Page No.	
Date	

Assignment No. 1A

Q.1 Derive the relation between lattice parameter 'a' and crystal density 'ρ'
A substance with fcc lattice has density 6250 kg/m^3 and molecular wt. 60.2. Calculate the lattice constant a.

→ Consider a cubic lattice of lattice constant 'a'.
If ρ is the density of the crystal then,
∴ Mass in each unit cell $= a^3\rho$ — (i)
where a^3 = volume of unit cell

If M is the molecular weight, N the Avagadro number then mass of each molecule $= \frac{M}{N}$

If n is the no. of molecules per unit cell, then

Mass in each unit cell $= \frac{nM}{N}$ — (ii)

from (i) & (ii), we get,

$$a^3 \rho = \frac{nM}{N}$$

$$a^3 = \frac{nM}{N\rho}$$

From this relation, the lattice constant 'a' can be calculated.

- $n = 4,$
  $M = 60.2 \ g/mol$
  $\rho = 6250 \ kg/m^3 = 6.25 \ g/cm^3$
  $N = 6.02 \times 10^{26} \ kg\text{-}mole = 6.02 \times 10^{23} /mole.$

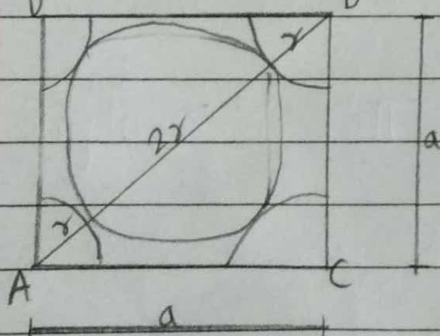
$$\therefore a^3 = \frac{4 \times 60.2}{6.02 \times 10^{23} \times 6.25}$$

$$a^3 = 64 \times 10^{-24}$$

$$a = 4 \times 10^{-8} \ cm$$

$$\therefore a = 4 \times 10^{-10} \ m$$
$$= 4 A^{\circ}$$

Q.2 Calculate the relation between atomic radius & lattice constant for BCC and FCC.



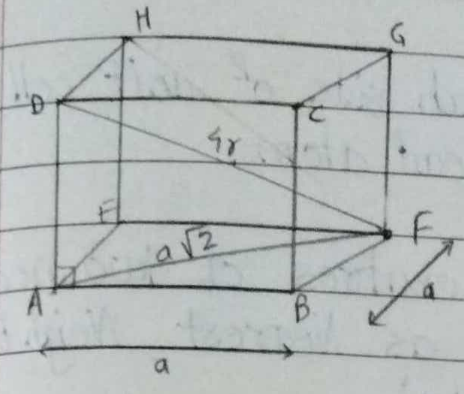
i) Face Centred Cubic Crystal.

$$AB^2 = AC^2 + BC^2$$
$$(4r)^2 = a^2 + a^2$$
$$16r^2 = 2a^2$$
$$r^2 = \frac{2a^2}{16}$$

$$r = \frac{a\sqrt{2}}{4} \times \frac{\sqrt{2}}{\sqrt{2}}$$

$$r = \frac{a}{2\sqrt{2}} \quad \Big| \quad \therefore a = 2\sqrt{2}\,r$$

ii) Base Centred Cubic Crystal.



cositer right angled ΔABF

$\therefore AF^2 = AB^2 + BF^2$

$= a^2 + a^2$

$= 2a^2$

$AF = \sqrt{2}\, a.$

now, consider right angled ΔDAF

$\therefore DF^2 = AD^2 + AF^2.$

$(4r)^2 = a^2 + (a\sqrt{2})^2$

$16r^2 = 3a^2$

$r^2 = \dfrac{3a^2}{16}$

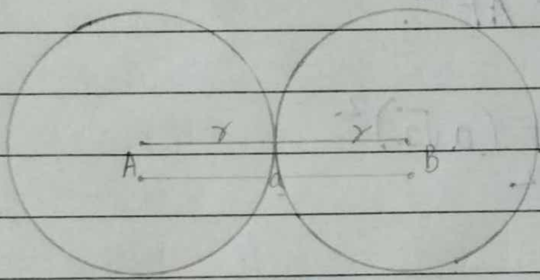
$\therefore r = \dfrac{a\sqrt{3}}{4}.$

$\therefore a = \dfrac{4}{\sqrt{3}} r.$

Q.3 Define atomic radius. Calculate atomic radii in SC, BCC and FCC lattices with suitable diagrams.

Lead exhibits FCC structure. Each side of unit cell is of 4.95 A°. Calculate radius of lead atom.

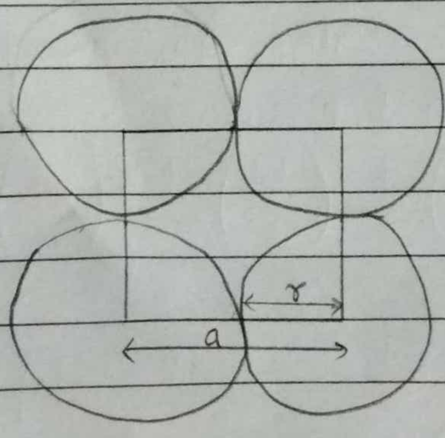
→ The distance between the centres of two nearest neighbouring atoms is called as Nearest Neighbour Distance, It is denoted by 'a'.



$a = 2r$.

If 'r' is considered to be radius of atom then $a = 2r$ i.e. the nearest neighbour distance is twice of the radius of atoms.

i) Simple Cubic Cell :

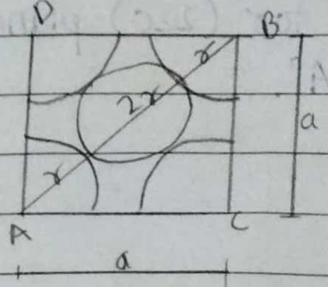


$$a = 2r$$

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

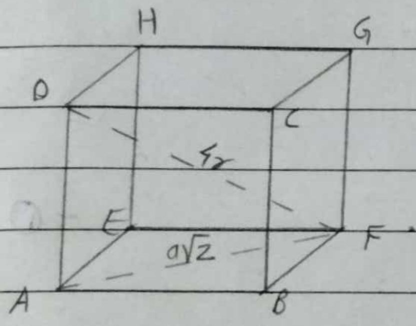
Page No. | Date

ii) Face Centered Cubic Cell :



$$AB^2 = AC^2 + BC^2$$
$$(r + 2r + r)^2 = a^2 + a^2$$
$$(4r)^2 = 2a^2$$
$$16r^2 = 2a^2$$
$$r = \frac{a\sqrt{2}}{4}.$$

iii) Body Centered Cubic Cell :



Consider right angled ΔABF.

$$AF^2 = AB^2 + BF^2$$
$$= a^2 + a^2$$
$$= 2a^2$$
$$AF = a\sqrt{2}.$$

now, consider righ angled ΔDAF.

$$DF^2 = AD^2 + AF^2$$
$$(4r)^2 = a^2 + (a\sqrt{2})^2$$
$$16r^2 = 3a^2$$

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

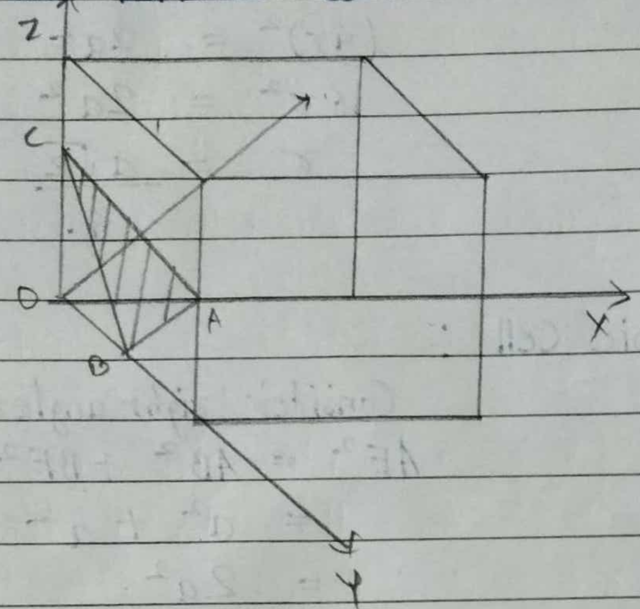
• $a = 4.95\ A^\circ$, FCC structure.

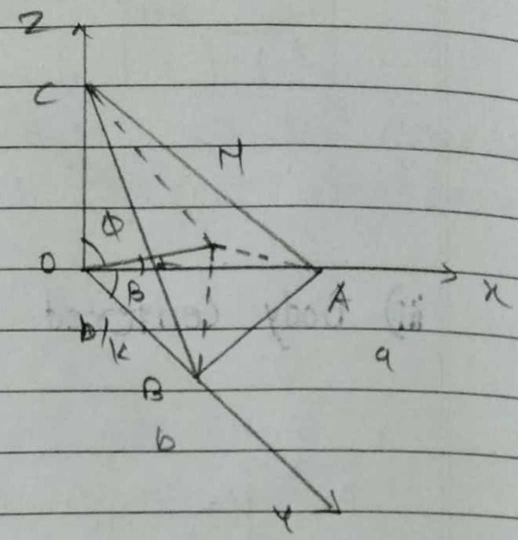
$\therefore\ r = \frac{a\sqrt{2}}{4} \times \frac{\sqrt{2}}{\sqrt{2}} = \frac{a}{2\sqrt{2}} = \frac{4.95 \times 10^{-10}}{2\sqrt{2}} = 1.75 \times 10^{-10}$

$\therefore$ radius of lead atom is $1.75\ A^\circ$

Page No.
Date

Q.4 Derive the relation between interplaner spacing 'd' defined by Miller Indices (hkl) and lattice parameter 'a'. Calculate the interplaner spacing for (220) plane where the lattice constant is 4.938 A°.





$$\cos \alpha = \frac{d}{a/h} = \frac{hd}{a} \quad -①$$

$$\cos \beta = \frac{d}{b/k} = \frac{kd}{b} \quad -②$$

$$\cos \phi = \frac{d}{c/l} = \frac{ld}{c} \quad -③$$

By cosine rule

$$\cos^2\alpha + \cos^2\beta + \cos^2\phi = 1$$

$$\left(\frac{hd}{a}\right)^2 + \left(\frac{kd}{b}\right)^2 + \left(\frac{ld}{c}\right)^2 = 1$$

$$d^2\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) = 1$$

Page No.
Date

$$d^2 = \frac{1}{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)}$$

$$d^2 = \frac{1}{\frac{h^2+k^2+l^2}{a^2}}$$

$$d^2 = \frac{a^2}{h^2+k^2+l^2}$$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$\therefore d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

This is the relation between interplaner spacing 'd' defined by Miller Indices (hkl) and lattice parameter 'a'.

- $a = 4.938\ A^\circ$; $hkl = 220$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{4.938\ A}{\sqrt{2^2+2^2+0^2}} = \frac{4.938}{\sqrt{8}} = 1.746\ A^\circ$$

Page No.
Date

Q.5 Define Packing Density. Find the packing density in SC, BCC, FCC lattices.

→ Packing Density is defined as ratio of volume of atoms per unit cell to the total volume of the unit cell.

i) Packing Density for Simple Cubic Crystal.

Volume of atom $= \frac{4}{3} \pi r^3$

volume of cube $= l \times b \times h$.

volume of cell $= a^3$

$= 8 r^3$.

$$P.D = \frac{4/3 \pi r^3}{8 r^3}$$

$$= \frac{\pi}{6}$$

ii) P.D for Body Centered Cubic Crystal.

volume of atom $= 4/3 \pi r^3 \times 2$

volume of unit cell $= a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3 = \frac{64 r^3}{3\sqrt{3}}$

$$P.D = \frac{2 \times \frac{4}{3} \pi r^3}{\frac{64 r^3}{3\sqrt{3}}} = \frac{\sqrt{3}\, \pi}{8}$$

Page No.
Date

iii) P.D for Face Centered Cubic Crystal.

volume of atom $= 4 \times \frac{4}{3} \pi r^3$

volume of cube $= a^3$
$= (\sqrt{2} \times 2 \times r)^3$
$= 16\sqrt{2}\, r^3$

$$P.D = \frac{4 \times 4/3\, \pi r^3}{16\sqrt{2}\, r^3}$$

$$= \frac{\pi}{3\sqrt{2}} \times \frac{\sqrt{2}}{\sqrt{2}}$$

$$= \frac{\sqrt{2}}{6} \pi.$$

Q.6 Derive the relation between crystal density 'ρ' & lattice parameter 'a'.
The density of copper is 8980 kg/m^3 and unit cell dimension is 3.61 A°. Atomic weight of copper is 63.54. Determine crystal structure.

→ Consider a cubic lattice of lattice constant 'a'
If ρ is the density of the crystal then,
∴ Mass in each unit cell $= a^3 \rho$
where a^3 = volume of unit cell

If M is the molecular weight, N is the Avagadro number then mass of each molecule $= \frac{M}{N}$

If n is the no. of molecules per unit cell, then Mass in each unit cell $= \frac{nM}{N}$ – (ii)

from (i) & (ii), we get,

$$a^3 \rho = \frac{nM}{N}$$

$$a^3 = \frac{nM}{N\rho}$$

From this relation, the lattice constant 'a' can be calculated.

• Density $(\rho) = 8980$, $M = 63.54$, $N = 6.02 \times 10^{26}$
$a = 3.61 \times 10^{-10}$ m.

$$n = \frac{N \rho a^3}{M} = \frac{(6.02 \times 10^{26})(8980)(3.61 \times 10^{-10})}{63.54}.$$

$n = 4$ atoms / unit cell.

∴ It is Face Centered Cubic Crystal.

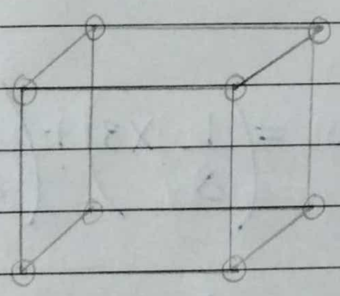
Q7 What is primitive and non premitive unit cells ? Find the number of atoms per unit cell in SC, BCC, FCC lattices.

→ i) Primitive Cell : Primitive cell is a type of unit cell which contains only one lattice point.

ii) Non-Primitive cell : The no. of additional lattice point per unit cell, may be more than one is Non-primitive cell.

1) Simple Cubic Crystal : One lattice point at each of the eight corners of unit cell. This type of unit cell is called SCC.

No. of atoms per unit :

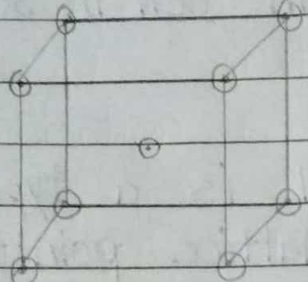


No. of atoms $= \frac{1}{8} \times 8 = 1$

→ No. of atoms for SCC is 1

2) Body Centered Cubic Crystal : There is one lattice point at each of the 8 corners and one at the center of cubic cell. is known as BCC.

No. of atoms per unit

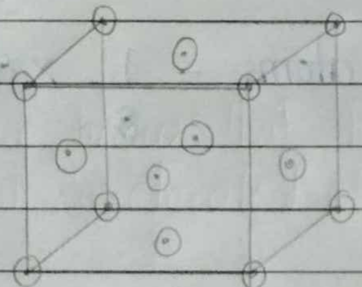


$$\text{No. of atoms} = \frac{1}{8} \times 8 + 1 = 2.$$

No. of atoms present in BCC is <u>2</u>.

3) Face Centered Cubic Crystal : There is one lattice point at each of the 8 corners and one lattice point at centers of each of 6 faces of cubic cell is known as FCC.

No. of atoms per unit.



$$\text{No. of atoms} = \left(\frac{1}{8} \times 8\right) + \left(\frac{1}{2} \times 6\right)$$

$$= 4.$$

No. of atoms present in FCC is <u>4.</u>