HCP,

$$V_{HCP} = \frac{V}{6} = \frac{6 \times \sqrt{3}\, a^2 c}{4} = \frac{\sqrt{3}}{4} a^2 c = \frac{\sqrt{3}}{4} \times (2.956)^2 \times 4.683$$

$$= 17.71 \mathring{A}$$

% change in volume

Phase BCC → HCP

Vol: FCC

$$= \frac{|V_{HCP} - V_{BCC}|}{V_{BCC}} \times 100$$

$$= \frac{|17.71 - 18.3|}{18.3} \times 100 = 0.032\%$$

5) $R_{BCC} = 1.258 \mathring{A}$

$R_{FCC} = 1.298 \mathring{A}$

$A_{Fe} = 56.05$ gm/mole

(a) Volume per atom for BCC i.e. $V_{BCC} = \frac{a_{BCC}^3}{2}$

where $a_{BCC} = \frac{4R_{BCC}}{\sqrt{3}}$.

$$\therefore V_{BCC} = \left(\frac{4R_{BCC}}{\sqrt{3}}\right)^3 \times \frac{1}{2} = \frac{(4 \times 1.258)^3}{(\sqrt{3})^3} \times \frac{1}{2} = 12.275$$

Similarly,

Volume per atom for FCC i.e. $V_{FCC} = \frac{a_{FCC}^3}{4}$

where $a_{FCC} = \frac{4R}{\sqrt{2}}$

So, $V_{FCC} = \left(\frac{4R}{\sqrt{2}}\right)^3 \times \frac{1}{4}$

$= \left(\frac{4 \times 1.298}{\sqrt{2}}\right)^3 \times \frac{1}{4} = 12.372 \, \text{Å}$

%age change in volume $= \frac{|V_{FCC} - V_{BCC}|}{V_{BCC}} \times 100$

$= \frac{|12.372 - 12.275|}{12.275} \times 100 = 0.$

(b) Linear change in ~~[illegible]~~ from BCC to FCC

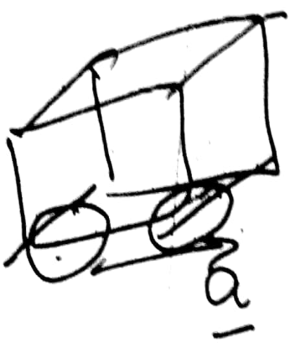
$a_{BCC} = \frac{4R_{BCC}}{\sqrt{3}} = \frac{4 \times 1.258}{\sqrt{3}} = 2.90 \, \text{Å}$

$a_{FCC} = \frac{4R_{FCC}}{\sqrt{2}} = \frac{4 \times 1.298}{\sqrt{2}} = 3.67 \, \text{Å}$ $\quad$ a fcc

%age linear change $= \frac{a_{FCC} - a_{BCC}}{a_{BCC}} \times 100$ $\quad$ 4r = BC

BCC

→ fc



$= \frac{|3.67 - 2.90|}{2.90} \times 100$ $\quad$ $a = \frac{4r}{\sqrt{3}}$

fc = a = $\frac{4}{r}$

$= \underline{26.61\%}$

Packing Efficiency $= \dfrac{\text{Volume of atoms in a unit cell}}{\text{Volume of unit cell}} \times 10$

$= \dfrac{\text{Volume of one atom} \times \text{No. of atoms per unit cell}}{\text{Volume of unit cell}}$

$= \dfrac{\frac{4}{3}\pi r^3 N}{a^3} \times 100 = \dfrac{4\pi r^3 N}{3a^3} \times 100$

(a) For FCC

$N = 4$

Radius of each atom, $r = \dfrac{\sqrt{2}}{4} a$

So Packing efficiency $= \dfrac{4 \times 3.14 \times \frac{2\sqrt{2}a^3}{64} \times 4}{a^3} \times 10$

$= \dfrac{4 \times 3.14 \times 2\sqrt{2} \times 4}{64} \times 100$

$= \dfrac{\sqrt{2} \times 3.14}{6} \times 100$

$= 0.74 \times 100$

$= 74\%$

(b) For HCP

Volume of atoms $= \frac{4}{3}\pi r^3 \times 6 = 8\pi r^3$

$= \dfrac{8\pi a^3}{8}$ $\left[\because r = \dfrac{a}{2}\right)$

Volume of unit cell $= \frac{3\sqrt{3}\,a^2 c}{2}$

Packing Efficiency $= \frac{8\pi a^3 \times 2}{8 \times 3\sqrt{3} a^2 c} \times 100$

$= \frac{2\pi a^3}{3\sqrt{3} a^2 c} \times 100 = \frac{2\pi}{3\sqrt{3}} \left(\frac{a}{c}\right) \times 100$

$= \frac{2\pi}{3\sqrt{3}} \sqrt{\frac{3}{8}} \times 100 \quad \left(\because \frac{a}{c} = \sqrt{\frac{3}{8}}\right)$

$= 0.74 \times 100$

$= 74\%$

(b) For BCC $N = 2$

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

Packing efficiency $= \frac{\frac{4}{3}\pi r^3 \times N \times 100}{a^3}$

$= \frac{4\pi (\sqrt{3}a)^3 \times 2}{3 \times 64\, a^3} \times 100$

$= \frac{4\pi\, 3\sqrt{3} a^3 \times 2}{3a^3 \times 64} \times 100$

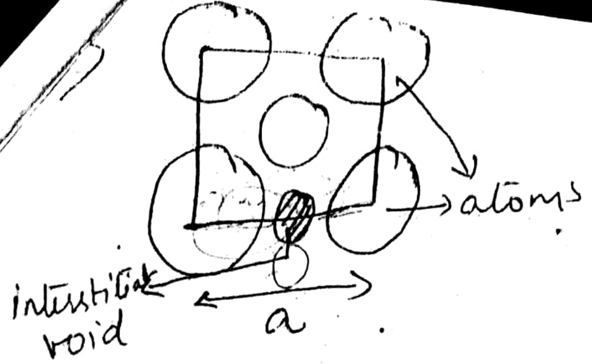
$= 100 \times \frac{\sqrt{3}\pi}{8} = 0.68 \times 100$

$= 68\%$

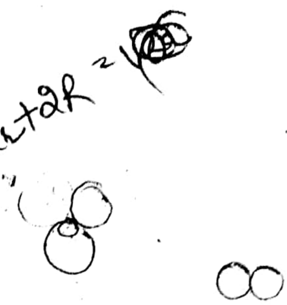
For SC $N = 1$, $r = \frac{a}{2}$

Packing efficiency $= \frac{4\pi r^3 N \times 100}{3a^3} = \frac{4\pi a^3 \times 1 \times 100}{3a^3 \times 8} = \frac{\pi}{6} \times 100 = 0.52 \times 100$

$= 52\%$



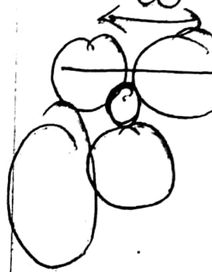
$2R+2r+2R =$



Let us say, Radius of atoms is R

Radius of sphere that occupied void $= r$

We have from Figure



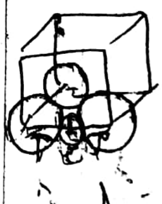
$$a = 2R+2r$$

For FCC $a = \frac{4R}{\sqrt{2}}$

$$\Rightarrow \frac{4R}{\sqrt{2}} = 2(R+r)$$

$$\frac{2R}{\sqrt{2}} = R+r$$

$$\sqrt{2}R = R+r$$



$$r = \sqrt{2}R - R$$

$$r = (\sqrt{2}-1)R$$

$$r =$$

For Ni $R = 1.25\,Å$

largest

Octahedral

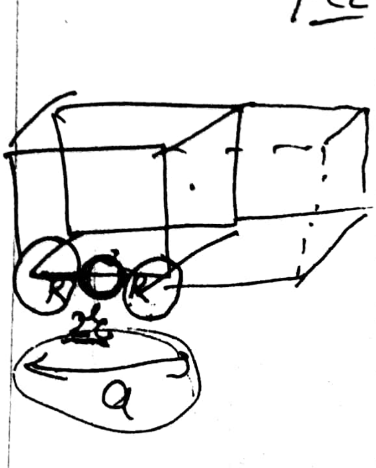
$\cancel{\Rightarrow r = 0.4}$

So, Radius of interstitial sphere without distortion is

FCC

$$r = 0.414 \times 1.25$$

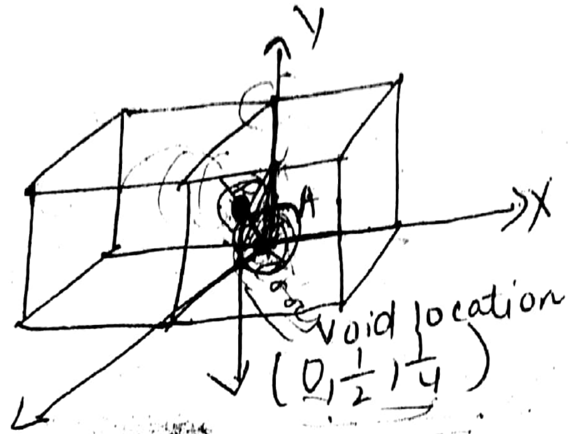
$$= 0.5175\,Å$$



$r \rightarrow$

$2r$

8)



Atom A is at position (0, 0, 0) and void is at loc (0, 1/2, 1/4)

So, Let us say, Radius of ~~Inters~~ atom is R
Radius of sphere is r

From fig,

$$R+r = \sqrt{(0-0)^2+\left(\frac{a}{2}-0\right)^2+\left(\frac{a}{4}-0\right)^2}$$

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

$$R+r = a\sqrt{\frac{5}{16}}$$

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

$$R+r = \frac{4R}{\sqrt{3}}\sqrt{\frac{5}{16}}$$

$$R+r = \frac{4R\sqrt{5}}{4\times\sqrt{3}}$$

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

$$r = \sqrt{\frac{5}{3}}R - R = 0.2925R \text{ Ans.}$$

b) $\rho_{Al} = 2700\ kg\ m^{-3} = \frac{2700 \times 1000}{10^6}\ gm/cm^3 = 2.7\ gm\,cm^{-3}$

For FCC $n = 4$

$A_{Al} = 26.98\ gm/mole$

$$\rho = \frac{n \times A_{Al}}{V \times N_A}$$

$$V = \frac{n \times A_{Al}}{\rho \times N_A}$$

$$= \frac{4 \times 26.98}{\frac{2700 \times 1000}{10^6} \times 6.023 \times 10^{23}} = 6.636 \times 10^{-23}\ cm^3$$

For FCC,

$$V = a^3$$

$$a^3 = 6.636 \times 10^{-23}\ cm^3$$

$$a = (6.636 \times 10^{-23})^{1/3}\ cm^3$$

$$= 4.04\ \mathring{A} = 4.04 \times 10^{-10}\ m$$

$d = \frac{\sqrt{3}}{2} b$

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

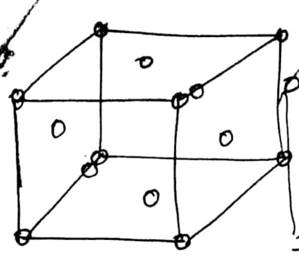
Now, $\sqrt{2}a = 4r$

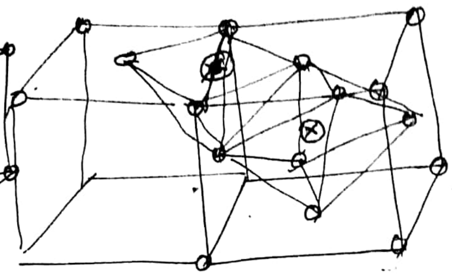
$$a = 2\sqrt{2}r$$

$$r = \frac{a}{2\sqrt{2}} = \frac{4.04}{2 \times \sqrt{2}} = 1.4315\ \mathring{A}$$

$$2r = d = \frac{a}{\sqrt{2}} = \frac{4.04 \cancel{\times 10^{-10}}}{\sqrt{2}}$$

$$d = 2.863\ \mathring{A}$$

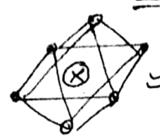




FCC ← BC site + FC

$\underline{1\ OV} + 3 \times 12 \times \frac{1}{4}$

$= \underline{\underline{4}}$



$\underline{\underline{0.414R}}$

$\boxed{AB} \rightarrow$

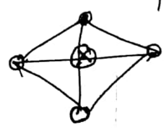
RS + OV

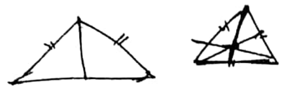
(4) (4)

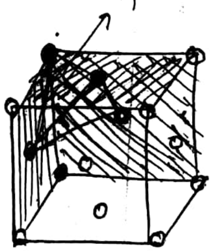
NaCl

(4) OV

TV







TV

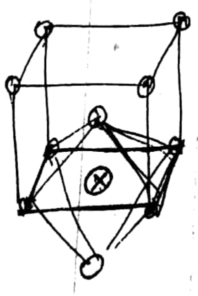
TV $\underline{\underline{8}}$

$\underline{\underline{0.225R}}$

$AB_2 \rightarrow \underline{\underline{TiO_2}}$

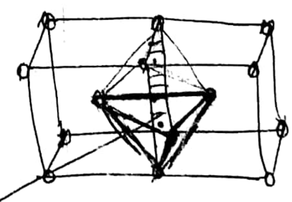
A → regular site (4)

B → TV. (8)



BCC ← FC site (OV)

$6 \times \frac{1}{2} = \underline{\underline{3}}$



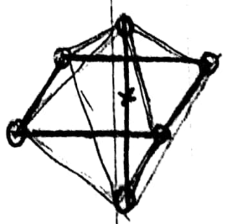
$24 \times \frac{1}{2} = \underline{\underline{12}}$ ← TV

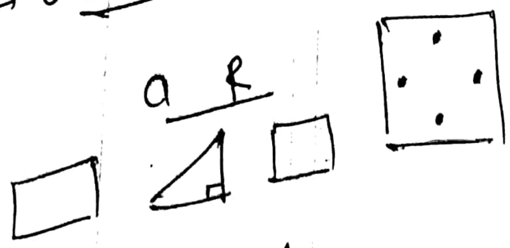
distorted TV

TV → $\underline{.225R}$

OV → $\underline{0.168R}$

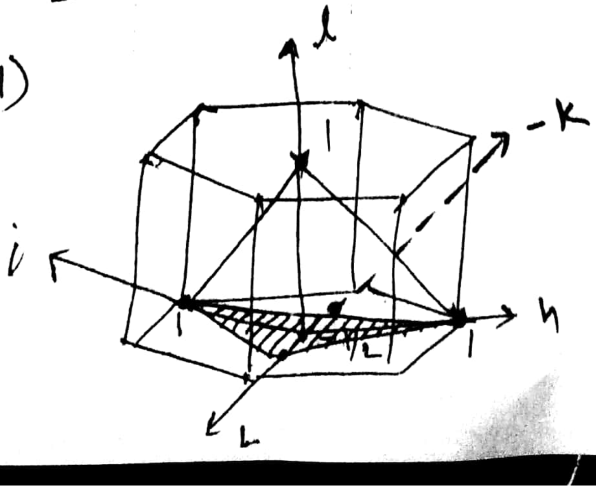
a R





(1 $\bar{2}$ 1 0 1)

h -1/2 1 1



$\boxed{h+k+i=0}$

(1 2 1 0)