3/12/2024

Unit 4

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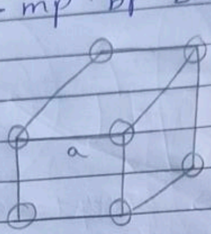
Crystal structure

Solid → Crystalline – mp · bp · Lusture

Solid → Amorphous

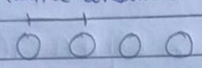


No. of atoms per unit cell $= \frac{1}{8} \times 8$

$= 1$ atom.

Bond length

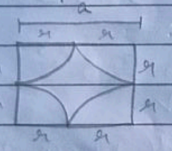
lattice constant



Interatomic distance $= a_0$

r = radius of atom

Volume of atom $= 1 \times \frac{4}{3}\pi r^3$



$a = 2r$

Volume of unit cell $= (\text{side})^3$

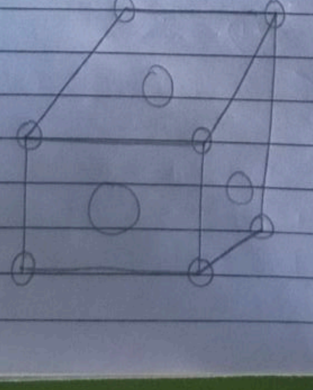
$= a^3 = (2r)^3 = 8r^3$

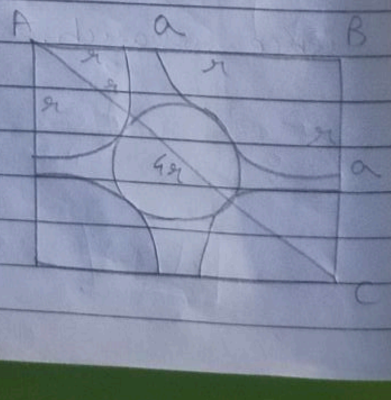
Atomic packing fraction $= \frac{\text{Volume of all atoms}}{\text{Volume of unit cell}}$

$= \frac{\cancel{4}/3\, \pi r^3}{2\, \cancel{8}\, r^3} = \frac{\pi}{6} = 0.52$

$= 52\%$

Face Centered cubic (FCC) structure





(67) BCC

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In ΔABC, $AB^2 + BC^2 = AC^2$

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

$$2a^2 = 16r^2$$

$$a^2 = 8r$$

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

No. of atoms in unit cell $= \frac{1}{2} \cdot 6 + \frac{1}{8} \cdot 8$

$= 3 + 1 = \boxed{4}$

Volume of unit cell $= (\text{side})^3 = a^3$

$= (2\sqrt{2}r)^3 = 8 \cdot 2 \cdot \sqrt{2} r^3$

$= 16\sqrt{2} r^3$.

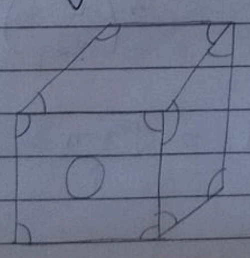
Volume of all atoms $= 4 \times \frac{4}{3} \pi r^3$

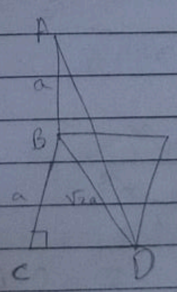
Atomic packing fraction $= \frac{\text{Volume of all atoms}}{\text{Volume of unit cell}}$

$= \frac{4 \times \frac{4}{3} \pi \cancel{r^3}}{16\sqrt{2} \cancel{r^3}} = \frac{\pi}{3\sqrt{2}} = 0.74$

$= 74\%$

Body Centered cubic (BCC) structure





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In ΔBCD, $\angle BCD = 90^\circ$

$$BC^2 + CD^2 = BD^2$$
$$a^2 + a^2 = BD^2$$
$$2a^2 = BD^2 \qquad \therefore \boxed{BD = \sqrt{2}a}$$

In ΔABD, $AB^2 + BD^2 = AD^2$
$$a^2 + 2a^2 = AD^2$$
$$3a^2 = AD^2$$
$$\therefore \boxed{AD = \sqrt{3}a}$$

~~Volume of atom = $\sqrt{3} \times \frac{4}{3}$~~

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

$\therefore$ No. of atom in unit cell $= \frac{1}{8} \times 8 + 1 \cdot 1$
$$= 1 + 1 = 2$$

Atomic packing fraction (APF) $= \dfrac{\text{Vol of atoms}}{\text{Vol of unit cell}}$

$$= \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{8\pi r^3}{3a^3} = \frac{8\pi r^3}{3\left(\frac{4}{\sqrt{3}} r\right)^3}$$

$$= \frac{8\pi \cancel{r^3}}{\cancel{3} \times \frac{64}{\cancel{3}\sqrt{3}} \cancel{r^3}} = \frac{8\sqrt{3}\pi}{64} = \frac{\sqrt{3}\pi}{8}$$

$$= 0.68 = \boxed{68\%}$$

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Crystal structure	No. of atoms per unit cell	APF	Coordination no.	Void
SCC	1	52%	6	48%
FCC	4	74%	12	26%
BCC	2	67%	8	33%

Coordination number ⇒ No. of nearest neighbour

As FCC has 74% APF as compared to BCC (67%), FCC structure should be ~~more~~ stronger than BCC.

Difference

	FCC	BCC
1	eg: Aluminium (Al)	eg: Iron (Fe)
2	Octahedral plane	Diagonal plane
3	Density: 2.70 g/cm^3	Density: 7.86 g/cm^3
4	Ductility is more than BCC	Ductility is less than FCC
5	Conductivity is more	Conductivity is less
6	APF = 74%	APF is 67%
7	Void = 26%	Void = 33%
8	Coordination no. = 12	Coordination no. = 8
9	No. of atoms = 4	No. of atoms = 2

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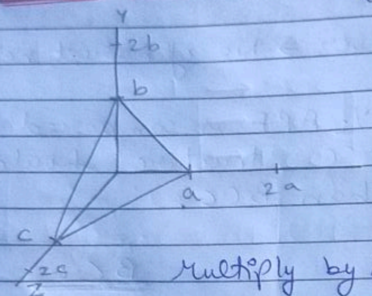
At room temperature, iron is BCC & also aluminium is FCC.

* Learn more about diffraction & scattering

Miller Indices (Assignment No. 07)



(a, b, c) ↳ Intercepts

Inverse ⇒ $\frac{1}{a}$ $\frac{1}{b}$ $\frac{1}{c}$

Multiply by LCM

(h, K, l)

eg $\boxed{(2, 3, 4)}$ ⇒ ①

Intercepts are (2, 3, 4)

Taking inverse

$\frac{1}{2}$ $\frac{1}{3}$ $\frac{1}{4}$

Taking LCM
Multiply by 12

$\frac{12}{2}$ $\frac{12}{3}$ $\frac{12}{4}$

6 4 3

Miller indices are
(6 4 3)

$\boxed{(4, 6, 8)}$ ⇒ ②

Intercepts are (4, 6, 8)

Taking inverse

$\frac{1}{4}$ $\frac{1}{6}$ $\frac{1}{8}$

Taking LCM
Multiply by 24

$\frac{24}{4}$ $\frac{24}{6}$ $\frac{24}{8}$

6 4 3

Miller indices are
(6 4 3)

① = ②

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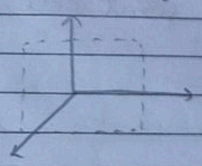
$(6 \ 4 \ \boxed{-3})$ use $(6 \ 4 \ \boxed{\bar{3}})$ Ke format mein likhna rehta hai

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

(1, 1, 0) ∴ z axis ko infinity pe cut kar raha hai

same as x & y axis



(0 0 1) z axis pe cut
(0 1 0) y axis pe cut
(1 0 0) x axis pe cut

↳ Interatomic distance x, y, z axis same

Relation between density (ρ) and lattice constant (a)

$$\text{Density} = \frac{\text{Mass of unit cell}}{\text{Volume of unit cell}}$$

$$\rho = \frac{\text{Mass of unit cell}}{a^3}$$

Mass of unit cell = ρa^3 —— (1)

Mass of one atom = ?

$N_A = 6.023 \times 10^{23}$ atoms/mole
↳ Avagadro's number.

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Molar mass = Moleculer weight (gm) = M

i.e.

6.023×10^{23} atoms weight = M

$\therefore$ Weight of atom mass $= \frac{M}{6.023 \times 10^{23}} = \frac{M}{N_A}$

Let n = no. of atoms in unit cell

= 1 $\longrightarrow$ SCC

= 2 $\longrightarrow$ BCC

= 4 $\longrightarrow$ FCC

Mass of one unit cell = No. of atom per unit cell × Mass of one atom

$= n \cdot \frac{M}{N_A}$ —— (2)

From eq^n (1) & (2)

$\rho a^3 = n \cdot \frac{M}{N_A}$

$\therefore a^3 = \frac{n \cdot M}{\rho N_A}$

$\therefore$ $\boxed{a = \sqrt[3]{\frac{n \cdot M}{\rho \cdot N_A}}}$

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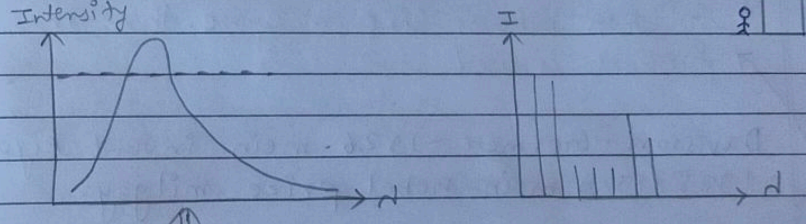
- De-Broglie hypothesis
- Wave function and its physical significance
- Heisenberg's uncertainty principle and its applications.
- Schrodinger's time dependent and time dependent equation
- Introduction to quantum computing

★ History of Quantum Mechanics

Max Planck → 1895

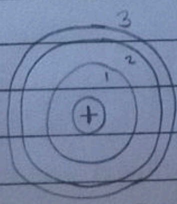
Black body ← 100% radiation
→ emit



absorption/emission spectra

$h = 6.63 \times 10^{-34}$ J·s → constant

Therotical adjustment



Niel's Bohr

Nucleus se 1 jyada distance pe rahega
2 aur 1 ke bich ka distance thoda kam
3 aur 2 ke bich ka distance aur jyada kam

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$\rho(\nu) = \frac{8\pi h \nu^3}{(\quad)}$ i.e. $E = h\nu$

$\therefore$ Density (ρ) $\propto$ Frequency (ν)

$\boxed{\rho \propto \nu}$

$E = h\nu = mc^2$

$= \frac{hc}{\lambda} = mc^2$ $\therefore$ $\lambda = \frac{h}{mc}$ photon

$\nu \approx c$ $\boxed{\lambda = \frac{h}{m\nu}}$ ... m = mass of particle

$\boxed{2d \sin\theta = n\lambda}$

W. C. Bragg's diffraction (William Charles)

W. L. Bragg's diffraction (William Lawrence)

electron behaves like a wave then this formula is used

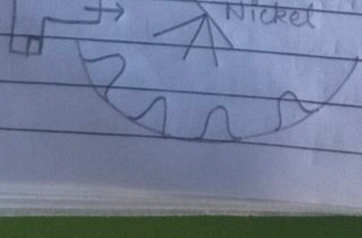
Davisson - Germer - 1926 mein invent kiya & 1928/1929 mein nobel prize milgaya.

Louis de Broglie - 1924 mein invent kiya.

1905 - $\boxed{E = mc^2}$ ... m = relative mass

m_0 = non relative mass

= rest mass.



in all direction

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eg $x + y = 7$

$2x + 3y = 9$

$\boxed{y = -5}$

$$2x + 3y = 9$$
$$-\,2x + 2y = 14$$
$$y = -5$$

$x + y = 7$

$x = 7 - y$

$x = 7 + 5$

$\boxed{x = 12}$

De - Broglie Hypothesis

Wave particle duality

$E = mc^2$ .... einstein

$E = h\nu$ .... Plank

$\frac{hc}{\lambda} = mc^2$ $\qquad \frac{h}{cm} = \lambda$ $\qquad \therefore \lambda = \frac{h}{mc}$

$\therefore \lambda = \frac{h}{mc}$ photon

for electron or subatomic particle,

$$\boxed{\lambda = \frac{h}{m\nu}}$$

Matter Wave —— x Real

Wave function

Schrodingar (1926) — ψ (x, y, z, t)

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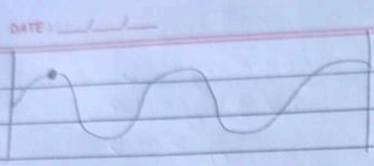
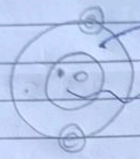


nucleus
10^{-14} m



Δx -
$\Delta p = m \cdot \Delta V$
e $\approx$ 2 to 4 MeV

Heisenberg's uncertainty Principle

$$\boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}}$$

$$\hbar = \frac{h}{2\pi}$$

$\Delta x \rightarrow 0$ $\Delta p \rightarrow 0$
$\Delta p \rightarrow \infty$ $\Delta x \rightarrow \infty$

★ Beta Decay

$${}_{Z}X^{A} \longrightarrow {}_{(Z+1)}Y^{A} + {}_{-1}\beta^{0} + \bar{\nu}$$

Problem: To prove that electron does not exist (reside) inside the nucleus.

Solution: Let us consider that electron resides inside the nucleus

Nuclear diameter $= 10^{-14}$ m

fixed nai bata sakte par probability bata sakte hai like in a class, Palak naam ka ladka hai par kahape baitha hai? Boys section. Par boys section mein kaha yeh nai pata, so probability hai ~~the~~ boys mein kahi toh bi baitha hai fixed nai bata sakte ki kahape baitha hai

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Max uncertainty in $x = (\Delta x)_{max}$

$= 10^{-14}\ m$

We know that,

HUP

$$(\Delta x)_{max} \quad (\Delta p)_{min} \geq \frac{\hbar}{2}$$

$$(\Delta p)_{min} \geq \frac{\hbar}{2(\Delta x)_{max}} \geq \frac{6.63 \times 10^{-34}\ J \cdot s}{2 \times 3.14 \times 2 \times 10^{-14} m}$$

$$(\Delta p)_{min} \geq \frac{6.63 \times 10^{\cancel{-14}}\ J \cdot s}{2 \times 3.14 \times 2 \times 10^{\cancel{34}}\ m} \quad 10^{20}$$

$$\geq \frac{6.63}{12.56} \times 10^{-20}\ \frac{J \cdot s}{m}$$

$$\geq 0.5278 \times 10^{-20}\ \frac{J \cdot s}{m}$$

$$\boxed{(\Delta p)_{min} \geq 0.527 \times 10^{-20}\ Js/m}$$

$$\boxed{\geq 5.28 \times 10^{-21}\ Kg\ m/s}$$

For realistic case,

$$E = \sqrt{p^2 c^2 + m_0^2 c^4}$$

$$E = p \cdot c$$

$$E_{min} = (\Delta p)_{min} \times c$$

$$= 5.28 \times 10^{-21}\ Kg \frac{m}{s} \times 3 \times 10^8 \frac{m}{s}$$

$$= 15.84 \times 10^{-13}\ Kg \frac{m^2}{s^2}$$

$$\boxed{E_{min} = 15.84 \times 10^{-13}\ J}$$

$$E_{min} = \frac{15.84 \times 10^{-13}}{1.6 \times 10^{-19}} \ eV$$

$$= 9.9 \times 10^{6} eV = 9.9 \ MeV$$

$$\boxed{E_{min} \approx 10 MeV}$$

experimentally, electron energy (Beta decay) is of the order of 2 to 4 MeV

$${}^{1}_{0}n \longrightarrow {}^{1}_{1}p + {}^{0}_{-1}e + {}^{0}_{0}\gamma$$

$$\psi = \psi(x, y, z, t)$$

light $\rightarrow \epsilon - \epsilon_0 \hat{j}$

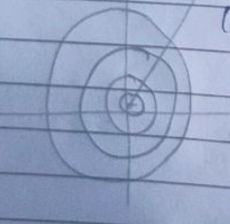
$$H = H_0 \hat{i}$$

$$\boxed{\text{Intensity} \propto (\text{amp})^2}$$

$$\iiint \psi^* \psi \, dx dy dz$$

= Probability of finding a particle in given region.

(r, θ, ϕ)



dx = line element

$dxdy$ = surface element

$dxdydz$ = volume element