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9/11/23

Basics of Material Science

[Sumeet
Tiwari Sir]

Introduction →

Material Science :-

- ↳ Material Science involve investigating the relationship that exist b/w the str. and properties of materials.
- material science does not deal with the strength & stiffness behaviour of engineering component s/a building, machines, Automobiles etc., rather it deals with the relationship b/w the structure and properties with which these structures components are made of. of materials

material →

- material can be defined as something that consist of matter. It is the stuff by which something can be made.
- the engineering materials can be classified as -
 - ① metal & alloys
 - ② ceramic & glass
 - ③ Organic polymers
 - ④ Composite.

Structure →

The structure of material usually relates to the arrangement of internal components s/a atoms, molecules, grains etc.

- usually structures are classified as -

① Macro structure :- "Examined with naked eye."

- the internal symmetry of crystalline material may reflect in the external form of crystal.

s/a flat faces of diamond & etc.

② microstructure \Rightarrow It is observed with the help of an optical microscope.

③ Crystal structure \Rightarrow

\rightarrow It tells us about the atomic arrangement in the crystal.

\rightarrow the smallest group of atoms by repeating which periodically in all the dirn, the crystal structure can be developed, this smallest group of atoms is k/a unit cell.

④ Atomic structure

↓
Electronic structure

↓
It tells us about the arrangement of e^- in various orbits of the atom.

↓
Nuclear structure.

↓
It tells us about the no of protons & neutrons inside the nucleus of an atom.

\Rightarrow It is studied by Nuclear spectroscopic techniques s/a Nuclear magnetic Resonance & Mossbauer studies etc.

Property \rightarrow

\hookrightarrow A property is a material trait in terms of the kind and magnitude of response to a specific imposed stimulus (excitation/Input).

\rightarrow Properties of solid material can be -

① mechanical property

② electrical "

③ Magnetic "

④ thermal "

⑤ optical "

⑥ Deteriorative "

10/11/23

CH-01] Atomic Str and Chemical Bonding

→ matter is made of very tiny particles called atoms which are indivisible structures

$\left\{ \begin{array}{l} A \rightarrow \text{not} \\ \text{tomio} \rightarrow \text{cuttable} \end{array} \right.$

→ Atoms can neither be created nor destroyed.

Subatomic particles

Electron

- -ve charged particle
- Charge = $-1.6 \times 10^{-19} \text{ C}$
- Mass = $9.1 \times 10^{-31} \text{ kg}$

Proton

- (+ve)ly charged particle
- Charge = $+1.6 \times 10^{-19} \text{ C}$
- Mass = $1.67 \times 10^{-27} \text{ kg}$
(17 to 18 times heavier)

Neutron

- neutral particle
- Charge = 0
- Mass = $1.67 \times 10^{-27} \text{ kg}$

Rutherford's atomic model →

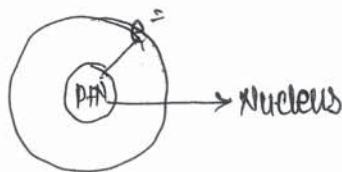
→ on the basis of famous α -particle scattering experiment, Rutherford proposed the nuclear model of atom.

→ Acc to this model the +ve charge and most of the mass is concentrated in extremely small region, this very small region was called 'Nucleus'.

→ the nucleus is surrounded by e^- which move with a very high speed in a circular path called orbits.

→ e^- & neutrons are held together by 'electrostatic forces of attraction'

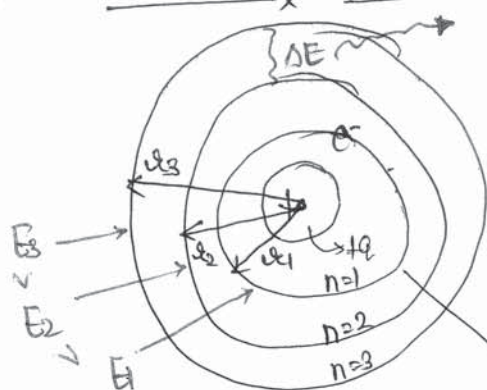
failed
(क्योंकि ये नहीं बता
सकता कि e^- nucleus
के चारों ओर कैसे घूम रहा है)



$$F = \frac{1}{4\pi\epsilon_0} \frac{(+q)(-q)}{r^2}$$

→ coulombic force of attraction
(Electrostatic force)

Bohr's Atomic Model for Hydrogen atom →



$$mve = \frac{nh}{2\pi}$$

→ e⁻ is moving only in those orbits where angular mom. is integral multiple of $\frac{h}{2\pi}$.

$h = \text{plank's Const}$

$$h = 6.62 \times 10^{-34} \text{ J-s}$$

Stationary states

↓
Allowed energy states.

$$p = \frac{mve}{2\pi r_1} = \frac{nh}{2\pi r_1}$$

$$K.E. = \frac{1}{2}mv^2$$

$$= \frac{p^2}{2m}$$

$$\Delta E \propto \nu$$

$$\Delta E = h\nu$$

↪ frequency.

(38)

Accs to Bohr's model →

(i) the e⁻ in H-atom can move around the nucleus in a circular path of fixed radius & Energy. these paths are called stationary states / orbits / Allowed Energy states

(ii) An e⁻ can move only in those orbits for which its angular momentum is integral multiple of $\frac{h}{2\pi}$.

i.e. why only certain fixed orbits are allowed

$$mve = \frac{nh}{2\pi}$$

(iii) when an e⁻ jumps from an orbit of higher energy to another orbit of lower energy then energy is released in the form of radiations & vice versa.

the amount of energy released / Absorbed is the difference of energy in two orbits.

$$E_2 - E_1 = h\nu = \frac{hc}{\lambda}$$

⇒ Bohr's orbital radius →

$$r_n = \frac{0.529 n^2}{Z} \text{ \AA}$$

Z = atomic no. of element

for hydrogen
 $Z=1$

$$r_n = 0.529 n^2 \text{ \AA}$$

⇒ Energy of e^- in Bohr's orbit →

$$E_n = \frac{-13.56 Z^2}{n^2} \text{ eV}$$

Z → atomic no. of element

eV → electron volt

unit of energy

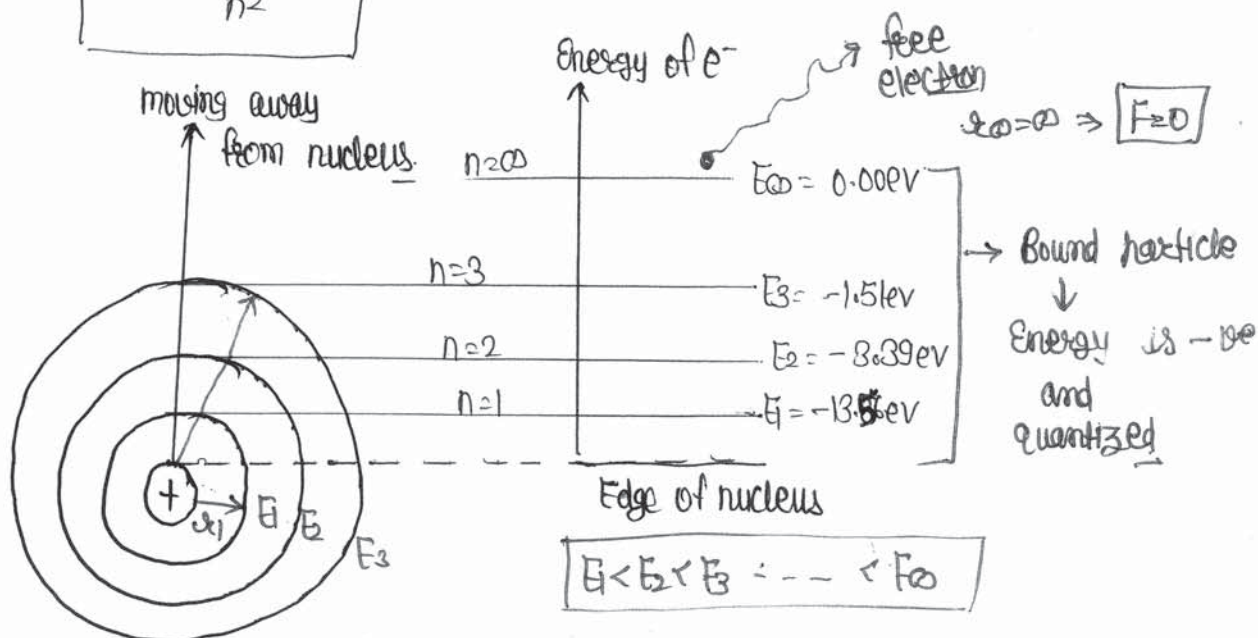
$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

for H atom

$Z=1$

$$E_n = -\frac{13.56}{n^2} \text{ eV}$$

⊗



- (i) In any atom greater the dist of an e^- from the nucleus, higher is its total Energy
 - (ii) An e^- orbiting very close to the nucleus in the first cell is tightly bound to the nucleus and possesses very small amount of Energy
 - (iii) so it would be difficult to knock out this e^- from its orbit.
- On the other hand an e^- orbiting far from the nucleus is loosely bound to the nucleus & posses 'greater' amount of energy

this is the reason why valence e⁻ participate in chemical rxⁿ & chemical bonding etc

Que. the radius of first bohr orbit of e⁻ in H-atom is 0.529 \AA
what is the radius of second bohr orbit in singly ionized Helium atom?

- Solⁿ
- a) 1.058 \AA c) 0.264 \AA
b) 10.58 \AA d) 0.0264 \AA

Solⁿ

$$r_n = \frac{0.529 n^2}{Z} \text{ \AA}$$

$Z=2$
 $n=2$

$$r_n = \frac{0.529 \times 4}{2} = 1.058 \text{ \AA}$$

⇒
wave particle duality →

Acc^r to de-Broglie

⇒ Based on wave particle duality Louis de Broglie proposed that particles of matter & a e⁻ could exhibit a wave

character in certain experiments

→ de Broglie proposed that a particle of momentum p has a wavelength given by

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

h → plank's Const

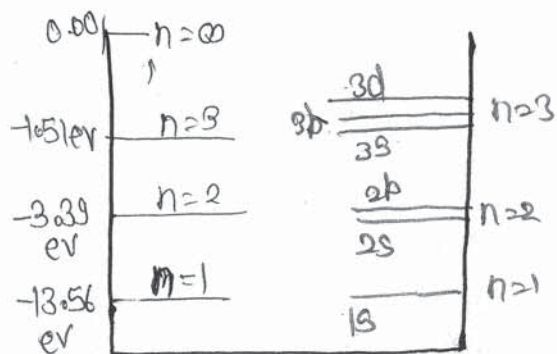
p → momentum

m → mass of particle

v → velocity " "

λ → de broglie wavelength

wave mechanical model →



→ In this model the e^- is considered to exhibit both wave like & particle like characteristics.

↳ With this model an e^- is no longer treated as a particle moving in a discrete orbital, rather position is considered to be probability of an e^- being at various locations around the nucleus.

↳ In other words position of an e^- is described by a probability distribution or e^- cloud.

⇒ the position of an e^- in wave mechanical model is described by four parameters called Quantum no's

→ * the size, shape and spatial orientation of an e^- 's probability density are specified by 3 of these quantum no's -

① First Quantum No. (n):-

→ It is also k/a principle quantum no.

→ $n = 1, 2, 3, 4, \dots$

→ It represents shells (orbits) (K, L, M, N, ...)

→ This quantum no represents the distance of e^- from the nucleus, or its position.

→ This quantum no is related to Bohr's model.

② Second quantum no. (l) → (Angular / Azimuthal quantum no.)

↳ It signifies subshells - s, p, d, f.

→ It is related to the shape of e^- subshell.

→ The no. of these subshells are restricted by the magnitude of n.

i.e.

$$l = 0 \text{ to } (n-1)$$

$n=1 \rightarrow l=0 \Rightarrow s\text{-subshell}$

$n=2 \rightarrow l=0, 1 \Rightarrow s, p, \text{ subshells}$

$n=3 \rightarrow l=0, 1, 2 \Rightarrow s, p, d\text{-subshells}$

③ third quantum no. $\rightarrow (m_l)$: (magnetic quantum no.)

\rightarrow the no. of energy states for each subshell is determined by third quantum no.

\Rightarrow there are (2l+1) of m_l ranging from -l to l.

s \rightarrow 1 energy state

p \rightarrow 3 energy states

d \rightarrow 5 energy states

f \rightarrow 7 energy states

\rightarrow In the absence of an external magnetic field the states within each subshell is identical.

However when a magnetic field is applied these subshell states split, each states consuming slightly diff^r energy

④ fourth quantum no. \rightarrow (spin quantum no.) (m_s):

\rightarrow Associated with each e^- is a spin moment which must be oriented either A.C.W or C.W.

\rightarrow related to this spin moment is the fourth quantum no for which two values are possible $+\frac{1}{2}$ & $-\frac{1}{2}$. one for each spin orientations.

Pauli's Exclusion principle \rightarrow

\rightarrow In any atom no two atom can have all the four quantum no to be same.

\rightarrow Each e^- will have different set of quantum no.