Ques.1

Cu has FCC structure and its atomic radius is 1.278Å. Calc ulate the theoretical density of Cu. Atomic weight of Cu is 63.54 gm/mole.

Ans.1

Cu has FCC structure

$N=6.022*10^{23}$

$R=1.278A^{0}$

$A=63.54$ g/mole

$V= a^3$

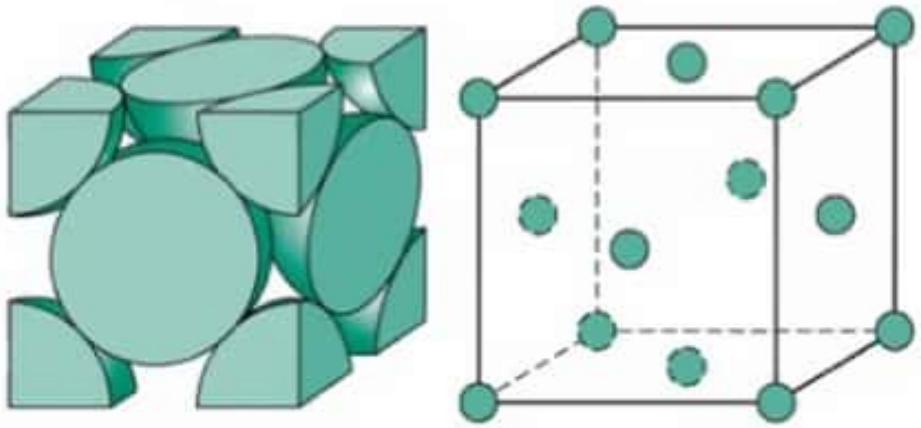
(Number of atoms in FCC unit cell)$n=4$

For FCC structure relation between atomic radius and length of cubic unit cell is

$a*\sqrt{2}=4R$

$$\rho=\frac{A*n}{N*V}=\frac{63.54 \times 4}{=a^3 \times 6.022*10^{23}}$$

$\rho=8.93$g/cc



Ques2.

Draw the section of graphite structure. All C-C bonds in the layer are 1.42 Å and the distance between layers is 3.44 Å. Calculate the density of graphite.

Ans.2.

Graphite has HCP structure with n=2 [2(6x1/6)]

C-C bond layer (a) =1.42 Å

Distance between layers (c) - 3.35 Å (6.70/2)

volume= Area of base*Height

=6*1/2*b*h*c

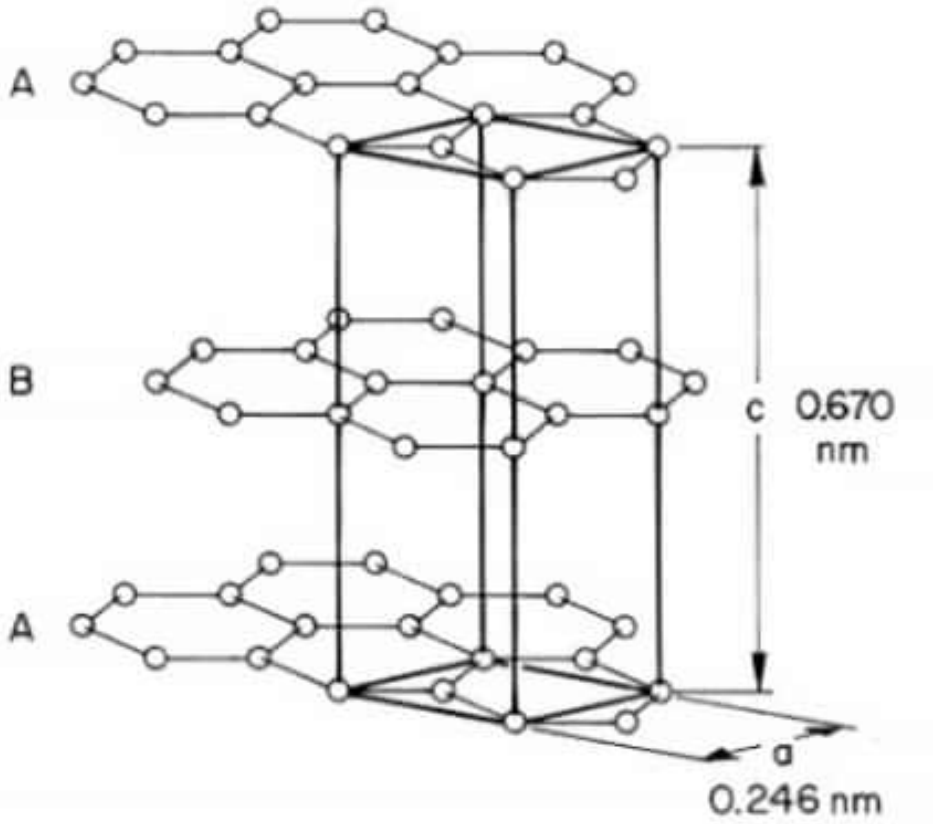
=6*1/2*a*$\sqrt{3}$a/2*c

=18.02*10^{-24} cm^3

(h= $\sqrt{3}$a/2)

$$\rho = \frac{A*n}{N*V} = \frac{12.11 \times 2}{18.02 \times 10^{-24} \times 6.022*10^{23}}$$

ρ = 2.211 gm/cc



Ques.5

Iron (atomic weight 56.05 gm/mole) change from BCC to FCC at 910 °C. At this atomic radius of iron is 1.258 Å in BCC and 1.298 Å in FCC. What is the percentage of

(a) volume change and

(b) linear change in iron when heated through this temperature range?

Ans.5

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FCC	BCC
$R_{FCC} = 1.298$ Å	$R_{BCC} = 1.258$ Å
$V_{FCC} = a^3/4$ (per atom)	$V_{BCC} = a^3/2$ (per atom)
$\sqrt{2}\,a = 4R$	$\sqrt{3}\,a = 4R$
V = 12.37 gm/cc	V = 12.25 gm/cc
$a_{FCC} = 3.671$ Å	$a_{BCC} = 2.905$ Å

% change in volume at 990 °C = $\frac{|V_{BCC} - V_{FCC}|}{V_{BCC}} \times 100 =$

$0.0097 \times 100 = 0.97\%$

Linear change in iron when heated through this temperature =

$$\frac{|a_{BCC} - a_{FCC}|}{a_{BCC}} \times 100 = 0.2636 \times 100 = 26.36\,\%$$

Ques.6

Calculate the packing efficiency of (a) close packed structures (FCC and HCP) (b) monoatomic BCC and SC crystals.

Face Centered Cubic (FCC)

- Close packed directions are face diagonals.

--Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

- Coordination # = 12

Close-packed directions:

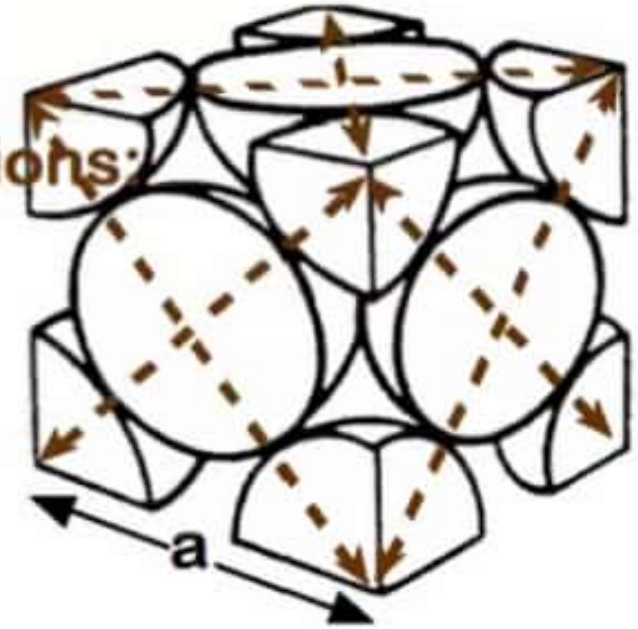
length = 4R

$= \sqrt{2}\, a$

Unit cell contains:

6 x 1/2 + 8 x 1/8

=4 atoms/unit ce

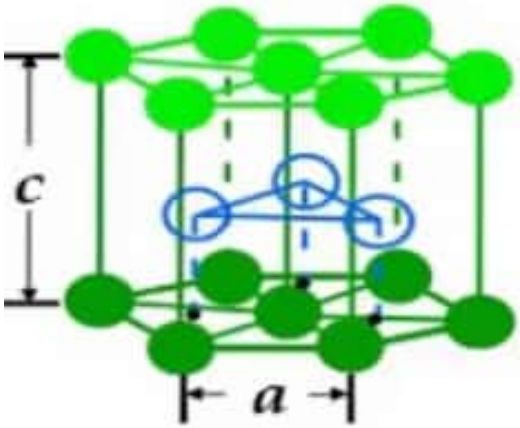


$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{4 \cdot \frac{4}{3}\pi (\sqrt{2}a/4)^3}{a^3}$$

- APF for a FCC = 0.74

APF for HCP



A sites

B sites

A sites

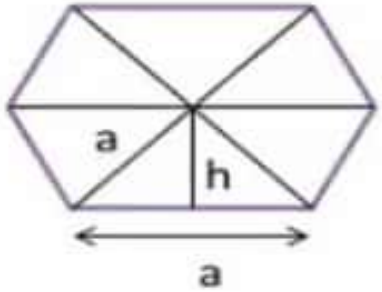
C=1.633a

Number of atoms in HCP unit cell=
(12*1/6)+(2*1/2)+3=6atoms

Vol.of HCP unit cell=
area of the hexagonal face X height of the hexagonal

Area of the hexagonal face=area of each triangle X6

a=2r



$$\text{Area of triangle} = \frac{bh}{2} = \frac{ah}{2} = \frac{1}{2}a.\frac{a\sqrt{3}}{2}$$

$$\text{Area of hexagon} = 6.\frac{a^2\sqrt{3}}{4}$$

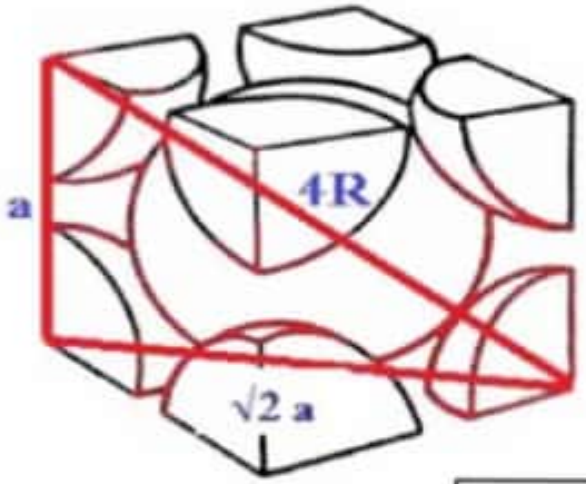
$$\text{Volume of HCP} = 6.\frac{a^2\sqrt{3}}{4}.C = 6.\frac{a^2\sqrt{3}}{4}.1.633a$$

$$\text{APF} = 6 * \frac{4\pi r^3}{3} / \left(\frac{\sqrt{3}}{4} * 6 * 1.633 * a3\right)$$

APF =0.74

Hari Prasad

- Let's calculate the atomic packing factor for BCC crystal:



Close-packed directions:

length = 4R

$= \sqrt{3}\, a$

Unit cell contains:

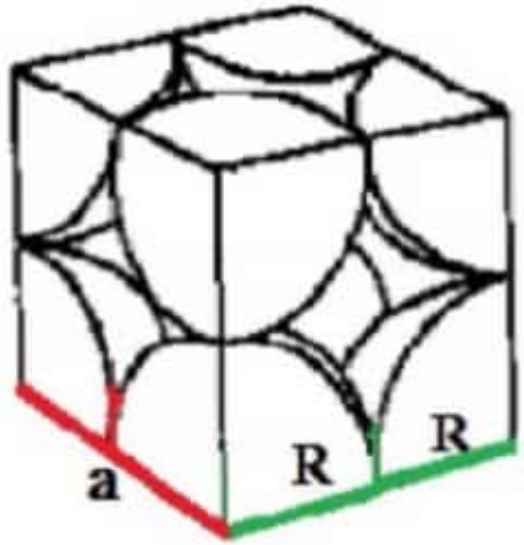
$= 1 + 8 \times 1/8$

$=$ **2 atoms/unit cell**

$$APF = \frac{\text{Atoms/unit cell} \times \text{Volume/atom}}{\text{Volume/unit cell}} = \frac{2 \times \frac{4}{3}\pi \left(\frac{a\sqrt{3}}{4}\right)^3}{a^3}$$

APF for a Body Centered Cubic Crystal Structure $= \pi\sqrt{3}/8 = 0.68$

APF OF Simple cubic



Close-packed directions:

length = 2R

= a

Unit cell contains:

= 8 x 1/8

= 1 atom/unit cell

Atoms/unit cell

$$APF = \frac{1 \times \frac{4}{3}\pi (a/2)^3}{a^3}$$

Volume/atom

Volume/unit cell

APF for a Simple Cubic Crystal Structure = π /6 = 0.52

Ques.7.

Find the diameter of the largest atom that would fit an interstitial void in FCC nickel without distortion.

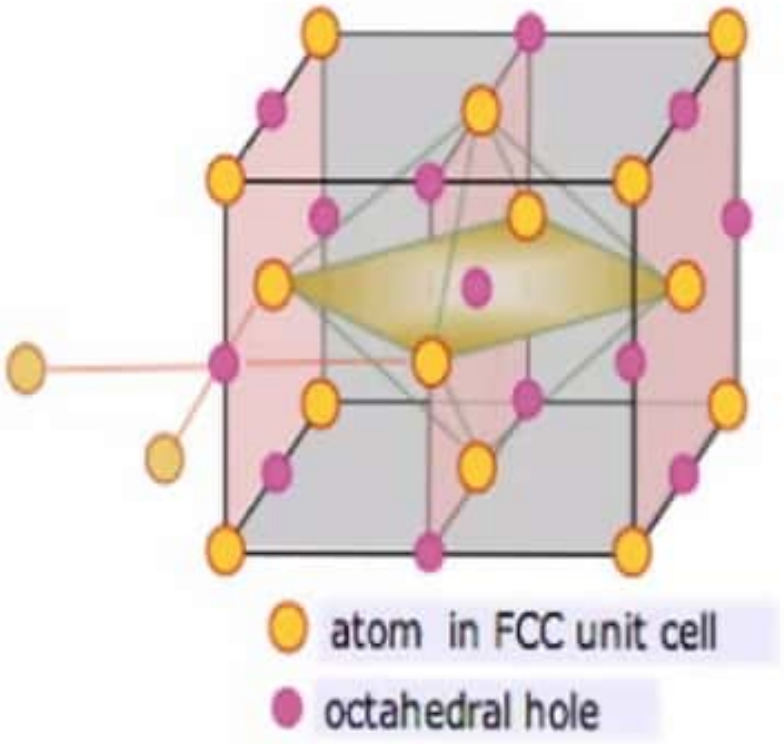
Ans.7.

Largest atom in the interstitial void of FCC Nickel without distortion

In FCC largest void is octahedral

$$\frac{R_{VOID}}{R_{ATOM}} = 0.414$$

$$R_{VOID} = 0.414 * R_{ni}$$



QUES.8.

Find the size of the largest sphere that will fit an interstitial void in a BCC crystal as a function of the atomic radius r. The void is located at (0, ½, ¼) and the other equivalent positions

Ans.8.

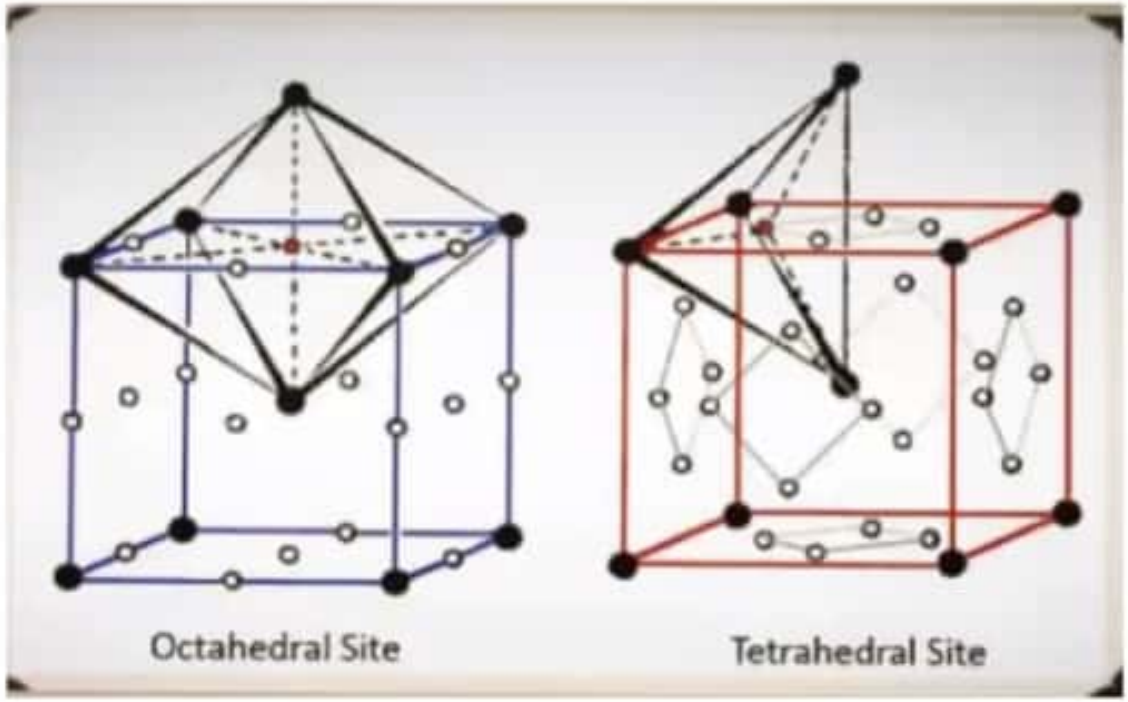
Largest void in BCC is located at

Tetrahedral void at $(0, \frac{1}{2}, \frac{1}{4})$

$\frac{R_{VOID}}{R_{ATOM}} = 0.225$

Octahedral void at $(\frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, 0, 0)$

$\frac{R_{VOID}}{R_{ATOM}} = 0.414$



Ques.9.

Aluminum has FCC structure. Its density is 2700 Kg/m^3. Calcul -ate the unit cell dimension and the atomic diameter.

Ans.9.

Al has FCC structure,

A_{al}=26.98 gm/mole

ρ=2700 Kg/m^3

$$\rho = \frac{A*n}{N*V}$$

$$2700 = \frac{26.98*4}{V*6.022*10^{23}}$$

V= 66.37*10^{-27} and $V=a^3$

a = 4.04 Å

For FCC $a\sqrt{2} = 4R$ R = 1.431 Å

D= 2R= 2.863 Å