UNIT-4 Quantum physics

Planck's quantum theory of black body radiation:

- * planck's hypothesis was introduced by Max planck in 1900.
- * It explains the law of black body radiation.

Planck's theory

Assumptions

* A black body radiation chamber consist of large number of oscillating particles and it vibrates with all frepuencies are called atomic oscillators.

* The frequency of radiation is same as the frequency of oscillation.

* An oscillator cannot absorb or emit energy in a continuous manner. It is in the multiplies of small units called quantum. It is called photon.

$$E \propto \nu$$

$$\boxed{E = h\nu}$$

* The oscillator vibrating with frequency can have discrete energy values.

$$\boxed{E_n = nh\nu = nE}$$

Planck's law of radiation

Statement

The energy density of heat radiation emitted at a temperature T in λ & $\lambda + d\lambda$ is given by

$$\boxed{E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5 \left(e^{hc/\lambda kT} - 1\right)} \, d\lambda}$$

Where h → Planck's constant

c → Velocity of light

k → Boltzmann constant

T → Temperature

Derivation of planck's law of radiation:

Consider a black body consist of large number of atomic oscillators.

Average energy $\boxed{\bar{E} = \frac{E}{N}}$ ——— ①

where $E \rightarrow$ Total
$N \rightarrow$ Number of oscillators.

According to maxwell energy distribution law, Number of oscillators is given by

$$N_n = N_0 e^{-E_n/kT} \quad \text{——} \ ②$$

where $N_0 \rightarrow$ Number of oscillators in ground state
$k \rightarrow$ Boltzmann constant
$T \rightarrow$ Absolute Temperature

We know that $N = N_0 + N_1 + N_2 + N_3 + \cdots\cdots$ ——

From eqn ②,

$$\left.\begin{aligned} n=0 &\Rightarrow N_0 = N_0 e^{-E_0/kT} \\ n=1 &\Rightarrow N_1 = N_0 e^{-E_1/kT} \\ n=2 &\Rightarrow N_2 = N_0 e^{-E_2/kT} \end{aligned}\right\} \text{——} \ ④$$

Sub eqn ④ in eqn ③ we get

$$N = N_0 e^{-E_0/kT} + N_0 e^{-E_1/kT} + N_0 e^{-E_2/kT} + \cdots\cdots$$

We know that $E_n = nh\nu$.

$$\left.\begin{aligned} n=0, &\quad E_0 = 0 \\ n=1, &\quad E_1 = h\nu \\ n=2, &\quad E_2 = 2h\nu \end{aligned}\right\} \text{——} \ ⑥$$

Sub eqn ⑥ in eqn ⑤ we get

$$N = N_0 e^{0} + N_0 e^{-h\nu/kT} + N_0 e^{-2h\nu/kT} + \cdots\cdots$$

$$N = N_0 + N_0 e^{-h\nu/kT} + N_0 e^{-2h\nu/kT} + \cdots\cdots$$

Sub $x = e^{-h\nu/kT}$

$$\therefore N = N_0 + N_0 x + N_0 x^2 + \cdots\cdots$$

$$= N_0 (1 + x + x^2 + \cdots\cdots)$$

$$= N_0 \left[\frac{1}{(1-x)}\right] \quad (\because \text{using binomial Series})$$

$$\boxed{N = \frac{N_0}{(1-x)}} \quad \text{——} \ ⑦$$

Total energy $\Rightarrow E = E_0 N_0 + E_1 N_1 + E_2 N_2 + \cdots\cdots$ —— ⑧

sub eqn ④ + ⑥ in eqn ⑧ we get

$$E = 0 \times N_0 e^{0} + h\nu N_0 e^{-h\nu/kT} + 2h\nu e^{-2h\nu/kT} + \cdots\cdots$$

$$E = h\nu N_0 e^{-h\nu/kT} + 2h\nu N_0 e^{-2h\nu/kT} + \cdots\cdots$$

sub $x = e^{-h\nu/kT}$

$$\therefore E = h\nu N_0 x + 2h\nu N_0 x^2 + \cdots\cdots$$

$$= h\nu N_0 x (1 + 2x + \cdots\cdots)$$

$$E = h\nu N_0 x \left[\frac{1}{(1-x)^2}\right] \quad (\because \text{using binomial Series})$$

$$\boxed{E = \frac{h\nu N_0 x}{(1-x)^2}} \quad \text{——} \ ⑨$$

Sub eqn ⑦ + ⑨ in eqn ① we get

$$\bar{E} = \frac{h\nu \cancel{N_0} x}{(1-x)^{\cancel{2}}} \times \frac{\cancel{(1-x)}}{\cancel{N_0}}$$

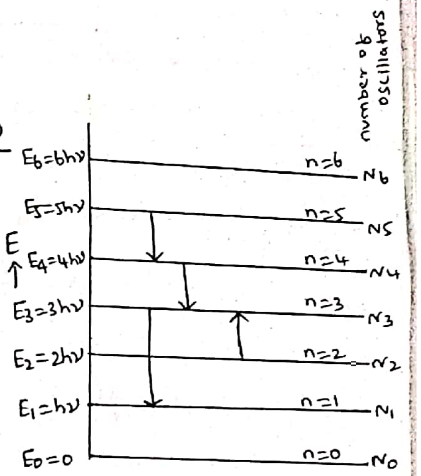
$$= \frac{h\nu x}{1-x}$$

$$\bar{E} = \frac{h\nu \cancel{x}}{\cancel{x}(1/x - 1)}$$

We know that $x = e^{-h\nu/kT}$

$$\therefore \bar{E} = \frac{h\nu}{\left[\frac{1}{e^{-h\nu/kT}} - 1\right]}$$

$$\boxed{\bar{E} = \frac{h\nu}{e^{h\nu/kT} - 1}} \quad \text{——} \ ⑩$$



Energy diagram of Planck's oscillator

Number of oscillators per unit volume is given by

$$\boxed{\frac{8\pi \, d\lambda}{\lambda^4}} \quad \text{——} \ ⑪$$

⑪

The energy density of radiation } = { Number of oscillators per unit volume } × {

$$E_\lambda \cancel{d\lambda} = \frac{8\pi \cancel{d\lambda}}{\lambda^4} \times \frac{h\nu}{e^{h\nu/kT}-1}$$

$$E_\lambda = \frac{8\pi h\nu}{\lambda^4 (e^{h\nu/kT}-1)}$$

Sub $\nu = \frac{c}{\lambda}$

$$\therefore E_\lambda = \frac{8\pi h\left(\frac{c}{\lambda}\right)}{\lambda^4 (e^{hc/\lambda kT}-1)}$$

$$\boxed{E_\lambda = \frac{8\pi hc}{\lambda^5 (e^{hc/\lambda kT}-1)}} \quad \text{———} \quad ⑫$$

The above equation represents planck's rad law in terms of wavelength.

Note

In terms of frequency,

$$\lambda = \frac{c}{\nu}, \quad d\lambda = \left|-\frac{c}{\nu^2} d\nu\right|$$

$$\therefore E_\nu \cancel{d\nu} = \frac{8\pi hc}{(c/\nu)^5} \times \frac{1}{e^{h\nu/kT}-1} \left[\left|-\frac{c}{\nu^2}\cancel{d\nu}\right|\right]$$

$$E_\nu = \frac{8\pi h\cancel{c} \times \nu^{\cancel{5}\,3}}{c^{\cancel{5}\,3}} \times \frac{\cancel{c}}{\nu^{\cancel{2}}} \cdot \frac{1}{e^{h\nu/kT}-1}$$

$$\boxed{E_\nu = \frac{8\pi h\nu^3}{c^3 (e^{h\nu/kT}-1)}} \quad \text{———} \quad ⑬$$

The above equation represents planck's radiation law in terms of frequency.

(i) Deduction of wiens displacement law:

* This law holds good for shorter wavelength.

* when λ is very small, $1/\lambda$ is large.

$$\therefore \frac{hc}{\lambda kT} >>> 1$$

$$e^{hc/\lambda kT} >>>> 1$$

so neglect 1 we get from eqn ⑫

$$\boxed{E_\lambda = \frac{8\pi hc}{\lambda^5 (e^{hc/\lambda kT})}}$$

(ii) Deduction of Rayleigh Jeans law:

* This law holds good for longer wavelength.

* when λ is very large, $\frac{1}{\lambda}$ is small.

$$\therefore \frac{hc}{\lambda kT} << 1$$

$$\therefore e^{hc/\lambda kT} = 1 + \frac{hc}{\lambda kT} \qquad (\because e^x = 1 + x + \dots)$$

so eqn ⑫ reduces to

$$E_\lambda = \frac{8\pi hc}{\lambda^5 \left[\cancel{1} + \frac{hc}{\lambda kT} - \cancel{1}\right]}$$

$$= \frac{8\pi \cancel{hc}\, \cancel{\lambda} kT}{\lambda^{\cancel{5}\,4} \cancel{hc}}$$

$$\boxed{E_\lambda = \frac{8\pi kT}{\lambda^4}}$$

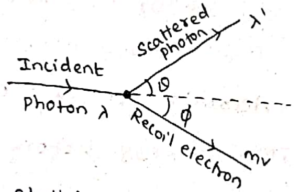
Compton Effect

Statement

When a beam of X-rays is scattered by a substance, the scattered radiation consists of two components, one has same wavelength λ as incident ray and the other has slightly longer wavelength λ'. This change in wavelength is called compton shift. This phenomenon is called compton effect.

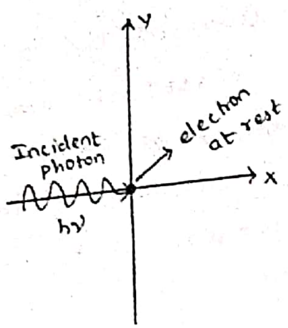
Explanation

- It was explained on the basis of quantum theory.
- It obey law of conservation of energy & momentum.
- when a photon of energy $h\nu$ collides with free electron at rest, the photon transfer some of the energy to electron.
- The electron gains kinetic energy and it recoils with velocity v.
- Hence the scattered photon has lower energy than incident photon.

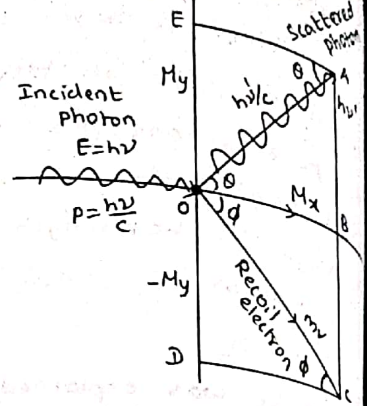


Theory of compton Effect

- consider an x-ray photon striking an electron at rest.
- It is scattered through an angle θ.
- consider the frequency of scattered photon is ν' & energy is $h\nu'$.
- During collision, the x-ray photon gives some amount of energy to free electron.
- The free electron gains energy & the recoil electron is formed with an angle ϕ.



Before collision



After collision

Total Energy Before Collision :

Energy of incident photon $= h\nu$

Energy of electron at rest $= m_0c^2$

Total energy before collision $= h\nu + m_0c^2$ —— ①

Total Energy After collision:

Energy of scattered photon $= h\nu'$

Energy of recoil electron $= mc^2$

Total Energy after collision $= h\nu' + mc^2$ —— ②

According to law of conservation of energy,

Total energy before collision = Total energy after coll

$$\boxed{h\nu + m_0c^2 = h\nu' + mc^2} \quad \text{——} ③$$

Total momentum along x-axis

Before collision

Momentum of photon along x-axis $= \frac{h\nu}{c}$

Momentum of electron along x-axis $= 0$

Total momentum along x-axis before collision $= \frac{h\nu}{c}$

After collision

Momentum of photon along x-axis $(\Delta ABO) = \frac{h\nu'}{c}$

Momentum of electron along x-axis $(\Delta OBC) = mv\cos\phi$

Total momentum along x-axis after collision is

$$= \frac{h\nu'}{c}\cos\theta + mv\cos\phi \quad \text{——} ⑤$$

Applying law of conservation of momentum,

$$\begin{Bmatrix}\text{Total momentum before} \\ \text{collision}\end{Bmatrix} = \begin{Bmatrix}\text{Total momentum} \\ \text{after collision}\end{Bmatrix}$$

$$\boxed{\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\theta + mv\cos\phi} \quad \text{——} ⑥$$

Total momentum along Y-axis

Before collision

Momentum of photon along Y-axis $= 0$

Momentum of electron along Y-axis $= 0$

Total momentum along Y-axis before collision $= 0$ —— ⑦

After collision

Momentum of photon along Y-axis $(\Delta OAE) = \frac{h\nu'}{c}\sin\theta$

Momentum of electron along Y-axis $(\Delta OCD) = -mv\sin\phi$

Total momentum along Y-axis after collision is

$$= \frac{h\nu'}{c}\sin\theta - mv\sin\phi \quad \text{——} ⑧$$

According to law of conservation of momentum,

$$\begin{Bmatrix}\text{Total momentum before} \\ \text{collision}\end{Bmatrix} = \begin{Bmatrix}\text{Total momentum} \\ \text{after collision}\end{Bmatrix}$$

$$\boxed{0 = \frac{h\nu'}{c}\sin\theta - mv\sin\phi} \quad \text{——} ⑨$$

eqn ⑥ reduces to

$$\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\theta + mv\cos\phi$$

$$\frac{h\nu}{c} - \frac{h\nu'}{c}\cos\theta = mv\cos\phi$$

$$h\nu - h\nu'\cos\theta = mcv\cos\phi$$

$$mcv\cos\phi = h(\nu - \nu'\cos\theta) \quad \text{——} ⑩$$

eqn ⑨ reduces to

$$0 = \frac{h\nu'}{c}\sin\theta - mv\sin\phi$$

$$mv\sin\phi = \frac{h\nu'}{c}\sin\theta$$

$$mcv\sin\phi = h\nu'\sin\theta \quad \text{——} \quad ⑪$$

$⑩^2 + ⑪^2 \Rightarrow$

$$(mcv\cos\phi)^2 + (mcv\sin\phi)^2 = h^2(\nu-\nu'\cos\theta)^2 + (h\nu'\sin\theta)^2$$

$$m^2c^2v^2\cos^2\phi + m^2c^2v^2\sin^2\phi = h^2\left[\nu^2+\nu'^2\cos^2\theta - 2\nu\nu'\cos\theta\right] + h^2\nu'^2\sin^2\theta$$

$$m^2c^2v^2\underbrace{(\cos^2\phi+\sin^2\phi)}_{1} = h^2\left[\nu^2+\nu'^2\cos^2\theta - 2\nu\nu'\cos\theta + \nu'^2\sin^2\theta\right]$$

$$m^2c^2v^2 = h^2\left[\nu^2 - 2\nu\nu'\cos\theta + \nu'^2\underbrace{(\cos^2\theta+\sin^2\theta)}_{1}\right]$$

$$m^2c^2v^2 = h^2\left[\nu^2 - 2\nu\nu'\cos\theta + \nu'^2\right] \quad \text{——} \quad ⑬$$

eqn ③ reduces to

$$h\nu + m_oc^2 = h\nu' + mc^2$$

$$mc^2 = m_oc^2 + h\nu - h\nu'$$

$$mc^2 = m_oc^2 + h(\nu-\nu') \quad \text{——} \quad ⑭$$

squaring,

$$m^2c^4 = \left[m_oc^2 + h(\nu-\nu')\right]^2$$

$$= m_o^2c^4 + h^2(\nu-\nu')^2 + 2hm_oc^2(\nu-\nu')$$

$$m^2c^4 = m_o^2c^4 + h^2(\nu^2+\nu'^2-2\nu\nu') + 2hm_oc^2(\nu$$

eqn ⑮ – eqn ⑬

$$m^2c^4 - m^2c^2v^2 = m_o^2c^4 + h^2(\nu^2+\nu'^2-2\nu\nu') + 2hm_oc^2(\nu-\nu') - h^2(\nu^2-2\nu\nu'\cos\theta+\nu'^2)$$

$$m^2c^2(c^2-v^2) = m_o^2c^4 + \cancel{h^2\nu^2} + \cancel{h^2\nu'^2} - 2h^2\nu\nu' + 2hm_oc^2(\nu-\nu') - \cancel{h^2\nu^2} + 2h^2\nu\nu'\cos\theta - \cancel{h^2\nu'^2}$$

$$m^2c^2(c^2-v^2) = m_o^2c^4 - 2h^2\nu\nu'(1-\cos\theta) + 2hm_oc^2(\nu-\nu')$$

From theory of relativity,

$$\boxed{m = \frac{m_o}{\sqrt{1-\frac{v^2}{c^2}}}} \quad \text{——} \quad ⑰$$

squaring,

$$m^2 = \frac{m_o^2}{1-\frac{v^2}{c^2}}$$

$$m^2 = \frac{m_o^2}{\left(\frac{c^2-v^2}{c^2}\right)}$$

$$m^2(c^2-v^2) = m_o^2c^2$$

Multiplying c^2 on both sides,

$$m^2c^2(c^2-v^2) = m_o^2c^4 \quad \text{——} \quad ⑱$$

equating eqn ⑯ & eqn ⑱

$$\cancel{m_o^2c^4} = \cancel{m_o^2c^4} - 2h^2\nu\nu'(1-\cos\theta) + 2hm_oc^2(\nu-\nu')$$

$$\cancel{2}h^{\cancel{2}}\nu\nu'(1-\cos\theta) = \cancel{2}\cancel{h}m_oc^2(\nu-\nu')$$

$$\frac{\nu-\nu'}{\nu\nu'} = \frac{h}{m_oc^2}(1-\cos\theta)$$

$$\frac{\nu}{\nu\nu'} - \frac{\nu'}{\nu\nu'} = \frac{h}{m_oc^2}(1-\cos\theta)$$

$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_oc^2}(1-\cos\theta)$$

Multiplying c on both sides

$$\frac{c}{\nu'} - \frac{c}{\nu} = \frac{h\cancel{c}}{m_oc^2}(1-\cos\theta)$$

$$\lambda' - \lambda = \frac{h}{m_oc}(1-\cos\theta)$$

$$\boxed{d\lambda = \frac{h}{m_oc}(1-\cos\theta)}$$

Special cases :

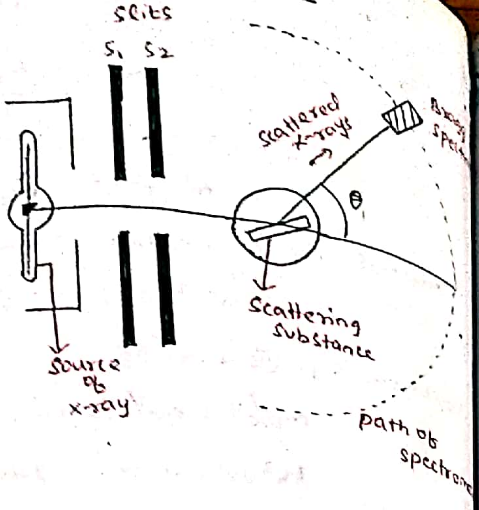
Case (i) when $\theta = 0$; $d\lambda = 0$

Case (ii) when $\theta = 90°$; $d\lambda = \frac{h}{m_oc} = 0.0243\,\text{Å}$ (compton wavelength)

Case (iii) when $\theta = 180°$; $d\lambda = \frac{h}{m_oc}(1+1) = \frac{2h}{m_oc} = 0.0486\,\text{Å}$.

Thus the change in wavelength is maximum at $\theta = 180°$.

Experimenta

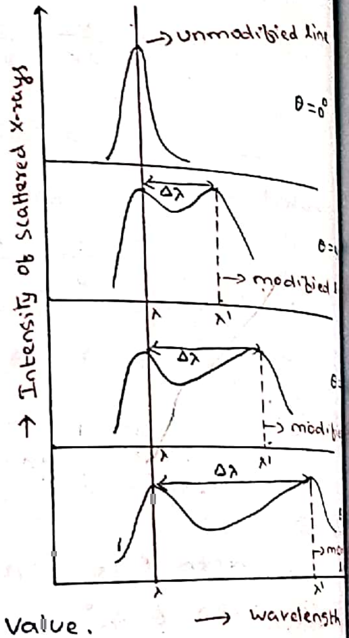


* A beam of monochromatic x-rays is made to incident on a scattering substance.

* The scattered x-rays are received by Bragg's spectrometer.

* The intensity is measured for various scattering angles.

* A graph is plotted between intensity and wavelength.



* It is found that the curves have two peaks, one corresponds to unmodified radiation and other corresponds to modified radiation.

* The difference between two peaks gives compton shift.

* Greater the scattering angle, greater the compton shift.

$$\boxed{\lambda'-\lambda = d\lambda = \frac{h}{m_0 c}(1-\cos\theta)}$$

* The change in wavelength $d\lambda = 0.0243\,\text{Å}$ at $\theta = 90^\circ$ is found good agreement with theoretical value.

* Thus, compton effect is experimentally verified.

Schroedinger wave Equation:

* It describes the wave nature of the particle in mathematical form.

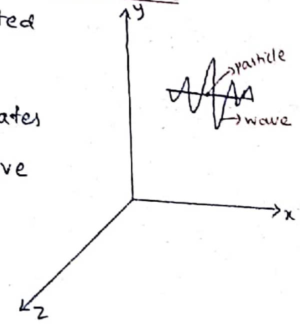
* It is the basic equation of motion for matter waves.

Forms of Schroedinger wave equation:

There are two forms of Schroedinger wave equation.

(i) Time independent wave equation
(ii) Time dependent wave equation

(i) Schroedinger time independent wave equation:



* consider a wave associated with a moving particle.

* Let x, y, z be the coordinates of the particle, ψ be the wave function at time t.

The classical differential equation for wave motion is

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \text{— ①}$$

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \left[\because \nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right.$$

└ ② Laplacian operator]

The solution of eqn ② is

$$\psi(x,y,z,t) = \psi_0(x,y,z)\,e^{-i\omega t}$$

$$\psi = \psi_0 e^{-i\omega t} \quad \text{— ③}$$

ψ_0 → amplitude
ω → angular velocity

Diff

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t} \quad \text{— ④}$$

Diff again w.r.to 't'

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega)\psi_0 e^{-i\omega t}$$

$$= -\omega^2\psi \quad \text{— ⑤}$$

Sub eqn ⑤ in eqn ②

$$\nabla^2\psi = \frac{1}{v^2}(-\omega^2\psi)$$

$$\nabla^2\psi + \frac{\omega^2}{v^2}\psi = 0 \quad \text{— ⑥}$$

Sub, $\omega = \frac{2\pi v}{\lambda}$

$$\frac{\omega}{v} = \frac{2\pi}{\lambda}$$

$$\frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2} \quad \text{— ⑦}$$

Sub eqn ⑦ in ⑥

$$\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0 \quad \text{— ⑧}$$

$$\lambda = \frac{h}{mv} \; ; \; \lambda^2 = \frac{h^2}{m^2v^2}$$

$$\nabla^2\psi + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \quad \text{— ⑨}$$

We know that

Total energy = potential energy + kinetic ener

$$E = V + \frac{1}{2}mv^2$$

$$\frac{1}{2}mv^2 = E - V$$

$$mv^2 = 2(E-V)$$

$$m^2v^2 = 2m(E-V) \quad \text{— ⑩}$$

sub eqn ⑩ in ⑨

$$\nabla^2\psi + \frac{4\pi^2}{h^2} \cdot 2m(E-V)\psi = 0$$

W.K.T $\hbar = h/2\pi \; ; \; \hbar^2 = \frac{h^2}{4\pi^2}$

$$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0} \quad \text{— ⑪}$$

If we consider 1D motion

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{— ⑫}$$

(ii) Schroedinger time dependent wave equation:

The Solution of classical differential eqn is

$$\psi(x,y,z,t) = \psi_0(x,y,z)e^{-i\omega t} \quad \text{— ①}$$

Diff w.r.to 't'

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t} \quad \text{— ②}$$

$$= -i(2\pi\nu)\psi_0 e^{-i\omega t}$$

$$= -2\pi i\nu\psi$$

$$= -2\pi i\left(\frac{E}{h}\right)\psi$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

×by i

$$i\frac{\partial \psi}{\partial t} = \frac{E}{\hbar}\psi$$

$$E\psi = i\hbar\frac{\partial \psi}{\partial t} \quad \text{— ③}$$

Schrodinger time independent eqn is

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi - V\psi$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad \text{——} \; ④$$

sub eqn ④ in ③

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\boxed{H\psi = E\psi}$$

where H → Hamiltonian operator

E → Energy operator.

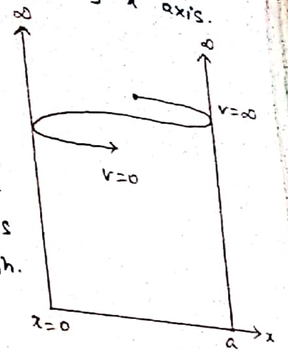
Particle in a one dimensional Rigid box :

* Consider a particle of mass m moving in a rigid box at $x=0$ and $x=a$ along x axis.

* The particle is moving back & forth between the walls.

* The potential energy of the particle inside the box is zero.

* The potential energy of the particle is infinite outside the walls because the walls are infinetely high.



The potential function is

$V(x) = 0$ for $0 < x < a$

$V(x) = \infty$ for $0 \geq x \geq a$

Schrodinger time independent wave equation for 1D is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{——} \; ①$$

Since $V=0$,

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

sub $\frac{2mE}{\hbar^2} = k^2$

$$\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{——} \; ②$$

The general solution is

$$\psi(x) = A\sin kx + B\cos kx \quad \text{——} \; ③$$

where A & B are constants. It is determined by applying boundary conditions.

Condition 1 : $\psi = 0$ at $x = 0$

$$0 = A\sin 0 + B\cos 0$$

$$\boxed{B=0}$$

$$0 = A \sin ka + 0$$

$$A \neq 0, \quad \sin ka = 0$$

$$\sin n\pi = 0$$

$$\therefore \quad ka = n\pi$$

$$k = \frac{n\pi}{a}$$

$$k^2 = \frac{n^2\pi^2}{a^2} \quad \text{——} \ ④$$

W.K.T $k^2 = \frac{2mE}{\hbar^2} = \frac{2mE \times 4\pi^2}{h^2}$

$$= \frac{8\pi^2 mE}{\hbar^2} \quad \text{——} \ ⑤$$

Equating ④ & ⑤

$$\frac{n^2\cancel{\pi^2}}{a^2} = \frac{8\cancel{\pi^2}mE}{h^2}$$

Energy of the particle $\Big\}$ $E_n = \frac{n^2h^2}{8ma^2}$

$$\psi_n(x) = A \sin \frac{n\pi x}{a}$$

Each value of En is called Eigen value & the corresponding ψn is called eigen function.

Normalisation of wave function:

The constant A is determined by normalisation of wave function.

The probability density $\psi^*\psi$ is

$$\psi^*\psi = A \sin \frac{n\pi x}{a} \times A \sin \frac{n\pi x}{a}$$

$$= A^2 \sin^2 \frac{n\pi x}{a}$$

∴ The probability of finding the particle inside the box of length a is

$$\int_0^a \psi^*\psi \, dx = 1$$

$$\int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$A^2 \int_0^a \left[\frac{1 - \cos \frac{2n\pi x}{a}}{2}\right] dx = 1$$

$$\frac{A^2}{2}\left[\int_0^a dx - \int_0^a \cos \frac{2n\pi x}{a} \, dx\right] = 1$$

$$\frac{A^2}{2}\left[(x)_0^a - \left(\frac{\sin \frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\right)_0^a\right] = 1$$

$$\frac{A^2}{2}(a) = 1$$

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

$$\boxed{A = \sqrt{\frac{2}{a}}}$$

The eigen function is

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

The above equation is called normalised eigen function.

Special cases:

(i) for n=1

$$E_1 = \frac{h^2}{8ma^2}$$

$$\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

(ii) for $n = 2$

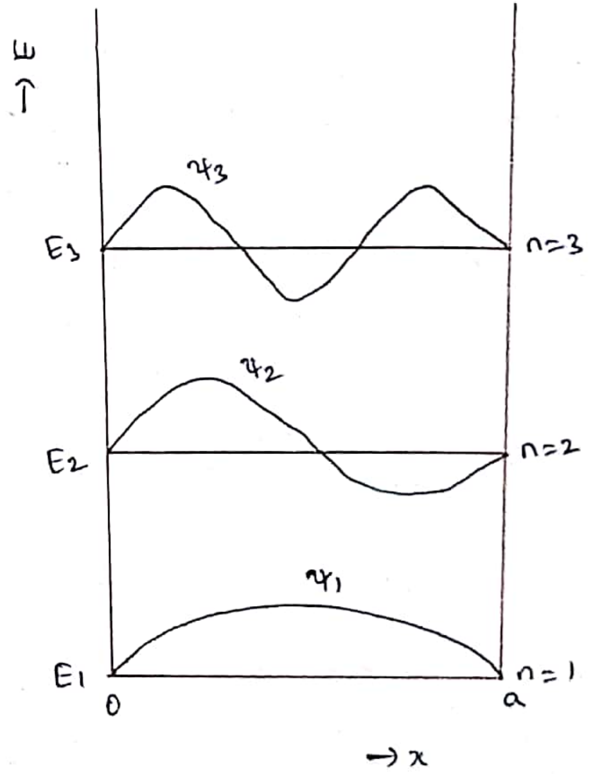
$$E_2 = \frac{4h^2}{8ma^2} = 4E_1$$

$$\psi_2(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{2\pi x}{a}\right)$$

(iii) for $n = 3$

$$E_3 = \frac{9h^2}{8ma^2} = 9E_1$$

$$\psi_3(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{3\pi x}{a}\right)$$



SCANNING TUNNELLING MICROSCOPE

- A Microscope is a device which is used to view the magnified image of the smaller object which cannot be clearly seen through the naked eye.
- In 1980, Gerd Binning and Heinrich Rohrer invented a new type of microscope called Scanning Tunnelling Microscope.

PRINCIPLE

- The basic principle is the tunnelling of electron between the sharp metallic tip of probe and surface of the sample.
- Here constant tunnelling current is maintained by adjusting the tip of the probe and sample with an air gap for electron to tunnel.
- It is used to scan atom by atom and line by line of the sample and the topography of the sample is recorded in the computer.

CONSTRUCTION

- It consists of a probe in which a small thin metal wire is etched such that the tip of the probe will have only one atom.
- The tip is connected to the scanner using a personal computer.
- The sample for which the image has to be recorded is kept below the tip of the probe at a particular distance in such a way that the tip should not touch the sample.
- Necessary circuit connections along with an amplifier are provided to measure the tunnelling current.

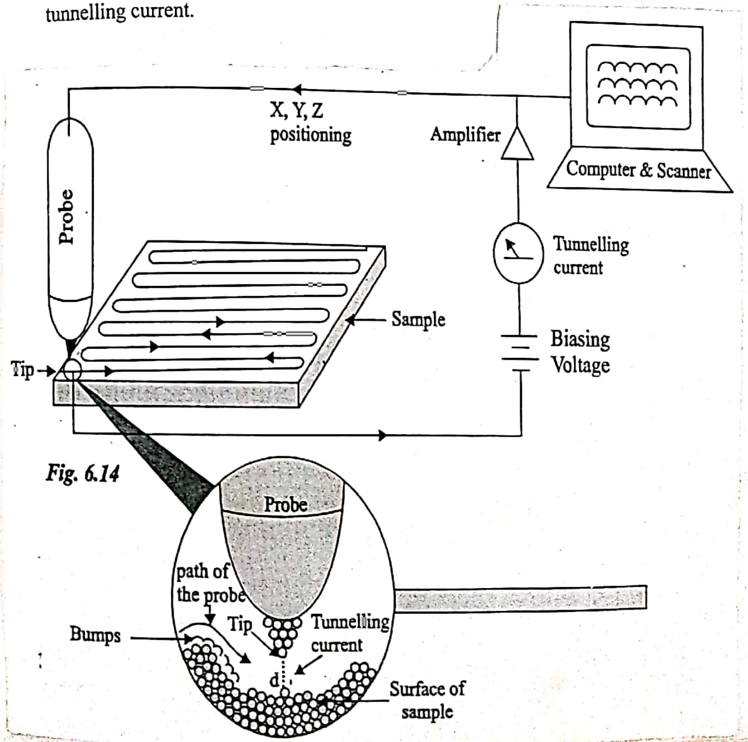


Fig. 6.14

WORKING

- The circuit is switched ON and necessary biasing voltage is given to the probe.
- Due to biasing, the electrons will tunnel or jump between the tip of the probe and sample and therefore produces small electric current called tunnelling current.
- The tunnelling current flows through the circuit only if the tip is in contact with sample through the small air gap at a distance of 'd'.
- The current produced is amplified and measured in computer.
- It is found that the current increases or decreases based on the distance between the tip of the probe and sample.
- The current in the circuit should be monitored in such a way that it should be maintained constant.
- Therefore, for maintaining constant current, the distance between the tip and the sample should be continuously adjusted.
- The fluctuations between the tip and sample is accurately recorded as a result, a bumps is obtained in the computer.
- In a similar way the tip is scanned atom by atom and line by line of the sample and the topography of the sample is recorded in the sample.
- It does not show the picture of the atom rather it records only the exact position of atoms.

ADVANTAGES

- It can scan the topography atom by atom.
- It is the latest technique.
- Very accurate measurement shall be obtained.
- Magnification is up to nanoscale.

DISADVANTAGES

- Even a very small sound will disturb the measurement setup.
- It should be kept in vacuum because even a dust particle may damage the tip of the probe.
- Cost is high.
- More complex.

APPLICATIONS

- It is used to produce Integrated circuits.
- It is used in Bio medical devices.
- It is used in Research labs.
- They are used in material science.

Engineering Physics

UNIT-5 - Crystal Physics

Characteristics of Unit cell :

A unit cell is characterised by following properties.

- Number of atoms per unit cell
- Coordination number
- Nearest neighbouring distance & Atomic radius
- Atomic packing factor (APF) or density of packing.

Number of atoms per unit cell :

Total number of atoms present in the unit cell.

Coordination number :

→ number of nearest atoms directly surrounding a particular atom in a crystal.

→ It gives information about the packing of atom (i.e) whether it is closely packed or loosely packed.

→ If C.N is high → more closely packed.

→ If C.N is low → loosely packed.

Nearest neighbouring distance (2r) :

→ distance between the centres of 2 nearest neighbouring atoms.

→ It is denoted as $a = 2r$

Atomic radius (r) :

→ half of the nearest neighbouring distance.

→ It is denoted by r.

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

(iv) Atomic packing of Packing:

→ ratio of total volume occupied by the at in the unit cell to the total volume of unit cell.

$$APF = \frac{\text{Total volume occupied by the atoms in the unit cell } (v)}{\text{total volume of unit cell } (V)}$$

$$= \frac{\text{number of atoms per unit cell} \times \text{volume of 1 atom}}{\text{Total volume of unit cell.}}$$

→ It has no unit.

→ If packing factor is high → closely packed

→ If packing factor is low → Loosely packed.

Crystal structure :

Cubic - SC, BCC & FCC

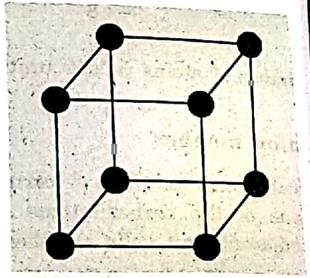
(a) Simple cubic structure :

* simplest & easiest crystal structure.

* one atom at each of 8 corners of unit cell.

* These atoms touch each other along cube edge.

(i) No. of atoms per unit cell :



* contains 8 atoms ; one atom at each corner of unit cell.

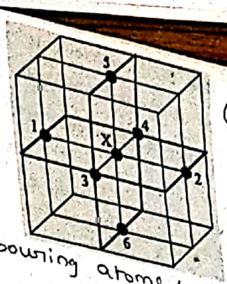
* Each corner atom is shared by 8 surrounding unit cell.

* Share of each unit cell = $\frac{1}{8}$ of each corner atom.

∴ Total number of atoms in one unit cell } = $\frac{1}{8} \times 8$ = 1 atom.

Hence number of atom per unit cell = 1

(ii) Coordination number :



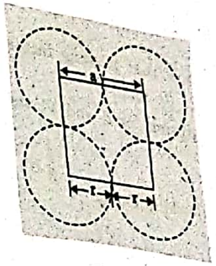
* It has 8 corner atoms.

* consider one of the corner atom. It is shared by 8 adjacent unit cell.

* There are 4 nearest neighbouring atoms & 2 more nearest neighbouring atoms one directly above & one directly below to x.

* Therefore the coordination number is 4+2 = 6

(iii) Atomic Radius :



* consider a face of a unit cell.

* atoms touch each other along the edges of the cube.

* distance between the centres of two nearest neighbouring atoms = a

∴ 2r = a

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

(iv) Atomic Packing Factor (APF):

$$APF = \frac{v}{V}$$

$$= \frac{\text{number of atoms per unit cell} \times \text{volume of 1 atom}}{\text{Total volume of unit cell}}$$

$$= \frac{1 \times \frac{4}{3}\pi r^3}{a^3}$$

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

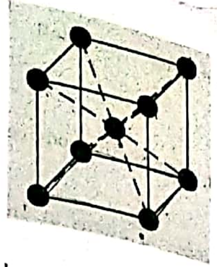
$$= \frac{\frac{\cancel{4}}{3}\pi \times \frac{\cancel{a^3}}{\cancel{8}2}}{\cancel{a^3}}$$

$$= \pi/6 = 0.52 = 52\%$$

* 52% of volume is occupied by atoms 48% of volume is vacant.

* Example : Polonium (Po)

(b) Body centred cubic



The unit cell consist of one atom at each corner of the cube and one atom at the body centre.

(i) Number of atoms per unit cell:

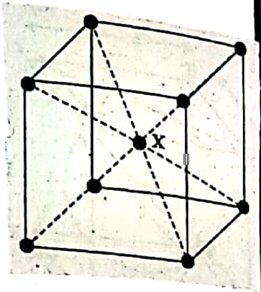
* Each corner atom is shared by surrounding unit cell $\Big\} = \frac{1}{8} \times 8 = 1$

* The atom present at the body centre $\Big\} = 1$

$\overline{\quad 2 \quad}$

$\therefore$ Number of atoms per unit cell $= 2$

(ii) Coordination number:



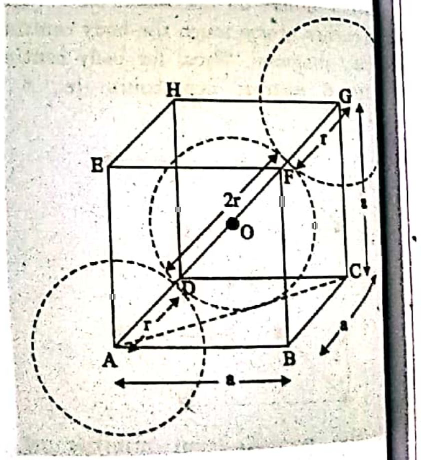
* consider an atom x present at the body centre of unit cell.

* Eight atoms are present at the eight corners of unit cell.

* These corner atoms touch the body centred atom along the diagonal.

$\therefore$ Coordination number $= 8$

(iii) Atomic radius:



* The corner atom do not touch each other and each corner atom touches the central atom.

* The nearest neighbouring atoms are corner atoms A and G and the body centre atom is o.

* Consider the atoms at A, G and centre O.

* These atoms lie in straight line along diagonal AG.

From right angled ΔABC,

$$AC^2 = AB^2 + BC^2$$
$$= a^2 + a^2$$
$$= 2a^2$$

From right angled ΔACG

$$AG^2 = AC^2 + CG^2$$
$$(4r)^2 = 2a^2 + a^2$$
$$16r^2 = 3a^2$$
$$r^2 = \frac{3a^2}{16}$$
$$\boxed{r = \frac{\sqrt{3}a}{4}}$$

(iv) Atomic Packing Factor: (APF):

$$APF = \frac{v}{V}$$

$$= \frac{\text{number of atoms per unit cell} \times \text{Volume of 1atom}}{\text{Total volume of unit cell}}$$

$$= \frac{2 \times \frac{4}{3}\pi r^3}{a^3}$$

$$= \frac{2 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}a}{4}\right)^3}{a^3}$$

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

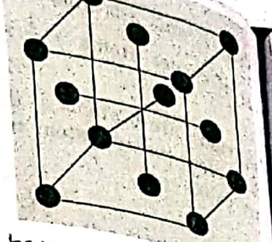
$$= \frac{\pi\sqrt{3}}{8} = 0.68 = 68\%$$

* 68% of volume is occupied by atoms.

32% of volume is vacant.

* Example: Tungsten, chromium.

* The unit cell consist of one atom at each corner of the cube and one atom at the centre of each face.



* The structure is close packed because each atom has 12 nearest neighbours.

(i) Number of atoms per unit cell :

* Each corner atom is surrounded by 8 unit cell $\left.\right\} = \frac{1}{8} \times 8 = 1$

* 6 atoms at the face centre of cubic, it is shared by 2 unit cell $\left.\right\} = \frac{1}{2} \times 6 = 3$

$$\overline{\underline{4}}$$

∴ Number of atoms per unit cell = 4.

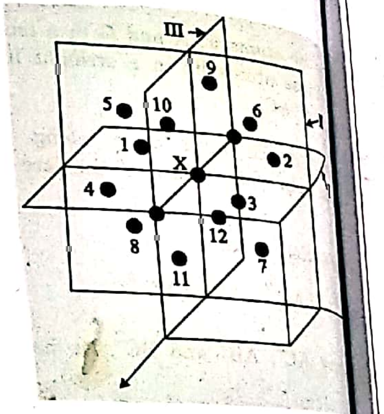
(ii) Coordination number :

* In FCC structure, it consist of 8 corner atoms and 6 face centred atoms.

* Consider corner atom (X).

* It consist of 3 planes

* Each plane consist of 4 face centred atoms.



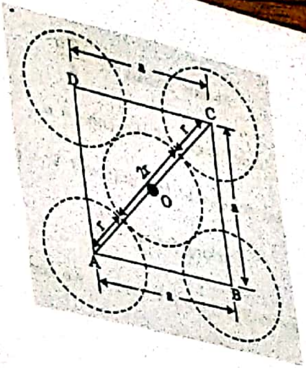
∴ Total number of nearest atom to any corner atom is 4+4+4 = 12

∴ coordination number = 12.

(iii) Atomic radius :

* The atoms touch each other along the diagonal.

* The neighbouring atoms are corner atom (A) & at the centre of adjacent face (O).



from right angled ΔABC

$AC^2 = AB^2 + BC^2$

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

$16r^2 = 2a^2$

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

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

(iv) Atomic Packing Factor (APF) :

$APF = \frac{v}{V}$

$= \frac{\text{number of atoms per unit cell} \times \text{volume of 1 atom}}{\text{Total volume of unit cell}}$

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

$= \frac{4 \times \frac{4}{3}\pi \left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}$

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

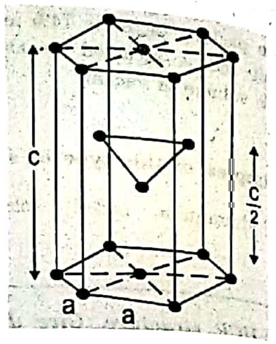
$= \frac{\pi\sqrt{2}}{6} = 0.74 = 74\%$

* 74% of volume is occupied by atoms

26% of volume is vacant

* Example : Copper, Aluminium.

Hexagonal close Packed (HCP) Structure :



- The unit cell has one atom at each of 12 corners of hexagon.
- one atom at the centre of two hexagonal faces.
- There are 3 atoms symmetrically arranged in the body of unit cell.
- There are three layers of atom (ie) bottom layer, middle layer and top layer.
- In bottom layer, the central atom has 6 nearest atom in the same plane.
- The middle layer is at a distance of c/2 from bottom layer and it consist of 3 atoms.
- The top layer is similar to bottom layer at a distance of c/2 from middle layer.

(i) Number of atoms per unit cell :

- Each corner atom is shared by 6 surrounding unit cell

∴ Number of atoms in upper hexagon due to corner atoms $\Big\} = \frac{1}{6} \times 6 = 1$

Number of atoms in lower hexagon due to corner atoms $\Big\} = \frac{1}{6} \times 6 = 1$

- Each central atom in upper and lower hexagon is shared by 2 unit cell.

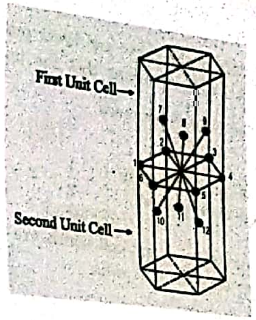
∴ Total number of central atoms in upper + lower planes $\Big\} = \frac{1}{2} \times 2 = 1$

- There are 3 atoms at body of unit cell which is not shared. It is given by $= \frac{3}{6}$

∴ Number of atoms per unit cell = 6

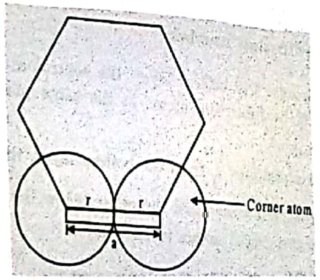
(ii) Coordination number:

- In bottom layer, the central atom has 6 nearest neighbouring atoms.
- At a distance of c/2 from the bottom layer, there are 2 layers one above and one below the bottom layer, it consist of 3 atoms in each layer.
- In total, there are 12 atoms present nearest to X.



∴ coordination number = 12

(iii) Atomic radius :



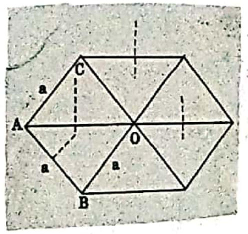
Atoms touch each other along the edges of hexagon.

$a = 2r$

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

(iv) Calculation of $\frac{c}{a}$ ratio :

- Let c is the height of the unit cell and a is the distance between two neighbouring atoms.

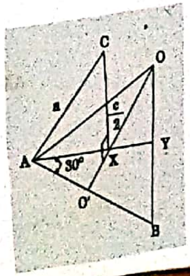


- Consider ΔABO in bottom layer.
- Let A, B, O are the lattice points at a distance of c/2.

Δ ABY , $\cos 30^\circ = \frac{AY}{AB}$

$AY = AB \cos 30^\circ = \frac{a\sqrt{3}}{2}$

$AY = \frac{a\sqrt{3}}{2}$



From fig, $AX = \frac{2}{3} AY$

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

$AX = \frac{a}{\sqrt{3}}$

ΔAXC,

$$AC^2 = AX^2 + XC^2$$

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

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$\frac{c^2}{4} = a^2 - \frac{a^2}{3}$$

$$\frac{c^2}{4} = \frac{3a^2 - a^2}{3}$$

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

$$\frac{c^2}{a^2} = \frac{8}{3}$$

$$\boxed{\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633}$$

(v) Packing factor :

$$APF = \frac{v}{V}$$

To find v :

$$v = 6 \times \frac{4}{3} \pi r^3$$

$$= 6 \times \frac{4}{3} \pi \left(\frac{a}{2}\right)^3$$

$$= \overset{\cancel{3}}{\cancel{6}} \times \frac{\cancel{4}}{\cancel{3}} \pi \frac{a^3}{\cancel{8}\,\cancel{4}}$$

$$\boxed{v = \pi a^3}$$

To find V :

Area of base = 6 × Area of ΔAOB

Area of $\Delta AOB = \frac{1}{2} (BO)(AY)$

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

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

$$\therefore \text{Area of base} = \overset{3}{\cancel{6}} \times \frac{a^2\sqrt{3}}{\cancel{4}\,2}$$

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

$\therefore$ volume of unit cell (V) = Base area x height

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

$$APF = \frac{v}{V}$$

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

$$= \frac{2\pi a}{3\sqrt{3}c}$$

$$= \frac{2\pi}{3\sqrt{3}}\left[\frac{a}{c}\right]$$

$$= \frac{2\pi}{3\cancel{\sqrt{3}}} \times \frac{\cancel{\sqrt{3}}}{\sqrt{8}}$$

$$= \frac{\cancel{2}\pi}{3} \times \frac{1}{\cancel{2}\sqrt{2}}$$

$$= \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

* 74% of volume is occupied by atoms

26% of volume is vacant

* Example : Magnesium

S.No	Properties	SC	BCC	FCC	HCP
1	Number of atoms Per unit cell	1	2	4	6
2	Coordination number	6	8	12	12
3	Atomic radius (r)	$\frac{a}{2}$	$\frac{\sqrt{3}a}{4}$	$\frac{\sqrt{2}a}{4}$	$\frac{a}{2}$
4	APF	0.52	0.68	0.74	0.74
5	Examples	Po	Tungsten, chromium	Copper, Aluminium	Magnesium

Diamond structure :

* It is an important crystal structure.

* Examples : Si and Ge.

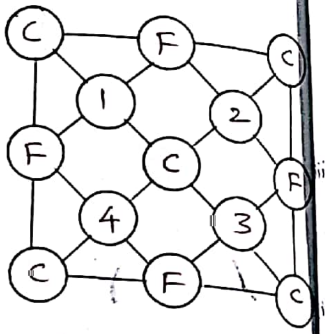
* Diamond structure is the combination of two interepenetrating fcc sub lattice.

* one sub lattice has origin (0,0,0)

* other sub lattice has origin $(\frac{a}{4},\frac{a}{4},\frac{a}{4})$

* It is a loosely packed structure.

(i) **Number of atoms per unit cell :**



There are 3 different atoms present in this structure.

→ corner atoms (i.e) C

→ face centred atoms (ie) F

→ four atoms present fully inside the unit cell (ie) 1,2,3,4.

Each corner atom is shared by 8 unit cell $\} = \frac{1}{8} \times 8 = 1$

Each face centred atom is shared by 2 unit cell $\} = \frac{1}{2} \times 6 = 3$

Extra atoms $= 4$

8

∴ Number of atoms per unit cell = 8

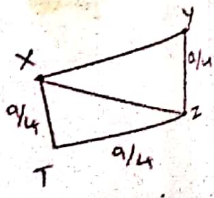
(ii) **Atomic radius :**

* The corner atoms & face centred atoms do not touch each other.

* But corner atom & face centred atoms have contact with the atoms 1,2,3,4.

* Consider atoms X & Y.

* Draw perpendicular to Y atom joining at the point Z.



from the figure,

$$XY^2 = XZ^2 + ZY^2$$

$$XY^2 = XT^2 + TZ^2 + ZY^2$$

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

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

$$4r^2 = \frac{3a^2}{16}$$

$$r^2 = \frac{3a^2}{64}$$

$$\boxed{r = \frac{\sqrt{3}a}{8}}$$

(iii) **Coordination number :**

The number of nearest neighbouring atom is 4. The coordination number is 4.

(iv) **Atomic Packing Factor :**

$$APF = \frac{v}{V}$$

$$= \frac{8 \times \frac{4}{3}\pi r^3}{a^3}$$

$$= \frac{8 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}a}{8}\right)^3}{a^3}$$

$$= \frac{\cancel{8} \times \frac{\cancel{4}}{\cancel{3}}\pi \times \frac{\cancel{3}\sqrt{3}\cancel{a^3}}{\cancel{8}\times 8 \times \cancel{8}_2}}{\cancel{a^3}}$$

$$= \frac{\pi\sqrt{3}}{16} = 0.34$$

* 34% of volume is occupied by atoms
66% of volume is vacant.

* Since APF is low, it is very loosely packed structure.

Miller Indices :

It is a set of three numbers to designate a plane in a crystal. This set of three numbers is called miller Indices. (ie) (h k l)

Procedure for finding Miller Indices :

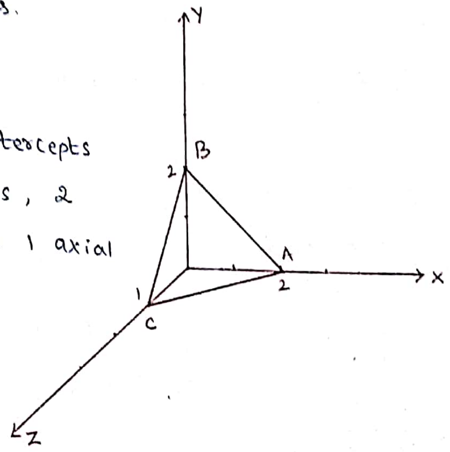
step 1 : Find the intercepts of the plane along the Coordinate axes x, y, z.

step 2 : Take the reciprocal of these intercepts.

step 3 : Reduce the reciprocal into whole number by taking LCM.

step 4 : Write these integers within Parantheses to get Miller Indices.

Example :



* A plane ABC has intercepts of 2 axial units on x axis, 2 axial units on y axis and 1 axial units on z axes.

* In otherwords, the numerical parameters are 2, 2 and 1.

* Hence the orientation is 2,2,1

* Taking reciprocal of the above intercepts

$$\left(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{1}\right) \text{ or } 1\ 1\ 2$$

* These numbers are written in parantheses.

(1 1 2)

∴ The miller indices of the given plane is (1 1 2).

Miller Indices of cubic crystal planes :

* when a plane is parallel to one of the coordinate axes, it is said to meet at infinity. Miller indices for that axes is $\frac{1}{\infty} = 0$.

* when the intercepts of the plane is on the negative part, miller indices is distinguised by a bar put directly over it.

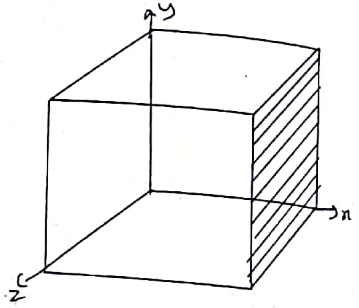
Examples :

(i) * Intercepts $1 : \infty : \infty$

* Reciprocal $\frac{1}{1} : \frac{1}{\infty} : \frac{1}{\infty}$

$1 : 0 : 0$

* Miller Indices (1 0 0)

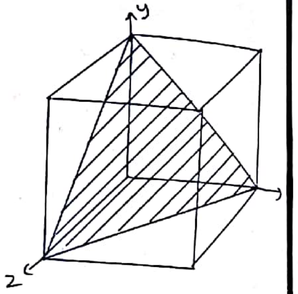


(ii) * Intercepts $1 : 1 : 1$

* Reciprocal $\frac{1}{1} : \frac{1}{1} : \frac{1}{1}$

$1 : 1 : 1$

* Miller indices (1 1 1)

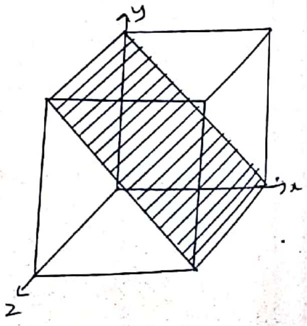


(iii) * Intercepts $1 : 1 : \infty$

* Reciprocal $\frac{1}{1} : \frac{1}{1} : \frac{1}{\infty}$

$1 : 1 : 0$

* Miller Indices (1 1 0)



d spacing in cubic lattice :

* Consider a cubic crystal of length 'a' and plane ABC.

* This plane belongs to the family of planes whose miller indices are (h k l).

* The Perpendicular drawn from the origin represents the interplanar spacing 'd'.

* The plane ABC makes OA, OB + OC as intercepts on reference axes OX, OY + OZ.

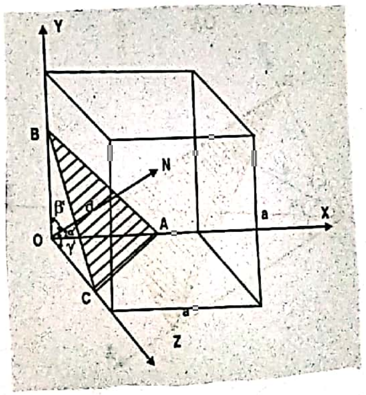
* α', β' and γ' are the angles between the axes OX, OY, OZ + ON.

* We know that miller indices of a plane are the smallest integers of the reciprocal of the intercepts.

$$OA : OB : OC = \frac{1}{h} : \frac{1}{k} : \frac{1}{l}$$

$$= \frac{a}{h} : \frac{a}{k} : \frac{a}{l}$$

$$\therefore \; OA = \frac{a}{h} \; ; \; OB = \frac{a}{k} \; ; \; OC = \frac{a}{l}.$$



From the right angled $\Delta OAN, OBN, OCN$,

$$\cos\alpha' = \frac{ON}{OA} = \frac{d}{a/h} = \frac{dh}{a}$$

$$\cos\beta' = \frac{ON}{OB} = \frac{d}{a/k} = \frac{dk}{a}$$

$$\cos\gamma' = \frac{ON}{OC} = \frac{d}{a/l} = \frac{dl}{a}$$

From the law of direction cosines,

$$\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1.$$

$$\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

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

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

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

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

This is the relation between interplanar spacing 'd', cube edge 'a' and Miller indices (h k l).

CRYSTAL GROWTH

MELT GROWTH:

It is the process of crystallisation by fusion and resolidification of starting materials.

TYPES OF MELT GROWTH:

- Czochralski Technique
- Bridgman Technique
- Verneuil Technique
- Zone Melting Technique

(i) CZOCHRALSKI TECHNIQUE:

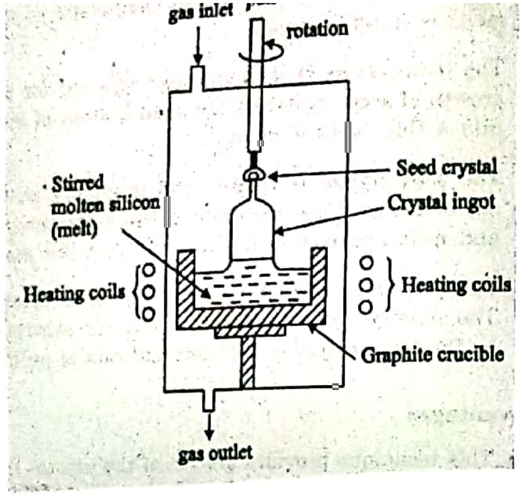
- Principle
- Description and working
- Advantages
- Disadvantages
- Examples

PRINCIPLE:

It is a crystal pulling technique from melt. This is initiated by seed crystal.

DESCRIPTION AND WORKING:

- The apparatus consists of Crucible, Heating coils, Seed crystal and Crystal holder.
- The pure material is taken in the crucible.
- The material is heated by using heating coils.
- Hence the melt is obtained in the crucible.
- Now the seed crystal is introduced in to melt by using crystal holder.
- A small portion of the seed crystal is initially melted.
- Therefore a single crystal is obtained.
- The diameter of the grown crystal is controlled by temperature of the melt.
- So large size cylindrical shaped grown crystal is obtained. This is called crystal ingot.



ADVANTAGES:

- Defect free crystal is obtained.
- It can produce large single crystal.
- It enables easy control of atmosphere.

DISADVANTAGES:

- High vapour pressure can be produced.
- It may produce contamination of melt.

EXAMPLES:

- Silicon & Germanium

(ii) BRIDGMAN TECHNIQUE:

- Principle
- Types
- Description and working
- Advantages
- Disadvantages
- Examples

PRINCIPLE:

The selective cooling of molten material by solidification along a particular direction.

TYPES:

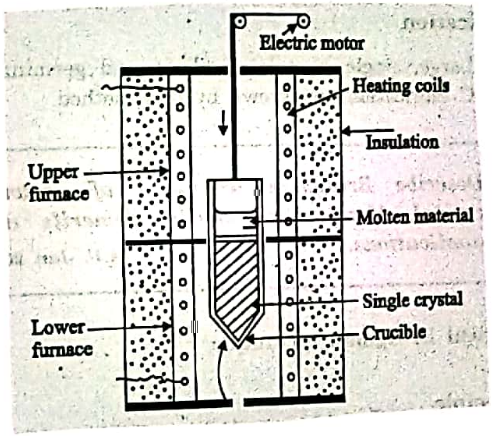
- Vertical Bridgman Technique
- Horizontal Bridgman Technique

In both techniques the melt is frozen from one end by any one of the following methods.

- Moving the furnace
- Moving the crucible
- Keeping both furnace and crucible stationary and cooling the furnace.

DESCRIPTION AND WORKING:

- The material is taken in a cylindrical crucible which is made up of platinum.
- The crucible is suspended in the upper furnace until the material is completely melted.
- The crucible is slowly lowered from upper furnace to lower furnace with the help of electric motor.
- The crucible enters the lower furnace, then its starts to form crystal.
- As the crucible is continuously lowered until all the melt becomes solid crystal.
- Thus a bulk single pure crystal is obtained.



ADVANTAGES:

- Simple technique
- Crucible can be evacuated and sealed, hence oxidation is prevented.
- Control over vapour pressure

DISADVANTAGES:

- Crystal perfection is not better than seed.
- No visibility of material during growth.

EXAMPLES:

Sodium chloride and Potassium chloride.

SOLUTION GROWTH:

TYPES:

- Low temperature solution growth (35^{0}C-100^{0}C)
- High temperature solution growth (about 1200^{0}C)

TYPES OF LOW TEMPERATURE SOLUTION GROWTH:

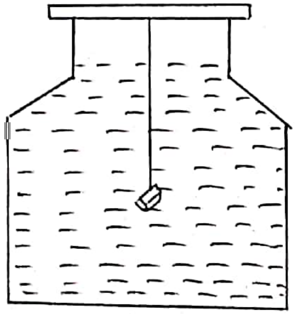
- Slow cooling method
- Slow evaporation method

SLOW COOLING METHOD:

- It is the easiest method to grow bulk single crystal from solution.
- This technique needs only vessel.
- The temperature is in the range of 45^{0}C-75^{0}C and the lower limit of cooling is room temperature.

SLOW EVAPORATION METHOD:

- The saturated solution is kept at a particular temperature and provision is made for evaporation.
- The basic apparatus called Manson jar crystalliser is shown in figure.
- The temperature stabilisation is about 0.05^{0}C and rate of evaporation is few mm^3/h.



ADVANTAGES:

- Simple and convenient method.
- Defect free crystal is possible.
- Growth of prism type crystal is possible.

DISADVANTAGES:

- The growth substance should not react with solvent.
- Small crystals are also formed on the walls of the vessel near the surface of the liquid.
- Quality of the crystal may be affected.

CRYSTAL DEFECTS (OR) CRYSTAL IMPERFECTIONS:

- If atoms are not arranged in a perfectly regular manner in a solid is called crystal defects.
- The various types of defects in crystals are
  - ✓ Lattice vibrations
  - ✓ Point defect (or) Zero dimensional defects
  - ✓ Line defect (or)One dimensional defects
  - ✓ Surface defect (or) Plane defect (or) Two dimensional defects
  - ✓ Volume defect (or) Bulk defect (or) Three dimensional defects

(a) LATTICE VIBRATIONS:

- Atoms are not stationery in their lattice positions, but vibrate about their mean position.
- These vibrations affect the electrical, specific heat and magnetic properties of the materials.

(b) POINT DEFECT (OR) ZERO DIMENSIONAL DEFECTS

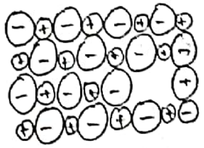
- The defect which takes place due to imperfect packing of atoms during crystallization.
- There are three types of point defect.
  - ✓ Vacancies
  - ✓ Interstitial
  - ✓ Impurities

(i)VACANCIES

- It is the simplest point defect referring to a one or more missing atom.
- This is due to imperfect packing during crystallization and thermal vibrations of atoms at high temperature.
- It is classified into two types.
  - ✓ Schottky defect
  - ✓ Frenkel defect

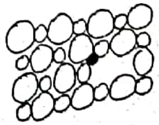
(I) SCHOTTKY DEFECT:

- ✓ It refers to the missing of pair of positive and negative ions in an ionic crystal.



(II) FRENKEL DEFECT

- ✓ It refers to the shift of cation from the regular site to interstitial site.
- ✓ It occurs in ionic crystal.
- ✓ It increases the electrical conductivity.



(ii) INTERSTITIAL DEFECT

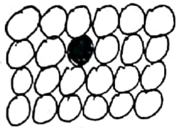
- When an extra atom occupies interstitial space within the crystal structure without removing parent atom is called interstitial defect.
- It has two types.
  - ✓ Self-interstitial
  - ✓ Foreign interstitial

(I) SELF-INTERSTITIAL

✓ If an atom from same crystal occupies interstitial site is called Self-interstitial.

(II) FOREIGN INTERSTITIAL

✓ If the impurity atoms occupies interstitial site is called Foreign interstitial



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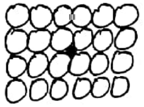


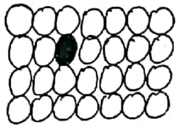
II

(iii) IMPURITIES

- When the foreign atoms (impurities) are added to crystal lattices, they are called impurities. This is called impurity defect.
- It is of two types.
  - ✓ Substitutional impurity
  - ✓ Interstitial impurity

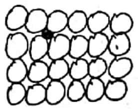
(I)SUBSTITUTIONAL IMPURITY

- It refers to the foreign atom that replaces parent atom in the lattice.
- Example: n type and p type semiconductors have Substitutional impurity from fifth group and third group elements.



(I)INTERSTITIAL IMPURITY

- It is the small size atom occupying the empty space in parent crystal without affecting the parent atom.
- This atom is smaller than parent atom.



(C)LINE DEFECT (OR) ONE DIMENSIONAL DEFECTS

- The defect due to dislocation of atoms along a line is called line defect.
- In line defect, a portion of line of atoms is missing from the regular site.
- There are two types of line defect.
  - ✓ Edge dislocation
  - ✓ Screw dislocation

(i) EDGE DISLOCATION

- ✓ An edge dislocation arises when one of the atomic planes forms only partially and does not extend through the entire crystal.
- ✓ The atomic plane AB terminates at B.
- ✓ It is viewed as an extra plane inserted in between a set of parallel planes.
- ✓ The edge of such a plane forms a line defect is called edge dislocation.
- ✓ There are two types.
  - Positive edge dislocation
  - Negative edge dislocation

(I) POSITIVE EDGE DISLOCATION

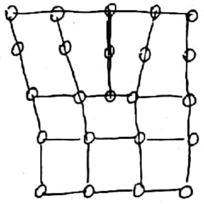
- ✓ If the extra plane of atoms is above the slip plane of the crystal is called positive edge dislocation.
- ✓ It is denoted by $\perp$

(II) NEGATIVE EDGE DISLOCATION

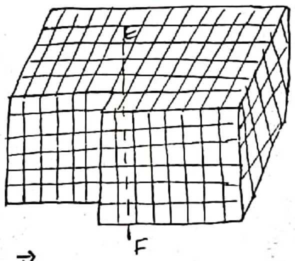
- ✓ If the extra plane of atoms is below the slip plane of the crystal is called negative edge dislocation.
- ✓ It is denoted by $\top$

(ii)SCREW DISLOCATION

- It is due to a displacement of atoms in one part of a crystal relative to rest of the crystal.
- It forms spiral ramp around dislocation line.
- The row of atoms marking the termination of the displacement is the screw dislocation.
- EF indicates dislocation line.
- If spiral motion of one part of crystal is in clockwise direction then dislocation is right handed and in anti-clockwise direction it is left hand.

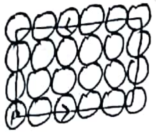


(i)



BURGER'S VECTOR

- The dislocation line are expressed by a burger vector $\vec{b}$
- It indicated the amount and direction of the shift in lattice on slip plane.
- By the presence of dislocation the burger circuit will not complete.



Perfect crytal

Dislocated crystal

(d) SURFACE DEFECT (OR) PLANE DEFECT (OR) TWO DIMENSIONAL DEFECTS

- The defect on the surface of the material is called surface defect.
- It is a two dimensional defect.
- It is of four types.
  - ✓ Grain boundaries
  - ✓ Tilt and Twist boundaries
  - ✓ Twin boundaries
  - ✓ Stacking fault

(i)GRAIN BOUNDARIES

- ✓ Whenever the grains of different orientations separate the general pattern of atoms and exhibit a boundary. the defect caused is called grain boundary.
- ✓ It is formed when two growing grain surface meet.
- ✓ This defect takes place during solidification.

(ii)TILT AND TWIST BOUNDARIES

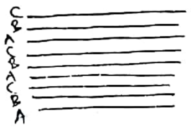
- ✓ Tilt boundary is an array of parallel edge dislocation of same sign arranged one above the other in an array. It is a type of low angle boundary.
- ✓ Twist boundary consists of atleast two sets of parallel screw dislocations lying in the boundary. It is a type of low angle boundary.

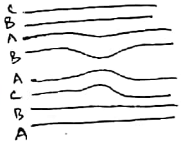
(iii)TWIN BOUNDARY

- ✓ The atomic arrangement of one side of boundary is mirror image of the arrangement of atoms on other side.

(iv) STACKING FAULT

- ✓ Whenever the stacking of atoms is not in proper sequence throughout the crystal, defect caused is called stacking fault.





(e) VOLUME DEFECT (OR) BULK DEFECT (OR) THREE DIMENSIONAL DEFECTS

- Whenever a cluster of atoms are missing, large vacancy is created.
- This is called volume defect.