MODERN PHYSICS

B.Sc. , PHYSICS, 3rd Year: Paper - IV

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FOREWORD

Since its establishment in 1976, Acharya Nagarjuna University has been forging ahead in the path of progress and dynamism, offering a variety of courses and research contributions. I am extremely happy that by gaining a B++ (80-85) grade from the NAAC in the year 2003, the Acharya Nagarjuna University is offering educational opportunities at the UG, PG levels apart from research degrees to students from over 285 affiliated colleges spread over the three districts of Guntur, Krishna and Prakasam.

The University has also started the Centre for Distance Education with the aim to bring higher education within reach of all. The centre will be a great help to those who cannot join in colleges, those who cannot afford the exorbitant fees as regular students, and even housewives desirous of pursuing higher studies. With the goal of brining education to the doorstep of all such people, Acharya Nagarjuna University has started offering B.A., and B.Com courses at the Degree level and M.A., M.Com., M.Sc., M.B.A., and L.L.M., courses at the PG level from the academic year 2003-2004 onwards.

To facilitate easier understanding by students studying through the distance mode, these self-instruction materials have been prepared by eminent and experienced teachers. The lessons have been drafted with great care and expertise in the stipulated time by these teachers. Constructive ideas and scholarly suggestions are welcome from students and teachers involved respectively. Such ideas will be incorporated for the greater efficacy of this distance mode of education. For clarification of doubts and feedback, weekly classes and contact classes will be arranged at the UG and PG levels respectively.

It is my aim that students getting higher education through the centre for Distance Education should improve their qualification, have better employment opportunities and in turn facilitate the country's progress. It is my fond desire that in the years to come, the Centre for Distance Education will go from strength to strength in the form of new courses and by catering to larger number of people. My congratulations to all the Directors, Academic Coordinators, Editors and Lesson-writers of the Centre who have helped in these endeavours.

Prof. P. Rajasekhar
Vice - Chancellor, FAC
Acharya Nagarjuna University

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ACHARYA NAGARJUNA UNIVERSITY
CENTRE FOR DISTANCE EDUCATION

B.Sc., Physics III Year
Paper – IV : (Modern Physics) For Maths Combination

UNIT – I

1. Atomic Physics and Molecular Physics

Spectra of Hydrogen, deuteron and alkali atoms spectral terms, doublet find structure, screening constant for alkali spectra for s,p,d and f states, selection rules.

Singlet and triplet fine structure in alkaline earth spectra, L-S and J-J Couplings.

Week spectra : Continuous X-Ray spectrum and its dependence on voltage, Duance and Hunt's law. Characterisitics X-rays. Moseley's law, doublet structure of X-Ray spectra, X-Ray absorption spectra.

Molecular Physics : Discrete set of electronic energies of molecules, quantisation of vibrational and rotational energies, determination of internuclear distance, pure rotational and rotation vibration spectra. Dissociation limit for the ground other electronic states, transition rules for pure vibration and electronic vibration spectra. Raman effect, Stokes and anti-Stokes lines. Complimentary character of Raman and infrared spectra, experimental arrangements for Raman spectroscopy.

Spectroscopic techniques : Sources of excitation, prism and grating spectrographs for visible, UV and IR, absorption spectroscopy, double beam instruments. different recording systems.

2. Quantum mechanics

Photoelectric, Ritz combination principle in spectra, stability of an atom Planck's radiation law, Einstein's explanation of photoelectric effect. Broglie's quantisation of angular momentum and its applications to hydrogen atom, limitations of Bohr's theory.

Wave-particle duality uncertainty principle : de Broglie's hypothesis for matter waves; the concept of wave and group velocities, evidence for diffraction and interference of 'particles', experimental demonstration of matter waves.

Consequence of de Broglie's concepts; quantisation in hydrogen atom, energies of a particle in a box, wave packets, Heisenberg's uncertainty relation for p and x, its extension to energy and time. Consequence of uncertainty relation gamma ray microscope, diffraction at a slit, particle in a box, position of electron in a Bohr orbit.

Quantum Mechanics : Schrodinger's equation. Postulatory basis of quantum mechanics; operators, expectation values, transition probabilities, applications to particle in a one- and three dimensional boxes, harmonie oscillator, relection at a step potential, transmission across a potential barrier.

3. Nuclear Physics :

Interaction of charged particles and neutrons with matter, working of nuclear detectors, (G-M counter, proportional counter and scintillation counter, cloud chambers, spark chamber, emulsions.

Contd.

Structure of nuclei, basic properties (I, h, Q and binding energy), deuteron binding energy. p-p and n-p scattering and general concepts of nuclear forces. Beta decay, range of alpha particle, Geiger – Nuttal law. Gamow's explanation of beta decay, alpha decay and continuous and discrete spectra.

Nuclear reactions, channels, compound nucleus, direct reaction (concepts)

Shell model : liquid drop model, fission and fusion (concepts), energy production in stars by p-p and carbon cycles (concepts).

4. Solid –State Physics

Crystalline nature of matter, crystal systems, Bravais lattices, miller indices – diffraction of X-rays. Laue method, powder diffraction method – simple crystal structures (NaCl, CsCl and Diamond) – Types of bonding in crystals, characteristics of crystals with different bondings – lattice energy of ionic crystals – moderlung constant – Born potential calculation of repulsive exponent, Born-Haber cycle – magnetic properties of materials – Dia, para and Ferro magnetic materials, Weiss theory of ferromagnetism – ideas of magnetic domains, anti ferromagnetism and ferri magnetism – super conductivity – Zero resistance.

Reference books :

1. Introductory of Atomic Spectra-	H.F. White
2. Spectroscopy	Straughen and Walker
3. Quantum Mechanics	Mathaws and Venkatesan
4. Introduction to Quantum Mechanics	Pauling and Wilson
5. Physics of Atom	Wher and Richards
6. Introduction to Solid state physics	Kittel
7. Nuclear Physics	Tayal
8. Elements of modern Physics	Patil
9. Introduction to Modern Physics	H.S. Mani and G.K. Mehta
10. Prospective of Modern Physics	A. Beiser
11. Atomic and Nuclear Physics	T.A. Littlefield and N. Thoriey

B.Sc., IIIrd Year – Paper – IV

1. e/m of an electron by Thomson method.
2. Energy gap of an intrinsic semiconductor.
3. Energy gap of semi conductor using a junction diode
4. Temperature characterisitics of thermistor
5. R.C. Coupled amplifier
6. Logic gates AND, OR NOT, X-OR gates.
7. Verification of truth tables for half and full adders.
8. Phase shift Oscillator
9. Hysteresis curve of transformer core
10. Determination of Planck's constant (photocell)
11. Study of spectra of hydrogen spectrum (Rydberg constant)
12. Study of absoption of α and β rays
13. Hall –probe method for measurement of magnetic field
14. Absorption spectrum of iodine vapour
15. Study of alkaline earth spectra using a concave grating

CONTENTS

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Unit-I ATOMIC PHYSICS

Unit-II QUANTUM MECHANICS

Unit-III NUCLEAR PHYSICS

Unit-IV SOLID STATE PHYSICS

LAB MANUAL –P-1V

UNIT - I

LESSON - 1

SPECTRA OF ALKALI AND ALKALINE ELEMENTS

OBJECTIVES :

After completing the study of this lesson the student will be able to

1) **Know about spectra, types of spectra and spectra of hydrogen**
2) **Understand the spectra of alkali and alkaline spectra.**
3) **Understand the salient features of alkali spectra.**
4) **Obtain expressions for spectral forms of alkali spectra.**
5) **Know the selection rules.**
6) **Understand the coupling schemes.**

STRUCTURE :

1.1 INTRODUCTION :

In this chapter we discuss the types of spectra and spectra of hydrogen. Later we discuss about the spectra of alkali and alkaline elements.

The general spectrum is defined as orderly arrangment of colours. Here we concerned with the light spectrum. When a beam of composite light or white light is passed through a prism or grating the light splits into its component colours. The spectra maybe divided into two principal classes, namely, (1) emissioin spectra, (2) absoprtion spectra.

Both the emission and absorption spectra are subdivided into three types, namely, (1) continuous spectra, (2) band spectra, (3) line spectra.

The atomic spectra consists of a large number of discrete parallel lines. The simplest atomic spectra is that of hydrogen. After hydrogen, the next simplest spectra are of monovalent atoms of alkali metals Lithium (Li), Sodium (Na), Potassium (K), Rubidium (Rb), Cesium (Cs) etc. They belong to first group of periodic table. The outermost shell contain a single electron and hence their spectra are characteristic of single valence electron like hydrogen atom.

The alkaline earth elements are Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba) and Mercury (Hg). They have two electrons in their outermost shell. The spectra of alkaline earth elements resemble the spectra of helium atom. The spectra of alkaline earths consists of a very large number of lines and each spectrum consists of two types of spectral lines, singlets and triplets.

1.2. TYPES OF SPECTRA :

Spectrum : The regular arragnement of colours is known as spectra.

When a beam of composite light or white light is passed through a prism or grating the light splits into its component colours and produce the regular arrangement of colours on screen.

The spectra may be divided into two classes, namely :

1. Emission spectra
2. Absorption spectra

1.3. SPECTRA OF HYDROGEN :

When the hydrogen atom is subjected to external energy, the electron jumps from lower energy state to a higher energy state i.e., the hydrogen atom is excited. The excited state is not stable, hence the electron returns to its ground state in about 10^{-8} seconds. The excess of energy is now radiated in the from of radiations of different wavelengths. These different wavelengths constitute a hydrogen spectrum.

Spectra of hydrogen is the simplest atomic spectra.The different wavelengths constitute spectral series which are characteristics of the atom emitting them.

The wavelengths of the different members of the series can be calculate from the following Rydberg relations

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H\left[\frac{1}{m^2} - \frac{1}{n^2}\right]$$

where m and n are integers. $\bar{\upsilon}$ is the wave number. By giving different values of m and n, we can obtain different regions of hydrogen spectrum. R_H is called, the Rydberg constant (1.097×10^7 m^{-1}).

i)Lyman Series : This series consists of all wavelengths which are emitted when an electron jumps from an outer orbit to the first orbit i.e. the electron jumps to K orbit give rise to Lyman series.

$$\bar{\upsilon} = R_H\left[\frac{1}{1^2} - \frac{1}{n^2}\right] \qquad n = 2, 3 \ldots\ldots\ldots \infty$$

ii) Balmer series : This series consists of all wavelengths which are emitted when an electron jumps from an outer orbit to the second orbit i.e., the electron jumps to L orbit give rise to Balmer series.

$$\bar{\upsilon} = R_H\left[\frac{1}{2^2} - \frac{1}{n^2}\right] \qquad n = 3, 4, 5 \ldots\ldots\ldots \infty$$

iii) Paschen series : This series consists of all wavelengths which are emitted when an electron jumps from an outer orbit to the third orbit i.e. the electron jumps to M orbit give rise to Paschen series.

$$\bar{\upsilon} = R_H\left[\frac{1}{3^2} - \frac{1}{n^2}\right] \qquad n = 4, 5, 6 \ldots\ldots\ldots \infty$$

iv) Brackett series : This series consists of all wavelengths which are emitted when an electron jumps from outer orbit to the fourth orbit i.e. the electron jumps to N orbit give rise to Brackett series.

$$\bar{\upsilon} = R_H\left[\frac{1}{4^2} - \frac{1}{n^2}\right] \qquad n = 5, 6, 7 \ldots\ldots\ldots \infty$$

v) Pfund series : This series consists of all wavelengths which are emitted when an electron jumps from outer orbit to the fifth orbit i.e. the electron jumps to O orbit gives rise to Pfund series.

$$\bar{\upsilon} = R_H\left[\frac{1}{5^2} - \frac{1}{n^2}\right] \qquad n = 6, 7, 8 \ldots\ldots\ldots \infty$$

Balmer series falls in visible region, Lyman series falls in ultraviolet, Paschen and Brackett series falls in infra red series.

Diagrammatic representation of series spectrum of hydrogen atom:

Figure(1.3.1) shows the orbital diagram of spectral series of hydrogen atom.

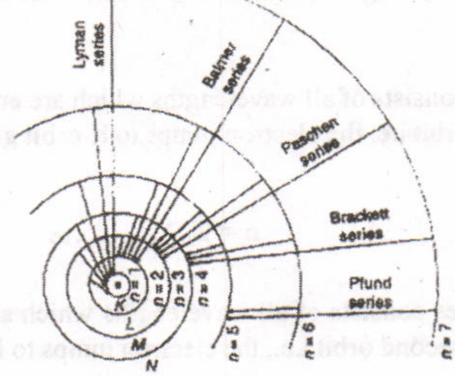


FIG 1.3.1

Figure(1.3.2) shows the energy level diagram of spectral series of hydrogen atom.

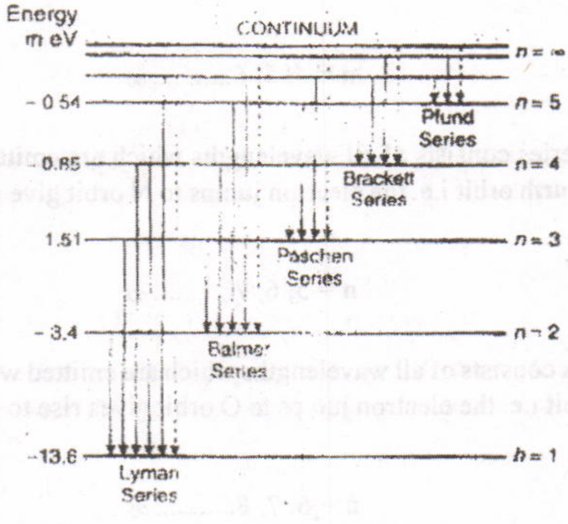


FIG 1.3.2

1.4 ALKALI ATOMS SPECTRAL TERMS :

In alkali atoms the valençe electron is under the influence of the net effective field of the nucleus and the core electron. Because of this the atom reduces to a hydrogen like atom with a nucleus of charge $(Z - \sigma)e$, where σ is the screening effect of the core. For a large value of n, the value of $(Z - \sigma)$

approaches unity and the energy levels of the alkali atom will be nearer to those of hydrogen atom.

As the electron comes closure to the nucleus, it penetrates into the atomic trunk and consequently the attractive force on the electron also changes. The penetration of orbits is shown in figure(1.4.1).

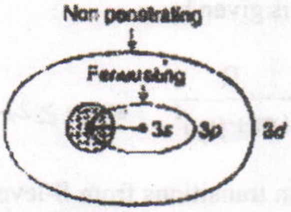


Fig.1.4.1

The term value for alkali atoms is expressed as

$$T_n = \frac{R}{n_{eff}^2}$$

The spectral term can so be expressed as

$$T_n = \frac{R}{(m+\mu)^2}$$

where m is currently related to n but not equal to n and μ is called quantum effect.

The lines in the spectrum of an alkali atom can be grouped into four series in visible region and converge to a common limit.

The wave numbers of these series interms of their term values an expressed as

1. **Principal series :** The series arises from the transitions between various P-levels and lowest S-level. The lowest S-level has the lowest possible value for the energy. This represent the ground state of atom.

   The term values for S-states is

$$T_s = \frac{R}{(1+\mu_s)^2}$$

where R is Rydberg constant and μ_s is the characteristic constant for the sharp series.

The fine values for P-state is

$$T_p = \frac{R}{(m+\mu_p)^2}$$

where μ_p is the characteristic constant of principal series, it is an integer ≥ 2 and $T_s > T_p$.

The wave number of principal series is given by

$$\nu_p = T_s - T_p = \frac{R}{(1+\mu_s)^2} - \frac{R}{(m+\mu_p)^2} \quad \text{at } (m \geq 2) \text{----- (1)}$$

2. Sharp Series : This series arises from transitions from S-levels to the lowest P-levels.

The wave number of sharp series is given by

$$\nu_s = \frac{R}{(2+\mu_p)^2} - \frac{R}{(m+\mu_s)^2} \quad \text{at } (m \geq 2) \quad \text{-------- (2)}$$

where μ_s is characteristic constant of Sharp series.

3. Diffuse Series : This series arises from transitions between the various transitions between D-levels and lowest P-levels.

The wave number of diffuse series is given by'

$$\nu_D = \frac{R}{(2+\mu_p)^2} - \frac{R}{(m+\mu_D)^2} \quad \text{at } (m \geq 3) \quad \text{-------- (3)}$$

where μ_D is characteristic constant of Diffuse series.

4.Fundamental Series : This series arises from transitions from various F-levels to lowest D-levels.

The wave number of fundamental series is given by

$$\nu_F = \frac{R}{(3+\mu_D)} - \frac{R}{(m+\mu_F)^2} \quad \text{at } (m \geq 4) \quad \text{-------- (4)}$$

where μ_F is characteristic constant of fundamental series.

1.5. Doublet Fine Structure in Alkali Spectra :

The lines of optical spectra of alkali atoms show a fine structure splitting. This splitting is small for lighter atom and increases rapidly with increasing atomic number. All lines of the sharp series are close doublets and each line of principal series is also a doublet. The lines of diffuse and fundamental series show a three component fine structure which are called as compound doublets.

In alkali spectra, S-levels is single while P, D, F....levels are doublet levels. The splitting of the levels is due to the spin of electron.

The spin magnetic moment of optically active electron interacts with the internal magnetic field ereated by moving electron through nuclear electric field. The phenomenon is known as spin orbit intraction. Due to interaction, orbital angular momentum $\bar{l}$ of the optical electron is coupled with spin angular momentum $\bar{s}$ to form resultant $\bar{j}$.

The quantum number j values are

$$j = l + s$$
$$= l \pm ½$$

The splitting of each energy level into two levels due to

$j = l + ½$ and $j = l - ½$ values.

For S-level $l = 0$ then there is an expectation for S-level between two splitted level $j = +½$ and $j = -½$.

The table-1.5 shows the complete notation of the levels.

Level	l	s	Multiplicity $(2s+1)$	j	Full notation
S	0	1/2	2	1/2	$^2S_{1/2}$
P	1	1/2	2	3/2, 1/2	$^2P_{3/2}$, $^2P_{1/2}$
D	2	1/2	2	5/2, 3/2	$^2D_{5/2}$, $^2D_{3/2}$
F	3	1/2	2	7/2, 5/2	$^2F_{7/2}$, $^2F_{5/2}$

TABLE-1.5

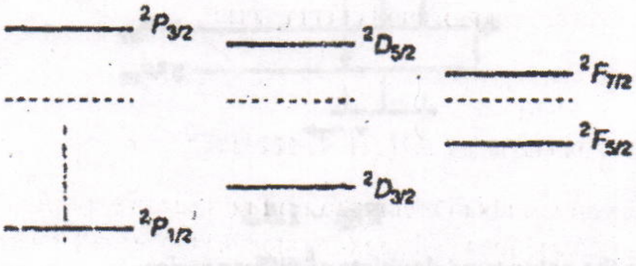


Fig.1.5.1

The figure(1.5.1) represent the splitting of alkali levels ^2P, ^2D and ^2F for a given n value.

The doublets of sharp series are formed by the transitions as

$$n\,^2S_{1/2} \rightarrow m\,^2P_{1/2} \text{ and } m\,^2P_{3/2} \text{ (with } n > m)$$

The principal series doublet are formed by the transitions as

$$n\,^2P_{3/2} \text{ and } n\,^2P_{1/2} \rightarrow m\,^2S_{1/2} \qquad \text{(with } n > m)$$

where n and m represents the total quantum numbers in vector atom model.

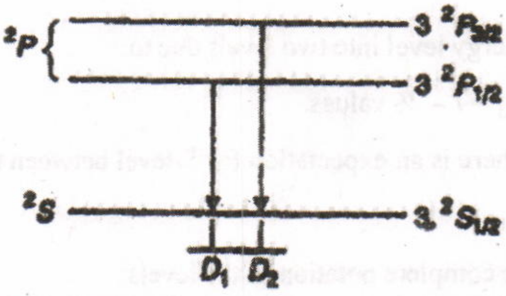


Fig. - 1.5.2

Figure (1.5.2) represents the first members of principal series in sodium D lines doublet.

The lines of diffuse and fundamental series show a three component structure and are called component doublets.

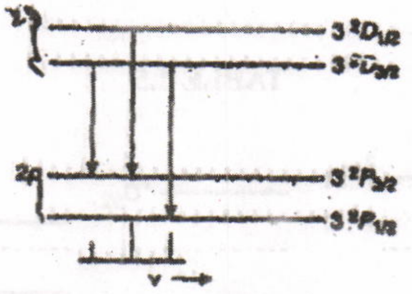


Fig. - 1.5.3

Figure (1.5.3) shows the compound doublets of diffuse series.

1.6 SCREENING CONSTANTS FOR ALKALI SPECTRA :

The effect of electrons in the inner shells that screen the inner charge is called screening effect or *internal screening effect.*

It is supposed that the L electrons (n = 2) move in an approximately coulomb field when the two K electrons (n = 1) behave as though they had coalesced with the nucleus, then by reducing the actual nuclear charge by 2e. The effective nuclear charge is (Z – 2)e. Consequently the spectral term gets modified as

$$T_n = \frac{R\,Z_{eff}^2}{n^2} = \frac{R(Z-b)^2}{n^2} \text{ ----------------} (1)$$

where 'b' is called the screening constant and the effect is called internal screening effect. The value of b is approximately 2 for screening by K electrons.

Similarly M electrons are screened by the L and K electrons from the nucleus and again the spectral term gets suitably modified.

In addition to internal screening effect there is also external screening effect. The outer shell of N-electrons with charge Ne can be regarded as surface of radius r. The potential energy U of an electron of charge e with in the outer shell of charge Ne. Then

$$U = \frac{Ne^2}{r} \text{ ----------------------} (2)$$

When both the effects are considered the total screening constant is taken as σ.

The spectral term is now considered as

$$T_n = \frac{R(Z-\sigma)^2}{n^2} \text{ -----------------------} (3)$$

1.7SELECTION RULES :

The transition rules in spectrascopy are known as selection rules.

Selection rules are the principles which do not allow all transitions from one energy state to another energy state to occur.

The transition rules for alkali spectra are

1. The orbital quantum number can change by ±1.

$$\Delta l = \pm 1$$

2. **The selection principle for spin quantum number S is given by $\Delta S = 0$.**

   It states that the transition between the levels having different multiplicites cannot take place.

3. **The selection princile for total quantum number j is that it may remain unchanged or it may change by unity.**

   The transitions are allowed for $\Delta j = 0$ or ± 1.

1.8 SINGLET AND TRIPLET FINE STRUCTURE IN ALKALINE EARTH SPECTRA

The spectra of alkaline earth elements resemble the spectra of helium atom. Due to two electrons in outermost shell, the spectra of alkaline earth consists of very large number of lines. The spectrum consists of two types of spectral lines, singlets and triplets. The lines of each type can be grouped into four series, namely, principal, sharp, diffuse and fundamental.

In the ground state of two valence electron system.

$n = 1$, $l = 0$ and $s = ½$ for each electron.

For two electrons system

$$L = l_1 + l_2 = 0$$

and $S = s_1 + s_2 = 0$ **or** 1

But Pauli's exclusion principle does not allow $S = 1$ state. Then the term symbol is $^1S_0$. Hence the ground state of alkaline earth only show singlet structure.

When the electron is excited, it comes to higher states. Then in first excited state (P state).

$$L = l_1 + l_2 = 1$$

$$S = s_1 + s_2 = 0 \text{ or } 1$$

a) Wtih $S = 0$, $J = L + S = 1$ we get singlet state $^1P_1$.

b) With $S = 1$, $J = 2, 1, 0$ $[(1 + 1), 1, (1 - 1)]$ we get $^3P_2$, $^3P_1$, $^3P_0$. This is triplet state.

Let us now consider the second excited state (D state). In this case $L = 2$, $S = 0$ or 1.

i). with $L=2$, $S=0$ and $J=2$, the state is $^1D_2$ This is singlet state.

ii). with $L=2$, $S= 1$ and $J= (3,2,1)$, the state are $^3D_3$, $^3D_2$, $^3D_1$. This is a triplet state.

In singlet state the spins are anti parallel and in triplet state the spins are parallel.

In fine structure of triplets,

i). all members of sharp series are composed of three lines and approach a triplet limit

ii). all members of principal series are composed of three lines with decreasing separation and have a single limit.

iii) all members of diffuse and fundamental series contain six lines, three strong lines and three satellites with triple limit.

1.9 COUPLING SCHEMES :

An atom contains a large number of electrons with different orbit and spin angular momenta. The total angular momentum J is the vector sum of these individual momenta. The method of combination depends on the coupling between the orbital and spin angular momenta.

There are two types of coupling, namely

1. L-S coupling or Russell - Saunders coupling
2. j-j coupling

a) L-S Coupling or Russel - Saunders Coupling :

This type of coupling occurs more frequently and hence it is known as normal coupling.

In this coupling all the orbital angular momentum vectors l of the electrons and resultant vector L, spin angular momentum vectors s and resultant vector S.

The total angular momentum of the atom is given by

$$J = L + S$$

where $L = l_1 + l_2 + l_3 + \ldots..$

$S = s_1 + s_2 + s_3 + \ldots..$

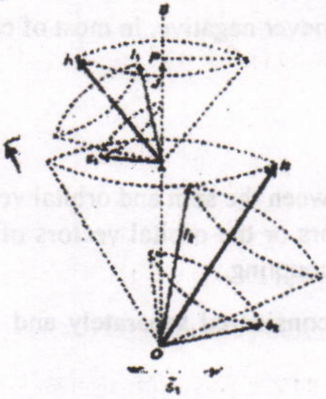


FIG. 1.9.1

Figure (1.9.1) shows the L-S coupling.

L is always an integer 0, 1, 2, 3,.......etc.

S is depends upon the number of electrons and direction of their spin vectors.

In case of two electrons system,

S = 1 when the spins are parallel

S = 0 when the spins are anti parallel

In case of three electrons system,

S = 3/2 when the spins are parallel

S = 1/2 when the spins are anti parallel

Table - 1.9 Shows the spin values of electrons.

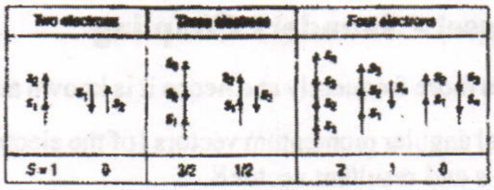


Table - 1.9

Then J = integer (0, 1, 2, 3 ....etc) when S is integer for even electron system.

J = half integer (1/2, 3/2, 5/2 ....etc) when S is half integer for odd electron system.

J is always positive and never negative. In most of cases L-S couling is effective.

b) j-j Coupling :

In certain cases the interaction between the spin and orbital vectors in each electron is stronger than the interactive between spin vectors or the orbital vectors of different electrons. In such cases j-j coupling is more suitable than L-S coupling.

In j-j coupling, each electron is considered separately and its angular momentum j is given by $j = l + s$.

The total angular momentum J of the atom would be vector sum of j vectors of electrons.

Then $j_1 = l_1 + s_1$

$j_2 = l_2 + s_2$

$j_3 = l_3 + s_3$

....

....

$$J = j_1 + j_2 + j_3 + ...$$

$$= \sum j$$

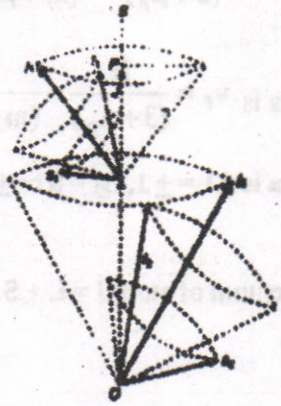


Fig. 1.9.2

Figure (1.9.2) shows j - j compling.

1.10 SUMMARY :

1. The regular arrangement of colours is called spectrum.
2. Atomic spectra consists of a large number of discrete parallel lines.
3. Spectra of hydrogen is the simplest atomic spectra
4. As the value of n increases, the energy levels of alkali metals approaches to that of hydrogen level.
5. Term value of alkali spectra is $T = \frac{R}{n_{eff}^2}$

   Term value of S-states is $T_S = \frac{R}{(l + \mu_S)^2}$

   Term value of P-states is $T_P = \frac{R}{(m + \mu_P)^2}$

6. Wave number of principal series is $\nu_P = T_S - T_P$

$$= \frac{R}{(l + \mu_S)^2} - \frac{R}{(m + \mu_P)^2}$$

Wave number of sharp series is $\nu_S = \frac{R}{(2+\mu_P)^2} - \frac{R}{(m+\mu_S)^2}$

Wave number of diffuse series is $\nu_D = \frac{R}{(2+\mu_P)^2} - \frac{R}{(m+\mu_D)^2}$

Wave number of fundamental series is $\nu_f = \frac{R}{(3+\mu_D)} - \frac{R}{(m+\mu_f)^2}$

7. The transition rules for alkali spectra is $\Delta l = \pm 1, \Delta j = 0$ or ± 1.

8. In L-S coupling, total angular momentum of atom $J = L + S$.

where $L = l_1 + l_2 + l_3 + \ldots\ldots\ldots$

$S = s_1 + s_2 + s_3 + \ldots\ldots\ldots$

9. In j-j coupling, total angular momentum of atom $J = j_1 + j_2 + j_3 + \ldots\ldots\ldots$

$$= \sum j$$

where $j_1 = l_1 + s_1, j_2 = l_2 + s_2, j_3 = l_3 + s_3$.

$$S = S_1 + S_2 + S_3 + \ldots\ldots\ldots$$

9. In j-n coupling, total angular momentum of atom $J = j_1 + j_2 + j_3 + \ldots\ldots\ldots$

$$= \sum j$$

where $j_1 = l_1 + s_1,\ j_2 = l_2 + s_2,\ j_3 = l_3 + s_3 \ldots\ldots\ldots\ldots\ldots\ldots$

1.11 KEY WORDS :

Spectrum, Spectral terms, Double fine structure, Screening constants, Selection rules, Singlet and triplet fine structure, Coupling schemes, L-S coupling, j-j coupling.

UNIT - I

LESSON - 2

X-RAY SPECTRA

OBJECTIVES :

After completing the study of this lesson the students will be able to

1. **Know about X-rays, Types of X-rays spectra.**
2. **Understand the Weak spectra and Continuous spectra of X-rays.**
3. **Obtain the expression for empirical law of Duane and Hunt.**
4. **Obtain the Moseley's equation.**
5. **Understand the Double structure of X-ray spectra and Absoprtion spectra of X-rays.**

STRUCTURE :

2.1 INTRODUCTION :

Rontgent in 1895 discovered X-rays when he was studying the phenomenon of discharge of electricity through rarefield gases. After performing a series of experiments Rontgen concludes that when a beam of fast moving electrons strike a solid target, an invisible high penetrating radiation is produced. Because of their unknown nature Rontgen called these rays as X-rays These rays are electromagnetic waves of very short wavelength.

X-rays are produced due to loss of kinetic energy when high velocity electrons strike the target materal of high atomic number. High penetrating X-rays termed as hard X-rays while low penetrating X-rays termed as soft X-rays

There are two types of X-ray tubes to produce X-rays, namely

i) the gas filled or Rontgen X-ray tube ii) the modern Coolidge tube or Hot filament tube

X-ray spectra may be divided into two types. They are

i) Characteristic of line spectra or Weak spectra ii) Continuous spectra.

Moseley carried out a systematic study of characteristic X-ray spectra of various metallic elements. A Bragg's spectrometer is used for this purpose and stated Moseley's law.

In the X-ray absorption spectra, the edges are characteristics of the absorbed element. X-ray absorption spectra is not a selective while the optical spectra is selective.

2.2 TYPES OF X-RAY SPECTRA :

a) Weak Spectra or Chracteristic Line Spectra :

The X-ray spectra consist of sharp lines and is the characteristic of target material is said to be weak spectra or characteristic spectra. Few of the fast moving electrons may penetrate the surface atoms of the target material and knockout of the tightly bound electrons even from the inner-most shells like K, L shells etc. of the atom. Then the vacancies so created may be filled by the electrons from higher shells. Thus electronic transitions take place. The energy difference is radiated in the form of X-rays of very small but of definite wavelength. The waelengths depend upon target material. The X-ray spectra consists of sharp lines and is the characteristic of target material. The characteristic X-rays are softer than the primary (continuous) X-rays. Thus the characteristic X-ray spectra is referred as weak spectra

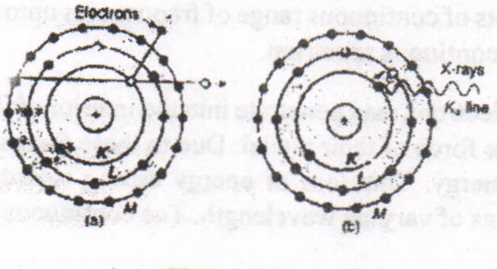


FIG 2.2.1

Figure (2.2.1) shows the fast moving electron knocks off one electron from K-shell and the vacancy is filled by electron from L-shell and produce K_α line of K-series. Similarly the vacancy maybe filled by electrons from more outer orbits.

The frequency of K_α line is given by the relation.

$$(E_K - E_L) = h\upsilon_1$$

If the energy of incident electron is sufficient to remove electron from L-shell then the vacancy filed by electron from M-shell and produce L_α line in L_s-series. The K, L, M , etc. series constitute the X-ray line spectra. Spectral series are shown in figure (2.2.2)

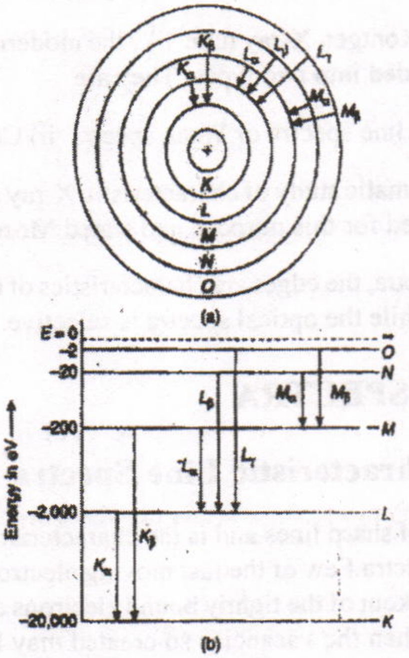


FIG. 2.2.2

b)Continuous Spectra :

The X-ray spectra consists of continuous range of frequencies upto maximum frequency or minimum wavelength is said to be contiuous spectrum.

Few of the fast moving electrons may penetrate into the interior of the atoms of target material and are attracted by the attractive force of their nuclei. Due to these forces the electrons are decelerated and this gives the loss of energy. This loss of energy during retardation is liberated in the form of electromagnetic radiations of varying wavelength. The continuous X-rays are also called as white X-rays.

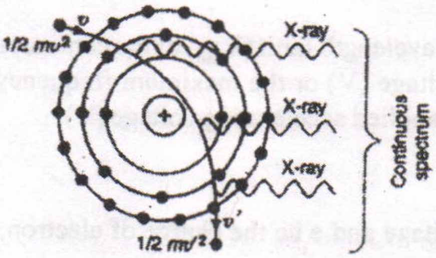


FIG. 2.2.3

Fig. (2.2.3) shows the liberation of X-rays of continuous spectrum.

Let the velocity of electron of mass m changes from v to v_1 due to retardation, then the energy of emitted photon is

$$h\upsilon = \frac{1}{2}mv^2 - \frac{1}{2}mv_1^2 \quad \text{----- (1)}$$

When electron moves very close to the nucleus, it lose a greater amount of energy and release a photon of high frequency.

When the electron is brought to rest by the forces, then the frequency of liberated photon is maximum.

$$\therefore \frac{1}{2}mv^2 = h\upsilon_{max} = \frac{ch}{\lambda_{min}} \quad \text{----- (2)}$$

Let V be the accelerating potential, e be the charge of electron then

$$\frac{1}{2}mv^2 = eV \quad \text{----- (3)}$$

From equations (2) and (3) $\frac{ch}{\lambda_{min}} = eV$

$$\therefore \text{minimum wavelength} = \lambda_{min} = \frac{ch}{eV}$$

$$\text{or maximum frequency } \upsilon_{max} = \frac{eV}{h} \quad \text{------------- (4)}$$

This is empirical law of Duane and Hunt.

Equation (4) shows that the frequency or wavelength of continuous spectra depends on accelerating voltage.

2.3 DUANE AND HUNT'S LAW :

It states that the minimum wavelength limit (λ_{min}) of the continuous X-rays is inversely proportional to the applied accelerating voltage (V) or the maximum frequency (υ_{max}) of the continuous X-rays is directly proportional to the applied accelerating voltage (V).

Let V be the accelerating voltage and e be the charge of electron, then

$$\text{Kinetic eneryg KE} = \frac{1}{2}mV^2 = h\upsilon_{max} = \frac{ch}{\lambda_{min}}$$

$$\text{or KE} = eV$$

$$\therefore h\upsilon_{max} = \frac{ch}{\lambda_{min}} = eV$$

$$\text{maximum frequency } \upsilon_{max} = \frac{eV}{h}$$

$$\text{minimum wavelength } \lambda_{min} = \frac{ch}{eV}$$

On substituting the values of $c = 3 \times 10^8$ m/s, $h = 6.62 \times 10^{-34}$ J-s and $e = 1.602 \times 10^{-19}$ C, we get

$$\lambda_{min} = \frac{3\times10^8 \times 6.02\times10^{-34}}{V[1.602\times10^{-19}]} = \frac{1.24\times10^{-6}}{V}\text{metre} = \left[\frac{12400}{V}\right]\text{Å}$$

It shows that λ_{min} doesnot depend upon the target material.

Figure 2.3.1(a) shows the graph of maximum frequency (υ_{max}) of continuous x-rays against the corresponding voltage. Figure 2.3.1(b) shows the variation of intensity as a function of wavelength for different accelerating potentials.

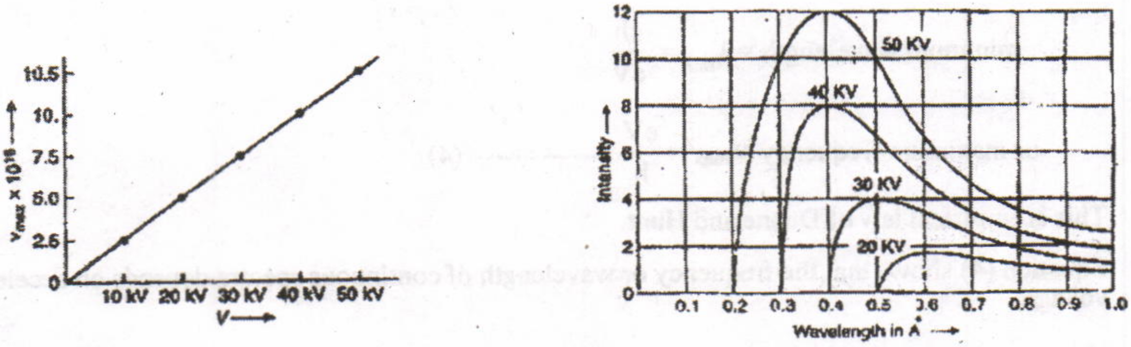


FIG. 2.3.1(a) (b)

2.4 CHARACTERISTICS OF X-RAYS :

1. They are elcctromagentic waves of very short wavelength.
2. They travel in straight lines with the velocity of light.
3. Under suitable conditions, X-rays are reflected and refracted like ordinary light.
4. They exhibit the property of interference, diffraction and polarisation like ordinary light.
5. They are not deflected by electric and magentic fields.
6. They cause fluorescence in many substances like barium, cadmium, zinc sulphide.
7. Thye can ionise the gas through which they pass.
8. When X-rays fall on heavy metals, they produce secondary X-rays.
9. X-rays have destructive effect on living tissue.
10. When X-rays fall on certain metals, they liberate photoelectrons.

2.5 MOSELEY'S LAW :

It states that the frequency of a spectral line in a characteristic X-ray spectrum varies directly as the square of atomic number (Z) of the element emitting it.

Moseley carried out a systemtic study of characteristic X-ray spectra of various metallic elements as targets in X-rays tube.

Fig. (2.5.1) shows the Moseley's diagram for K_α and K_β lines obtained by plotting $\sqrt{\upsilon}$ verses Z of different elements. The graph is a linear one.

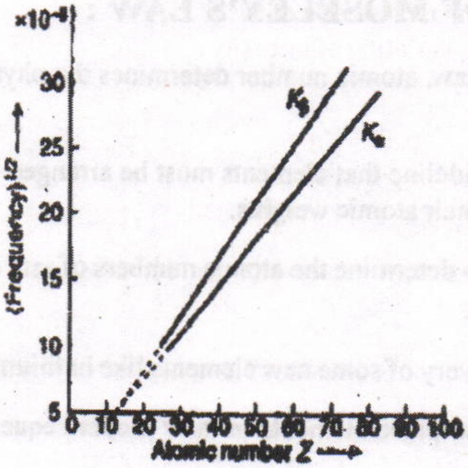


FIG. 2.5.1

Mathmatically, the relation between frequency and atomic number is given by

$$\upsilon \alpha (Z-a)^2$$

or $$\upsilon = b(Z-a)^2 \quad \text{----- (1)}$$

where υ is frequency of charactristic radiation

b is constant, which is different for different series

a is constant, known as screening constant and is difference for different series.

Relation (1) is known as Moseley's law or Moseley equation.

For K_{α} – line

Constant $b = 3R/4$ where R is Rydberg constant

$a = 1$

then $$\upsilon_{K_{\alpha}} = \frac{3R}{4}(Z-1)^2 \quad \text{----- (2)}$$

The exact form of Moseley's law is

$$\frac{1}{\lambda} = R(Z-\sigma)^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \quad \text{----- (3)}$$

where σ is correction factor, n_1 and n_2 are principal quantum numbers of the energy levels.

2.6 IMPORTANCE OF MOSELEY'S LAW :

1. According to Moseley's law, atomic number determines the physical and chemical properties of an element.
2. This law provides the guideline that elements must be arranged in periodic table according to their atomic numbers and not their atomic weights.
3. This law has been used to determine the atomic numbers of rare earth elements and also fixing their positions in periodic table.
4. This law had to the discovery of some new elements like hafnium (72), technitium (43) etc.
5. This law has been used to place elements in their proper sequence in the periodic table in certain questionable cases.

2.7 DOUBLE STRUCTURE OF X-RAY SPECTRA :

Moseley made a systematic study of the characteristic of K-radiation and found that K-radiatio consists of two distinct lines K_α and K_β. Later investigation showed that in heavier elements, each lin consists of two lines such as K_α line consists K_{α_1} and K_{α_2}. Similarly K_β line consists K_{β_1} and K_{β_2}. Thi is called as doublet structure of X-ray spectra. For these lines Moseley's law holds good.

$$\upsilon = b(Z - a)^2$$

For K_α lines, $b = \dfrac{3Rc}{4}$ **and** $a = 1$

For K_β lines, $b = \dfrac{8Rc}{9}$ **where R is Rydberg's constant.**

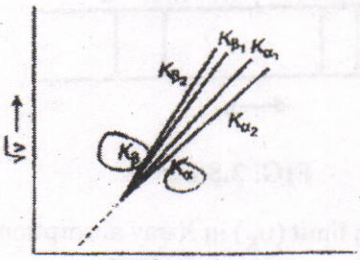


FIG. 2.7.1

Fig.(2.7.1) shows the doublet structure of K lines.

The similar kind of fine structure is observed in L, M and N series also.

In doublet structure, the K-series consists of single group, L-series consists of three sub groups, M series consists of five sub groups and so on. All these lines obey Moseley's law.

The doublet fine structure of X-ray spectra is shown in fig. (2.7.2)

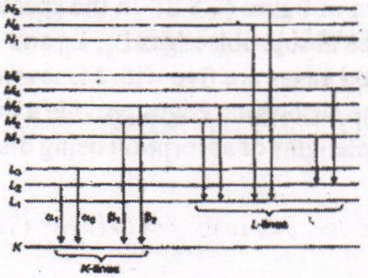


FIG. 2.7.2

2.8 X-RAY ABSORPTION SPECTRA :

The X-ray spectrum in which a continuous region of absorption bounded by sharp edge in the positior of the limit of the emission series is called X-ray absorption spectrum.

The sharp edges in the absorption spectrum are characteristics of the absorbed elements. These edges are called absorption edges. The frequency of the absorption edge in a series is called absorption limit. Frequencies higher than absorption limit are strongly absorbed while the lower frequencies are sightly absorbed.

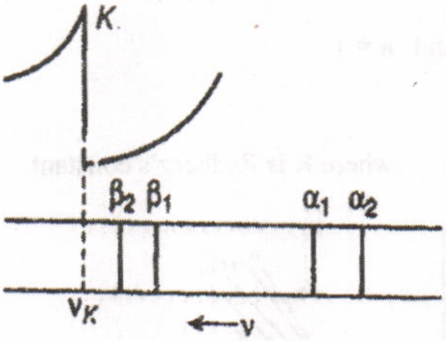


FIG. 2.8.1

Figure (2.8.1) shows the K-absorption limit (υ_K) in X-ray absorption spectra.

X-ray absorption spectra is not selective while the optical spectra is selective. When light pass through sodium vapour in hot state emits two D-lines while in cooler state produce two dark lines at same wavelengths. The case is reverse in X-ray absorption spectra.

The K-absorption edge observed in X-ray spectra of elements corresponds to photoelectric ejection of an electron from the K-shell of that element. Its frequency υ_K exactly gives the required energy W_K.

Each element gives only one K-absorption edge. This shows that K-shell has only a single energy level.

Let ρ is density of the material and μ is its absorption coefficient then

Mass absorption coefficient = μ/ρ

The X-ray absorption for lead is shown in figure (2.8.2). In the spectrum there is a continuum in L region. This continuum consists of three absoprtion edges L_I, L_{II} and L_{III}. These edges directly give three energy levels. Similarly absorption edges are five with M, seven with N, nine with O and so o can be observed in other cases. Thus the absorption edges provide a direct method of determining ray energy levels of elements. The wavelengths of absorption being discontinuous is the characterist of the chemical element.

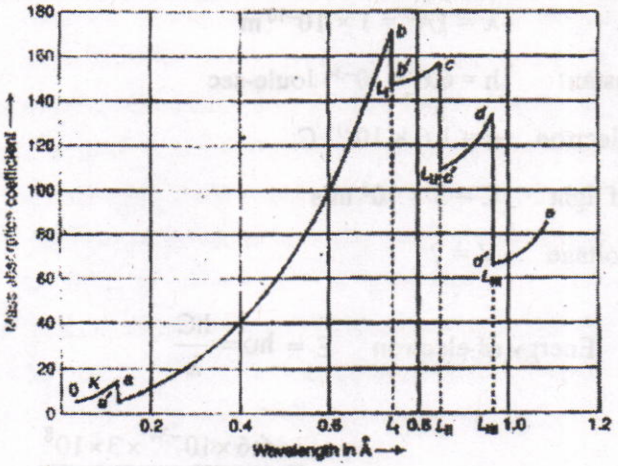


FIG. 2.8.2

.9 SOLVED EXAMPLES :

1. X-ray tube operated at 40KV emits a continuous X-ray spectrum with a short wavelength limit 0.310Å. Calculate the Planck's constant. [C = 3 × 10^8 m/s, e = 1.6 × 10^{-19} C].

(Ans : 6.61 × 10^{-34} Joule-sec)

l: Given that Voltage V = 40 KV = 40 × 10^3 volts

Minimum wavelength λ_{min} = 0.310Å

Velocity of light c = 3 × 10^8 m/s

Charge of electron e = 1.6 × 10^{-19} coulomb

Formula : Minimum wavelength $\lambda_{min} = \frac{ch}{eV}$

$$\text{Plancks constant } h = \left[\frac{eV}{c}\right]\lambda_{min}$$

$$= \left[\frac{1.6\times10^{-19}\times40\times10^{3}}{3\times10^{8}}\right]0.310\times10^{-10}$$

$$= \mathbf{6.61 \times 10^{-34}} \textbf{ Joule-sec.}$$

2. Find the operating voltage of X-ray tube to emit electron from cathode to give an X-ray of wavelength 1A^0 after striking the target ? [e = 1.6 × 10^{-19}C, C = 3 × 10^8 m/s and h = 6.6 × 10^{-34} Joule-sec]

(Ans : 12380 volt)

Wavelength $\lambda = 1A^0 = 1 \times 10^{-10}$ m

Plancks constant $h = 6.6 \times 10^{-34}$ Joule-sec

Charge of electron $e = 1.6 \times 10^{-19}$ C

Velocity =of light $C = 3 \times 10^8$ m/s

Operating voltage $V = ?$

Formula : Energy of electron $E = h\upsilon = \frac{hC}{\lambda}$

$$= \frac{6.6\times10^{-34}\times3\times10^8}{1\times10^{-10}}$$

Operating voltage $V = E/e$ $\because E = eV$

$$= \frac{19.8\times10^{-16}}{1.6\times10^{-19}} = 12380 \text{ volt}$$

3. If K_α - radiation of Mo (Z = 42) has a wavelength of 0.75A⁰. Calculate the corresponding wavelength of radiation coming out of Co (Z = 27). **(Ans = 1.86 A⁰)**

Sol: Given that

Atomic number of Mo is $Z_{Mo} = 42$

Atomic number of Co is $Z_{Co} = 27$

Wavelength of K_α - radiation $= \lambda_{Mo} = 0.75\ A^0$

$= 0.75 \times 10^{-10}$ m

Wavelength of K_α - radiation $= \lambda_{Co} = ?$

Formula : Moseley's law $\upsilon \propto (Z-1)^2$

(or) $\frac{1}{\lambda} \propto (Z-1)^2$ $\therefore \frac{\lambda_{Co}}{\lambda_{Mo}} = \left[\frac{Z_{Mo}-1}{Z_{Co}-1}\right]^2$

$$\therefore \frac{\lambda_{Co}}{\lambda_{Mo}} = \left[\frac{Z_{Mo}-1}{Z_{Co}-1}\right]^2$$

$$\lambda_{Co} = \lambda_{Mo}\left[\frac{Z_{Mo}-1}{Z_{Co}-1}\right]^2$$

$$=0.75\times10^{-10}\left[\frac{42-1}{27-1}\right]^2$$

$$=0.75\times10^{-10}\left[\frac{41}{26}\right]^2 \quad = 1.86\ A^0$$

4. Deduce the wavelength of K_α line for an atom of $Z = 92$ [$R = 1.1 \times 10^5\ cm^{-1}$].

(Ans : 0.1464 A^0)

Sol: Given that

Atomic number $Z = 92$

Rydberg constant $R = 1.1 \times 10^5\ cm^{-1}$

Wavelength of K_α line $= \lambda_{K_\alpha} = ?$

Formula : Moseley's law $\upsilon = b(z-a)^2$

$$\text{or} \qquad \frac{1}{\lambda} = b(z-a)^2$$

For K_α - line, $b = 3R/4$ and $a = 1$

$$\therefore \frac{1}{\lambda_{K_\alpha}} = \frac{3R}{4}\ [2-1]^2$$

$$= \frac{3\times1.1\times10^5}{4}\ [92-1]^2 = \frac{3\times1.1\times10^5[91]^2}{4}$$

$$\text{then} \qquad \lambda_{K_\alpha} = \frac{4}{3\times1.1\times10^5[91]^2} = 0.1464\times10^{-8}\ cm = 0.1464\ Å$$

5. What is the minimum wavelength of X-ray emitted by an X-ray tube operating at 120

(Ans : 0.1033 Å)

Sol: Given that Operating voltage $V = 120\ KV = 120 \times 10^3$ volt

Minimum wavelength $\lambda_{min} = ?$

Formula :

$$\text{Minimum wavelength } \lambda = \left[\frac{12{,}400}{V}\right] Å$$

$$= \left[\frac{12{,}400}{120 \times 10^3}\right] Å = 0.1033\ Å$$

6. In Uranium (Z = 92) the K absorption edge is 0.107Å and K_α line is 0.126Å. Determine th wavelength of L- absorption edge. **(Ans : 0.709 Å)**

Sol: Given that

Wavelength in K-absorption edge $\lambda_K = 0.107Å$

Wavelength of K_α line $\lambda_{K_\alpha} = 0.126\ Å$

Wavelength in L-absorption edge $\lambda_L = ?$

Formula : Energy $E = \frac{Ch}{\lambda_{K\alpha}} = -\left[\frac{12{,}400\ eV}{\lambda_{K\alpha} \text{ in } Å}\right]$

$$= -\left[\frac{12{,}400\ eV}{0.107\ Å}\right] = -115.9\ KeV$$

and $E_L - E_K = \frac{ch}{\lambda_{K_\alpha}}$

$$= \left[\frac{12{,}400 eV}{\lambda_{K_\alpha} \text{ in } Å}\right] = \left[\frac{12{,}400\ eV}{0.126\ Å}\right] = 98.4\ KeV$$

$$\therefore E_L = 98.4 + E_K$$

$$= 98.4 - 115.9 = -17.5\ KeV$$

$$\therefore \lambda_L = -\frac{ch}{E_L} = \frac{-12{,}400\ eV}{-17.5\ KeV} = 0.709\ Å$$

2.10 SUMMARY :

1. Rontgen in 1895 discovered X-rays.
2. X-ray tubes to produce X-rays are (i) gas filled X-ray tube, (ii) Coolidge tube.
3. Characteristic of line spectra or weak spectra.

   The frequency of K_α line is given by the relation. $(E_K - E_L) = h\upsilon_1$
4. Continuous spectra Minimum wavelength $\lambda_{min} = ch/eV$
5. Duane and Hunt's law ;

   Maximum frequency $\lambda_{max} = eV/h$

   Minimum wavelength $\lambda_{min} = ch/eV$

   $$= \left[\frac{12400}{V}\right]Å$$
6. Moseley's law

   Frequency $\upsilon = b(z-a)^2$

   $$\nu_{K_\alpha} = \frac{3R}{4}(z-1)^2$$

   Exact form of Moseley's law is $\frac{1}{\lambda} = R[Z-\sigma]^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$
7. Double structure of X-ray spectrum $\upsilon = b[z-a]^2$

   For K_α lines $b = 3Rc/4$ and $a = 1$

   For K_β lines $b = 8Rc/4$
8. Mass absorption coefficient of $= \mu / P = \frac{\text{absorption coefficeint}}{\text{density}}$

2.11 KEY WORDS :

X-rays, X-ray spectra, Weak spectra, Continuous spectra, Moseley's law, Duane and Hunt law, Absorption spectra.

2.12 SELF ASSESSMENT QUESTIONS

1. What are X-rays and state their properties ?
2. Explain weak spectrum and continuous spectrum of X-rays.
3. Explain the main features of X-ray absorption spectra.
4. State and explain Moseley's law.
5. Explain Duane and Hunt's law.
6. Explain double structure of X-ray spectra.

EXERCISES:

1. If the minimum wavelength recorded in X-ray spectrum of 50KV tube is 0.26Å, determin the Planck's constant. **(Ans : 6.56 × 10^{-34} J-S)**

[**Hint :** Maximum energy of emitted X-ray = $h\upsilon_{max} = hc/\lambda_{min}$

$= eV$

$$\therefore \frac{hC}{\lambda_{min}} = eV \text{ or } h = \frac{eV\lambda_{min}}{C} = \frac{1.6\times10^{-19}\times50\times10^{3}\times0.26\times10^{-10}}{3\times10^{8}} J-S]$$

2. Estimate the value of wavelength of K_α line of silver (Z = 47). Give R = 109737 cm^{-1}. **(Ans : 0.57Å)**

[**Hint :** For K_α line, $\frac{1}{\lambda_{K_\alpha}} = \frac{3R}{4}(Z-1)^2 = \frac{3\times109737}{4}(47-1)^2$

$$\lambda_{K_\alpha} = \frac{4}{3\times109737(46)^2} cm]$$

3. X-ray tube is operated at 18KV. Calculate the minimum velocity of electron bombarding at an cathode. **(Ans : 8 × 10^7 m/s)**

[**Hint :** Kinetic energy of electron $KE = \frac{1}{2}mV^2 = eV$

Velocity of electron $V = \sqrt{\frac{2eV}{m}} = \sqrt{\frac{2\times1.6\times10^{-19}\times18\times10^{3}}{9.1\times10^{-31}}}$]

.What element has K_α line of wavelength 1.785Å ? For K_α line a = 1, b = 3CR/4 and R = 1.097 × 10^7 m^{-1} ? **(Ans : 27 cobalt)**

[**Hint :** For K_α – line, $V_{K_\alpha} = b(z-a)^2$

$$V_{K_\alpha} = \frac{C}{\lambda_{K_\alpha}} = \frac{3CR}{4} = (Z-1)^2$$

$$\frac{1}{\lambda_{K_\alpha}} = \frac{3R}{4}(Z-1)^2$$

$$\therefore (Z-1)^2 = \frac{4}{3R\ \lambda_{K_\alpha}} = \frac{4}{3 \times 1.097 \times 10^7 \times 1.785 \times 10^{-10}}$$

$$Z - 1 = 26.]$$

The K_α and K_β of X-rays of molybdenum hae wavelength 0.71Å and 0.63Å respectively, find the wavelength of material. **(Ans : 5.58 Å)**

[**Hint :** Energy $E_{K_\alpha} = -\frac{Ch}{\lambda_{K_\alpha}} = -\frac{12,400}{0.71} = -1.746 \times 10^4$ eV

Energy $E_{K_\beta} = -\frac{Ch}{\lambda_{K_\beta}} = -\frac{12,400}{0.63} = -1.968 \times 10^4$ eV

Energy for L_α line $E_\alpha = E_{K_\beta} - E_{K_\alpha}$

$$= -[1.968 - 1.746] \times 10^4 = -0.222 \times 10^4 \text{ eV}$$

Wavelength of L_α line $\lambda_\alpha = -\frac{12400}{E_\alpha} = \frac{-12400}{-0.222 \times 10^4}$]

material of K-absorption edge is 0.15Å is irradiated with X-rays of 0.10Å. What is the maximun kinetic energy of photoelectron that are emitteo from K-shell.

(Ans : 41.3 KeV)

[**Hint :** In K-shell $E_K = \frac{CH}{\lambda_K} = \frac{12,400 \text{ eV}}{\lambda_K \text{ in Å}} = 82.7$ KeV

ıergy of incident photon $E_\upsilon = \frac{Ch}{\lambda} = \frac{12400\text{eV}}{\lambda \text{ in Å}} = 124$ KeV $\qquad KE_{mass} = E_0 - E_K$]

7. If K, L and M energy levels of platinum are 80,000 eV, 15,000 eV and 3,100 eV respectively, calculate the wavelength of K_α and K_β radiation respectively when platinum is used to emit these radiations.

(Ans : 0.190 Å, 0.179 Å)

[Hint : $h\upsilon_{K_\alpha} = (80{,}000 - 15{,}000)\text{eV} = 65{,}000 \text{ eV} = hC/\lambda_{K_\alpha}$

$$\therefore \lambda_{K_\alpha} = \frac{hC}{65{,}000 \text{ eV}} = \frac{6.62\times10^{-34}\times3\times10^{8}}{65{,}000\times1.6\times10^{-19}}$$

and $h\upsilon_{K_\beta} = (80{,}000 - 3100)\text{eV} = 76{,}900 \text{ eV} = hC/\lambda_{K_\beta}$

$$\therefore \lambda_{K_\beta} = \frac{hC}{76{,}900 \text{ eV}} = \frac{6.62\times10^{-34}\times3\times10^{8}}{76.900\times1.6\times10^{-19}}$$]

2.13 REFERENCE BOOKS:

1. Prospective of Modern Physics	A.Beiser
2. Induction to Modern Physics	M.S. Mani, G.K. Mehta
3. Elements of Modern Physics	Patil
4. Modern Physics	S.L. Gupta, S.Gupta

UNIT - I

LESSON- 3

MOLECULAR PHYSICS

OBJECTIVES :

After completing the study of this lesson the students will be able to

1. Understand about molecular spectra.
2. Quantization of rotational energies
3. Know the selection rules
4. Understand the vibration-rotation spectra
5. Determine the inter-nuclear distance
6. Know about Raman effect and its characteristics
7. Understand the quantum theory of Raman effect
8. Know the difference between Rayleight scattering and Raman scattering

STRUCTURE :

3.1 INTRODUCTION :

The spectra emitted by a element in its molecular state is called as molecular spectra. It arises from rotation of a molecule as a whole, vibrations of its constituent atoms relative to one another as well as from change in its electronic configuration. Molecular spectra generally fall in three regions, namely, (i) Microwave and far infrared region, (ii) Near infrared region, (iii) Visible or ultra violet region.

The internal energy of a molecule besides translational is of three kinds, namely, electronic, vibrational and rotational. Each energy is quantised. The total energy of a molecule is sume of these energies.

The vibrational energy arise due to nuclei vibration along the inter nuclear axis and rotational energy arise due to the system as a whole rotates about the centre of mass and then gives various rotational energy levels which gives a spectrum.The transitions between rotational energy states are possible by obey the selection rules $\Delta J = \pm 1$.

Rayleigh observed that the change in intensity of scattered light but there is no change in wavelength or frequency. C.V. Raman observed that the spectrum of scattered light consists of frequencies greater and smaller than the incident beam frequency. This is known as Raman effect.

3.2 MOLECULAR SPECTRA :

The spectra emitted by element in its molecular state is known as band or molecular spectra.

Molecular spectra arise from the rotation of molecule, vibrations of its atoms and changes in its electronic configuration.

Molecular spectra fall in three distinct regions, namely,

1. **Microwave and far Infrared Region :** The spectrum in this region is called as pure rotational spectrum. It consists of many equally spaced lines.

2. **Near Infrared Region :** The spectrum in this region is called as vibrational rotational spectrum. It consists of large number of bands and each band consists of closely spaced lines.

3. **Visible or Ultra-violet Region :** The spectrum in this region is called as electronic spectrum. It consists of bands and each band consists of several bands.

3.3 DISCRETE SET OF ELECTRONIC ENERGIES OF MOLECULES :

The total energy of a molecule consists of electronic energy (E_c), vibrational energy (E_v) and rotational energy (E_R). The vibrational energy arise due to nuclei vibration along the inter nuclear axis and rotational energy arise due to the system as a whole rotates about the centre of mass. The energy levels corresponding to these energies of molecules are discrete. The total energy of a molecule is the sum of three energies.

$$E = E_e + E_R + E_V$$

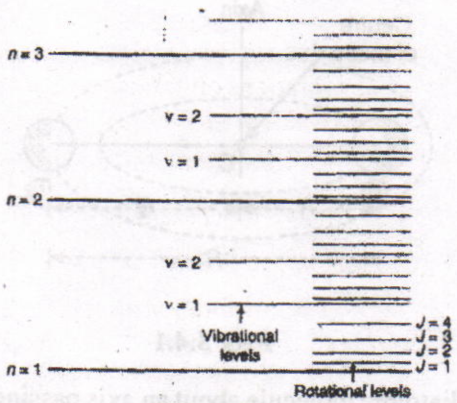


FIG. 3.3.1

Fig. 3.3.1 shows the electronic, vibrational and rotational energy levels in a diatomic molecule.

In the molecular spectra

1. A molecule has a number of discrete energy levels. A transition between two electronic levels results in a radiation which fall in ultraviolet region.

2. With each electronic level, a number of vibrational energy levels are asociated.

   A transition between two vibrational levels results in a radiation which fall in near infrared region.

   With each vibrational level a set of vibrational level is associated. A transition between two vibrated levels results in a radiation which fall in far infrared or microwave region.

   When the molecule suffers a transition from higher energy state (E) to a lower energy state (E^1), the difference of energy

$$\Delta E = E - E^1$$

is emitted as radiation of frequency

$$\nu = \frac{\Delta E}{h} = \frac{E - E^1}{h}$$ where h is Planck's constant.

3.4 QUANTIZATION OF ROTATIONAL ENERGIES :

A pure rotational spectra arises due to the transition between various rotational energy levels. When microwave radiation is incident on a molecule, the molecule absorb the energy rotates about its centre of mass and then gives various rotational energy levels, it gives a spectrum.

Energy levels of a diatomic molecule : The simplest molecule is a diatomic molecule. Let two atoms of mass m_1 and m_2 are separated by a distance R and bounded by attractive forces. This diatomic molecule behaves as a rigid rotator. It rotates about an axis passing through its cnetre of mass C and perpendciualr to the line joining the atoms as shown in figure (3.4.1)

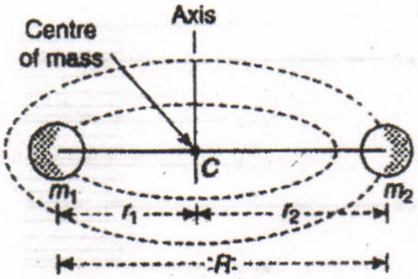


FIG 3.4.1

The moment of inertia of diatomic molecule about an axis passing through its centre of mass is given by

$$I = m_1 r_1^2 + m_2 r_2^2 \qquad \text{----- (1)}$$

As the system is balanced about its centre of gravity

$$m_1 r_1 = m_2 r_2 \qquad \text{----- (2)}$$

But $R = r_1 + r_2$ ----- (3)

From equations (2), (3),

$$r_1 = \left(\frac{m_2}{m_1 + m_2}\right) R$$

and $r_2 = \left(\frac{m_1}{m_1 + m_2}\right)R$

Substituting the values in equation (1), we get.

$$I = \left[\frac{m_1 m_2^2}{(m_1 + m_2)^2}\right]R^2 + \left[\frac{m_2 m_1^2}{(m_1 + m_2)^2}\right]R^2 = \left[\frac{m_1 m_2}{m_1 + m_2}\right]R^2$$

or $I = \mu R^2$ ----- (4)

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is reduced mass of the molecule.

The angular momentum of molecule is given by

$$L_r = I\omega$$

where ω is angular velocity.

The angular momentum of rotating molecule is quantized with values.

$$L_r = \left[\sqrt{J(J+1)}\right]\hbar \quad \text{----- (5)}$$

where $\hbar = h/2\pi$ and J is rotational quantum number. J has values of 0, 1, 2, 3, ...

In classical mechanics, the energy of rotation of a molecule is

$$E = ½ I\omega^2$$

Hence the energy levels of rotating molcule is given by

$$E_r = \frac{1}{2}I\omega^2 = \frac{1}{2I}(L_r)^2 = \frac{J(J+1)\hbar^2}{2I} \quad \text{----- (6)}$$

The solution of Schrodinger wave equation $\nabla^2\psi + \frac{8\pi^2\mu}{h^2}E\psi = 0$ gives the value of energy as

$$E = \frac{h^2}{8\pi^2\mu R^2}J(J+1)$$

$$= \frac{h^2}{8\pi^2 I}J(J+1) \quad \text{----- (7)}$$

where J = 0, 1, 2, 3 .... It gives a series of discrete energy levels with energies 0.2 $h^2/8\pi^2I$, 6 $h^2/8\pi^2I$, 12 $h^2/8\pi^2I$, ...

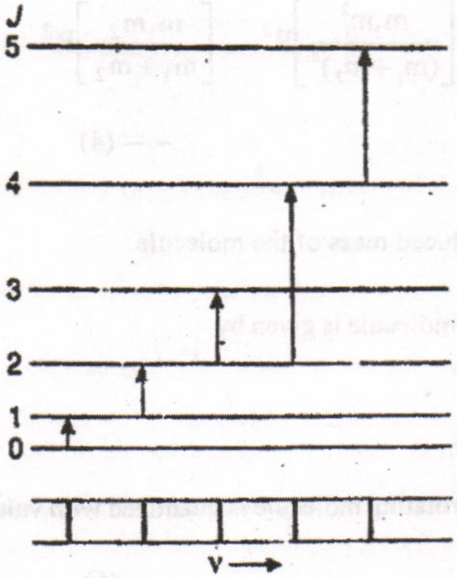


FIG. 3.4.2

Figure (3.4.2) shows the rotational energy levels of diatomic molecule and the spectrum.

The frequency of transition between levels of energy E_{J_1} and E_{J_2} states is given by

$$\upsilon = \frac{E_{J_1} - E_{J_2}}{h} = \frac{\Delta E}{h}$$

$$= \frac{1}{h}\left[\frac{h^2}{8\pi^2 I} J_1(J_1+1) - \frac{h^2}{8\pi^2 I} J_2(J_2+1)\right] = \frac{h}{8\pi^2 I}[J_1(J_1+1) - J_2(J_2+1)] \qquad \text{----- (8)}$$

For different values of J_1 and J_2, we get different lines in the spectrum of the molecule. This set of lines form the pure rotational spectrum of the molecule.

3.5 TRANSITION RULES FOR PURE ROTATIONAL SPECTRA :

The transitions are possible by obey the following selection rule

$\Delta J = +1$ for absorption $\qquad$ $\Delta J = -1$ for emission ----- (1)

The frquency of observed radiation due to transition between energy levels E_J and E_{J+1} is given by

$$\upsilon_1 = \frac{E_{J+1} - E_J}{h} = \frac{1}{h}\left[\frac{(J+1)(J+2)h^2}{8\pi^2 I} - \frac{J(J+1)h^2}{8\pi^2 I}\right]$$

$$= \frac{h}{8\pi^2 I}[2(J+1)] \quad \text{-- (2)}$$

Similarly the frequency of abosrbed radiation due to transitions between energy levels E_{J+1} and E_{J+2} is given by

$$\upsilon_2 = \frac{E_{J+2} - E_{J+1}}{h} = \frac{1}{h}\left[\frac{(J+2)(J+3)h^2}{8\pi^2 I} - \frac{(J+1)(J+2)h^2}{8\pi^2 I}\right]$$

$$= \frac{h}{8\pi^2 I}[2(J+2)] \quad \text{----- (3)}$$

The frequency difference is given

$$\Delta\upsilon = \upsilon_2 - \upsilon_1 = \frac{h}{4\pi^2 I} \quad \text{--------------- (4)}$$

Equation (4) is independent of J. This shows the lines in the spectrum are equally spaced.

3.6 VIBRATION - ROTATION SPECTRA :

When a molecule absorbs more energy,the molecule rotate rapidly. As a result the centrifugal force increases and pulls the atoms away from the centre of gravity. Now the atoms of molecule vibrate about their mean position. The absorption is also increases the vibrational energy of molecule and gives rise to the vibrational spectra.

The change in vibrational energy of molecule changed in rotational energy of molecule. The spectrum with the combination of rotational and vibrational effects is called as rotational-vibrational spectrum.

Vibration of Diatomic Molecule :

The simplest molecule is a diatomic molecule. Let two atoms of mass m_1 and m_2 are separated by a equlibrium distance r and bounded by attractive force. The vibrating diatomic molecule can be consider a linear harmonic oscillator. If the bond is changed from its equilibrium length r_e to a new length r.

The rotating forces on each atom of diatomic molecule are given by

$$m_1 \frac{d^2 r_1}{dt^2} = -K(r - r_e) \qquad \text{----- (1)}$$

and $$m_2 \frac{d^2 r_1}{dt^2} = -K(r - r_e) \qquad \text{----- (2)}$$

where K is known as force constant, r_1 and r_2 are positions of atoms relative to centre of mass.

Then $$r_1 = \frac{m_2 r}{m_1 + m_2}$$

and $$r_2 = \frac{m_1 r}{m_1 + m_2} \qquad \text{----- (3)}$$

Substitute the value of r_1 in equation (1), we get

$$\left(\frac{m_1 m_2}{m_1 + m_2}\right)\frac{d^2 r}{dt^2} = -K(r - r_e) \qquad \text{----- (4)}$$

But r_e = constant then $dr_e/dt = 0$

$$\therefore \frac{d^2 r}{dt^2} = \frac{d^2(r - r_e)}{dt^2} \qquad \text{----- (5)}$$

From equations (4), (5)

$$\left[\frac{m_1 m_2}{m_1 + m_2}\right]\frac{d^2(r - r_e)}{dt^2} = -K(r - r_e) \qquad \text{---- (6)}$$

then $$\mu \frac{d^2 x}{dt^2} = -Kx$$ where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ and $x = r - r_r$

or $$\mu \frac{d^2 x}{dt^2} + Kx = 0$$

or $$\frac{d^2 x}{dt^2} + \frac{K}{\mu} x = 0$$

or $$\frac{d^2x}{dt^2}+\omega^2x=0 \qquad \text{----- (7)}$$

where $\omega^2 = K/\mu$

Equation (7) is represent the equation of simple harmonic motion.

The frequency of vibration is given by

$$\upsilon_v = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}} \qquad \text{----- (8)}$$

Energy levels: Vibrational energies of molecule are quantized. The solution of Schroedinger equation $\nabla^2\psi+\frac{8\pi^2m}{h^2}E\psi=0$ gives the energy value of a linear harmonic oscillator. Then

$$E_V=\left[\upsilon+\frac{1}{2}\right]h\upsilon_v \qquad \text{----- (9)}$$

When υ is vibrational quantum number and having the values 0, 1, 2, 3, ...
Equation (9) can also be written as

$$E_v=\left[\upsilon+\frac{1}{2}\right]hc\varpi \qquad \text{----- (10)}$$

Where ϖ is the vibrational frequency of vibrating diatomic molecule expressed in wave number

If $\upsilon = 0,\ E_v=\frac{1}{2}hc\varpi$

It is clear that the minimum energy of oscillator is never zero even at absolute zero. This is known as zero point energy.

$$\therefore \text{Zero point energy} = \frac{1}{2}hc\varpi \qquad \text{----- (11)}$$

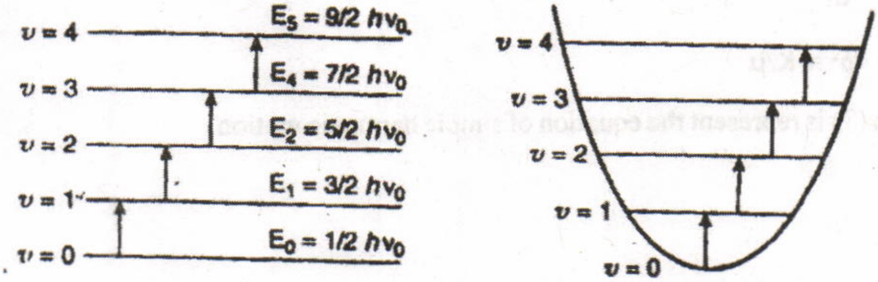


FIG. 3.6.1

Transition rules for vibration :

The selection rule for harmonic oscillator undergoing vibrational changes is

$$\Delta\upsilon = \pm 1$$

If the vibration involves a change in dipolemoment of the molecule, the change in vibrational energy gives an observable spectrum. Thus, vibrational spectra is observed only in hetronuclear diatomic molecule like HF, HCl, HBr etc.

Vibrational - Rotation spectrum of molecule :

Energy levels : Consider a diatomic molecule can execute rotation and vibrations independently without interactions between rotational and vibrational energies.

The total energy due to vibration and rotation is given by

$$E_{total} = E_\upsilon + E_r$$

$$= \left[\upsilon + \frac{1}{2}\right] h\upsilon_v + \frac{J(J+1)h^2}{8\pi^2 I}$$

Spectrum : The selection rule for transition between vibrational states is $\Delta\upsilon = \pm 1$ and $\Delta J = \pm 1$ for rotational states. The transition corresponding for $\Delta J = 0$ is forbidden.

Figure (3.6.2) shows the $J_2 = 0, 1, 2, 3, 4$ levels of diatomic molecule for $\upsilon_2 = 0$ and $J_1 = 0, 1, 2, 3, 4$ levels for $\upsilon_1 = 0$ and the allowed transitions.

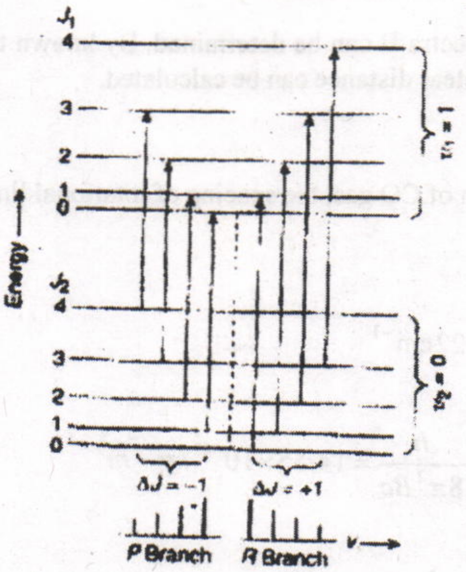


FIG. 3.6.2

3.7 DETERMINATION OF INTER-NUCLEAR DISTANCE :

The rotational spectra of rigid diatomic molecule consist of equidistant series of lines. When the molecule is raised from J to J + 1, the absorption is represented by

$$\Delta E = \frac{h^2}{8\pi^2 I}[(J+1)(J+2) - J(J+1)]$$

$$= \frac{h^2}{8\pi^2 I}[2(J+1)]$$

The wave number of radiation is given by

$$\nu = \frac{\Delta E}{hc}$$

$$= \frac{2h}{8\pi^2 Ic}[J+1]$$

$$= 2B(J+1)$$

where $B = \frac{h}{8\pi^2 Ic}$ **= constant.**

Hence, the spacing between lines is 2B.

From rotational spectra B can be determined. By known the vlaue of B, moment of inertia and bond lenght or internuclear distance can be calculated.

Example :

In the rotational spectra of CO gas, the spacing of rotational lines is 3.844/cm then

$$2B = 3.844\ /\ \text{cm}$$

$$\therefore B = \frac{3.844}{2} = 1.922\,\text{cm}^{-1}$$

$$\text{Moment of Inertia } I = \frac{h}{8\pi^2 Bc} = 14.55\times10^{-47}\,kg-m^2$$

But, $I = \mu r_b^{\,2}$

Where r_b = bond length or internuclear distance

$$\text{Internuclear distance } r_b = \sqrt{\frac{I}{\mu}}$$

$$= \left[\frac{14.55\times10^{-47}}{1.14\times10^{-26}}\right] = 1.13\times10^{-10}\,\text{m} = 0.113\,\text{nm}$$

3.8 RAMAN EFFECT :

The spectrum of scattered light consists of frequencies greater and smaller than the incident beam frequency is known as Raman effect. The spectrum of scattered light called as Raman spectrum. The new lines in the spectrum is known as Raman lines.

Figure (3.8.1) shows the Raman lines in spectrum.

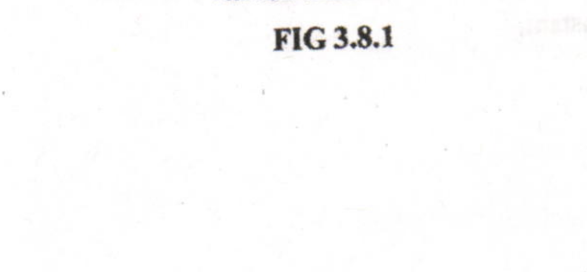


FIG 3.8.1

Anti-stroke lines : The lines of greater frequency than of the incident beam frequency in Raman lines is called as anti-stokes lines.

Stokes lines : The lines of smaller frequency than of the incident beam frequency in Raman lines is called as stokes lines.

The displacement of the lines are independent of frequency of incident light but are functions of the scattering substance. Thus the displacements are different for different scattering substances. So Raman displacements are characteristics of scattering substance.

3.9 CHARACTRISTICS OF RAMAN EFFECT :

1. The frequencies of Raman lines depend on the frequency of the incident light.
2. The displacement of Raman lines from original line depend on the nature of scattering substance.
3. The displacement of Raman lines is independent of the frequency of incident light.
4. The lines of greater frequency than of the incident beam frequency are called as anti-stokes lines.
5. The lines of smaller frequency than of the incident beam frequency are called as stokes lines.
6. The rotational or vibrational state of the molecule is changed due to scattering of light by it.
7. Raman effect is purely a molecular phenomenon.
8. Raman displacements are characteristics of scattering substance.
9. Raman lines are symmetrically situated on either side of the parent line at intervals corresponding to the characteristic frequency of molecule.
10. Rotational Raman lines are obtained with gases.
11. Vibrational Raman lines are obtained with liquids and solids.

3.10 APPLICATIONS OF RAMAN EFFECT :

1. To study the molecular structure of crystals and compounds.
2. To know the number of atoms in a molecule, their relative arrangement, relative masses and chemical bonds between them.
3. To study the composition in palstics, mixtures etc.
4. To decide about single, double or trible bond.
5. To study the spin and statistics of nuclei.

6. To study the binding forces between the atoms or groups of atoms in crystals.

7. To study the vibrational and rotational energy levels of homo nuclear molecules like nitrogen, oxyger etc.

3.11 EXPERIMENTAL STUDY OF RAMAN EFFECT :

The experimental arrangement for Raman effect is shown in figure (3.11.1). It consists of 1. Sourc 2. Raman tube 3. Spectrograph

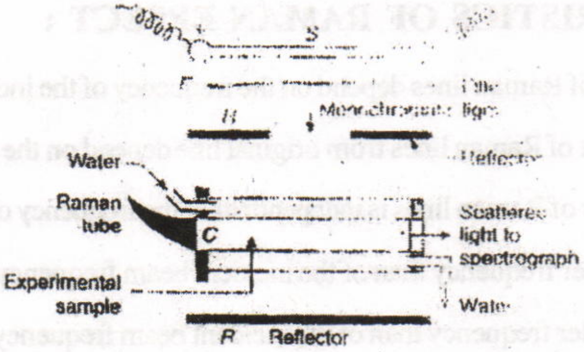


FIG 3.11.1

S is mercury arc lamp as a source of light. The light is passed through a filter F to obtain monochromat beam. The light from source pass through an opening in a metallic reflector is allowed to incident c Raman tube. The Raman tube is a glass tube of 10 to 15cm long and 1 or 2 cm diameter. Scattere light [illegible] through a flat glass surface at one end of tube. The other end of tube is made as hon shaped [illegible] ened outside to provide black background and the tube is surrounded by water jack with cold water circulation.

The experimental sample is placed inside Raman tube and the scattered beam emerges from flat er of tube is examin [illegible] spectrograph.

In the Raman tube gas sample is enclosed at a pressure of few cm of mercury or solid sample in tl form of powder mixed with liquid paraffin or solvent.

.12 QUANTUM THEORY OF RAMAN EFFECT :

On the basis of quantum theory Prof. Smekal in 1929 explained the Raman effect.

When a photon or light quanta of energy $h\upsilon_0$ hits a molecule.Then

1. The molecule doesnot absorb energy from photon but deviate it. Then there will be unmodif line in scattered beam.

2. When a photon hits a molecule, the molecule give some of its energy to photon. Then the energy molecule of decreases.

Let E_1 and E_2 be tne initial and final energies of molecule then

decrease in energy of molecule = $E_1 - E_2$

$\therefore$ energy of photon after hit a molecule = $h\upsilon_0 + (E_1 - E_2)$

Thus the frequency of scattered radiation is given by

$$v_{a.s} = \frac{h\upsilon_0 + (E_1 - E_2)}{h}$$

$$= \upsilon_0 + \frac{(E_1 - E_2)}{h} \qquad \text{----- (1)}$$

This shows that the frequency of scattered radiation is increased.

The frequency $\upsilon_{a.s}$ corresponds to frequency of anti-stokes line in Raman spectrum of the molecule.

3. The molecule may absorb some energy from photon.

Let the energy of molecule increases from E_2 to E_1 then,

Photon energy on absorption = $h\upsilon_0 - (E_1 - E_2)$

Thus the frequency of scattered radiation is given by

$$\upsilon_s = \frac{h\upsilon_0 - (E_1 - E_2)}{h}$$

$$= \upsilon_0 - \frac{(E_1 - E_2)}{h} \qquad \text{----- (2)}$$

This shows that the frequency of scattered radiation is decreased. The frequency υ_s corresponds frequency of stokes line in Raman spectrum of the molecule.

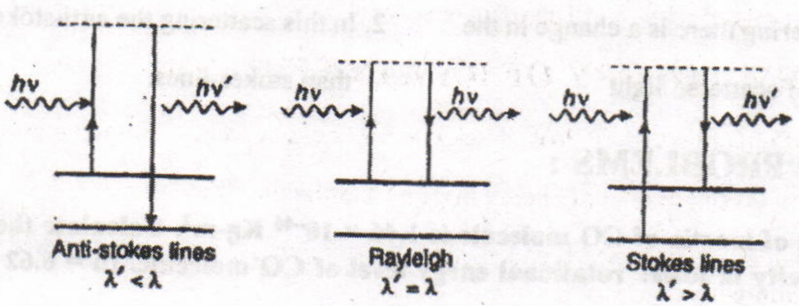


FIG 3.12.1

Figures (3.12.1) shows the three different situations.

Symmetry of Raman Lines :

Raman lines are symmetrically situated on either side of the parent line at intervals corresponding to the characteristic frequency of the molecule.

If E_1 and E_2 be the intrinsic energies of molecule before and after the photon hit it, then

$$E_1 - E_2 = nh\upsilon_m$$

where n = 1, 2, 3, ...etc.

υ_m = characteristic frequency of molecules

From equations (1) and (2) we get at n = 1

$$\upsilon_{a.s} = \upsilon_0 + \upsilon_m$$

and $\upsilon_s = \upsilon_0 - \upsilon_m$ ------ (3)

∴ Charactristic frequency of molecule $\upsilon_m = \upsilon_{a.s} - \upsilon_0$ or $\upsilon_m = \upsilon_0 - \upsilon_s$

Hence the Raman lines are symmetrically situated on either side of the parent line.

Rotational Raman lines are obtained with gases.

Vibrational Raman lines are obtained with liquids and solids.

.13 DIFFERENCE BETWEEN RAYLEIGH SCATTERING AND RAMAN SCATTERING :

Rayleigh Scattering	Raman Scattering
1. In this scattering the frequency of scattered light is always equal in incident rays	1. In this scattering the frequencies greater and smaller than of the incident beam frequency
2. In this scattering there is a change in the intensity of scattered light	2. In this scattering the anti-stokes lines are weaker than stokes lines.

14 SOLVED PROBLEMS :

1. The moment of inertia of CO molecule is 1.46×10^{-46} Kg-m^2. Calculate the enrgy in eV and angular velocity in lower rotational enrgy level of CO molecule. [$h = 6.62 \times 10^{-34}$ J-S]

(Ans : 2.37×10^{-4} eV, 7.21×10^{11} rad/sec)

Sol: Given that

Moment of inertia $I = 1.46 \times 10^{-46}$ kg-m^2

Planck's constant $h = 6.62 \times 10^{-34}$ J-s

In the lowest rotational energy level $J = 1$

Rotational energy $E_r = ?$

Angular velocity $\omega = ?$

Formula :

$$\text{Rotation energy } E_r = \frac{h^2}{8\pi^2 I}[J(J+1)]$$

$$= \frac{[6.62 \times 10^{-34}]^2[1(1+1)]}{8 \times (3.14)^2 \times (1.46 \times 10^{-46})}$$

$$= 2.37 \times 10^{-4} \text{ eV.}$$

$$\text{But } E_r = \frac{1}{2} I\omega^2 \quad \text{or } \omega = \sqrt{\frac{2E_r}{I}}$$

$$\therefore \text{Angular velocity } \omega = \left[\frac{2 \times 2.37 \times 10^{-4} \times 1.6 \times 10^{-19}}{1.46 \times 10^{-46}} \right] = 7.21 \times 10^{11} \text{ rad/sec.}$$

2. Calculate the frequency of vibration of CO molecule and spacing between its vibrational energy levels. Given that force constant K of bond in CO is 187 N/m and reduced mass of CO molecule μ is 1.14×10^{-26} Kg, $h = 6.63 \times 10^{-34}$ J-S.

[Ans : 2.04×10^{13} Hertz, 8.44×10^{-2} eV]

Sol: Given that

Force constant $K = 187$ N/m

Reduced mass $\mu = 1.14 \times 10^{-26}$ Kg

Planck's constant $h = 6.63 \times 10^{-34}$ J-S

Frequency of vibration $\upsilon = ?$

Spacing between levels $\Delta E = ?$

Formula :

$$\text{Frequency of vibration } \upsilon_V = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}}$$

$$= \frac{1}{2\times 3.14}\sqrt{\frac{187}{1.14\times 10^{-26}}}$$

$$= 2.04\times 10^{13} \text{ hertz}$$

Spacing between vibrational energy levels is

$$\Delta E = E_{\upsilon+1} - E_{\upsilon} = h\upsilon_{\upsilon}$$

$$= 6.63\times 10^{-34}\times 2.04\times 10^{13} \text{ Joule}$$

$$= 8.44\times 10^{-2} \text{ eV.}$$

3. The exciting line in an experiment is 5460 Å and the stokes line is at 5520Å. Find the wavelength of antistoke line. **[Ans : 5401 Å]**

Sol: Given that

Wavelength of exciting line $\lambda_0 = 5460$Å

$= 5460\times 10^{-8}$ cm

Wavelength of stokes line $\lambda_S = 5220$Å

$= 5220\times 10^{-8}$ cm

Wavelength of antistokes line $\lambda_{a.s} = ?$

Formula :

Wave number of displacement in Raman effect is

$\Delta\upsilon = \upsilon_0 - \upsilon_s$ for stokes line

$= \upsilon_{a.s} - \upsilon_0$ for anti-stokes line

$$\text{then } \upsilon_0 = \frac{1}{\lambda_0} = \frac{1}{5460\times 10^{-8}} = 18315 \text{ cm}^{-1}$$

$$\upsilon_s = \frac{1}{\lambda_s} = \frac{1}{5220\times 10^{-8}} = 18116 \text{ cm}^{-1}$$

$$\therefore \Delta u = \upsilon_0 - \upsilon_s = 18315 - 18116 = 199 \text{ cm}^{-1}$$

For anti-stokes line, $\upsilon_{a.s} = \Delta\upsilon + \upsilon_0$

$$= 199 + 18315 = 18514\ \text{cm}^{-1}$$

$\therefore$ Wavelength of antistokes line $\lambda_{a.s} = \dfrac{1}{\upsilon_{a.s}}$

$$= \frac{1}{18514} = 5.401\times10^{-5}\text{cm} = 5401\,\text{Å}$$

15 SUMMARY :

1. The spectra emitted by a element in its molecular state is called as molecular spectrum.
2. The total energy of a molecule $E = E_e + E_R + E_V$
3. Energy emitted in a transition $\Delta E = E - E^1 = h\upsilon$.
4. Frequency emitted radiation $\upsilon = \dfrac{\Delta E}{h} = \dfrac{E - E^1}{h}$.
5. Angular momentum of a rotating molecule quantized.

   $L_r = \hbar\sqrt{J(J+1)}$
6. Energy levels of rotating molecule $E_r = \dfrac{1}{2}Iw^2 = \dfrac{J(J+1)\hbar^2}{2I} = \dfrac{h^2}{8\pi^2 I}[J(J+1)]$
7. Frequency of vibration $\upsilon_0 = \dfrac{1}{2\pi}\sqrt{\dfrac{K}{\mu}}$
8. Transition rules for vibration $\Delta\upsilon = \pm1$
9. Total energy due to vibration and rotation is

$$E_{total} = E_\upsilon + E_r = \left[\upsilon + \frac{1}{2}\right]h\upsilon_\upsilon + \frac{J(J+1)h^2}{8\pi^2 I}$$

0. For stokes line $\upsilon_s = \upsilon_0 - \upsilon_m$

   For anti stokes line $\upsilon_{a.s} = \upsilon_0 + \upsilon_m$

3.16 KEY WORDS :

Molecular spectra, rotational spectra, selection rules, vibration spectra, inter nuclear distance, Raman effect, stokes line, anti-stokes line.

3.17 SELF-ASSESSMENT QUESTIONS :

1. **Give the elementary theory of rotational spectra of diatomic molecule.**
2. **Give the theory of origin of vibrational spectrum of a molecule.**
3. **Explain the vibration-rotation spectra.**
4. **Explain the transition rules for vibration and rotation spectra.**
5. **Explain how the inter-nuclear distance in a molecule can be estimates.**
6. **What is Raman effect and state its applications.**
7. **Give an elementary theory of Raman effect and experimental study of Raman effect.**

EXCERCISES:

1. **An experimental sample was exicted by 4358Å line of moving. A Raman line was observed at 4447Å. Calculate the Raman shift in cm^{-1}.** **(Ans : 460 cm^{-1})**

[Hint :

$$\text{Raman shift} = \upsilon - \upsilon_{stokes}$$

$$= \frac{1}{\lambda} - \frac{1}{\lambda_s}$$

$$= \frac{1}{4358\times10^{-8}} - \frac{1}{4447\times10^{-8}}]$$

At what wavelength would the antistoke line appears in the Raman spectrum of the sample when it was excited by 4358Å and a Raman line was observed at 4447Å. **(Ans : 4272 Å)**

[Hint :Raman shift $\Delta u = \upsilon - \upsilon_{stokes} = \frac{1}{\lambda} - \frac{1}{\lambda_s}$ $\frac{1}{4358\times10^{-8}} - \frac{1}{4447\times10^{-8}} = 460\text{cm}^{-1}$

$\upsilon_{a.s} = \Delta\upsilon + \upsilon = 460 + 2.295 \times 10^4$ $\lambda = \frac{1}{\upsilon_{a.s}}$Å]

3.18 REFERENCE BOOKS :

1. Physics of atom	Wher and Richards
2. Spectroscopy	Straughen and Walker
3. Introduction of Atomic Physics	H.F. White
4. Elements of Modern Physics	Patil

/*/*/*/

UNIT - I

LESSON- 4

SPECTROSCOPIC TECHNIQUES

OBJECTIVES :

After completing the study of this lesson the student will be able to

1. Know about the different spectrophotometers.
2. Understand the sources of excitation of ultraviolet, visible and IR radiation.
3. Know about filters and monochromators.
4. Understand the differnet recording systems or detectors.

STRUCTURE :

4.1 Introduction

4.2 Spectrophotometer

4.3 Sources of excitation of ultraviolet radiation

4.4 Sources of excitation of visible radiation

4.5 Sources of excitation for infrared radiation

4.6 Prism and grating spectrographs for visible, ultra violet and infrared regions.

4.7 Single beam and double beam instruments for absorption spectra.

4.8 Recording systems or detectors.

4.9 Ultraviolet and visible radiation detectors.

4.10 Infrared detectors

4.11 Summary

4.12 Key words

4.13 Self-Assessment Questions

4.14 Reference Books

4.1 INTRODUCTION :

A spectrophotograph is an instrument used to study the wavelength with distribution of radiation.

The instruments which are used to study the absorption or emission of electromagnetic radiation intensity as a function of wavelength are called spectrometer or spectrophotometers.

Sources of excitation are necessary to emit the radiations for ultraviolet radiation are hydrogen discharge tube, Deuterium lamps, mercury arc lamp, xenon discharge lamps and tungstn lamps. Incandescent tungsten filament lamp is a source for visible radiation. Sources of excitation for IR radiation are incandescent lamp, Nernst Glower, Globar source and Mercury arc.

An instrument which records the variation of intensity of electromagnetic radiation as a function of wavelength is known as detector. A detector absorb the energy of the photons that strike it and then convert this energy into measurable quantity. In general the detectors generate electrical signal which activates the recorders.

Photosensitive devices to detect the radiation are (i) photo tubes (ii) photovoltaic cell.

Infrared detectors suitable for absorption spectroscopy can be classified into two broad groups, namely, (i) thermal detector, (ii) photon detectors.

4.2 SPECTROPHOTOMETER :

The instrument used to study the absorption or emission of electromagnetic radiation intensity as a function of wavelength are called spectrophotometer.

The essential components of a spectrophotometer are

1. **Source of excitation**
2. **Collimating and Focusing system**
3. **Wavelength selection**
4. **Transparent container to hold the sample**
5. **Radiation detector**
6. **Recorder**

4.3 SOURCES OF EXCITATION FOR ULTRA VIOLET RADIATION

a) Hydrogen discharge lamps : It covers the wavelength range 3500 Å to 1200 Å.

This is a good source of UV-radiation. When electric discharge is passed through hydrogen gas in the lamp, the hydrogen molecules are excited to higher energy state and return to their original state by emitting UV radiation.

These lamps give two types of spectrum, namely, (i) Line spectrum, (ii) Continuous or broad band spectrum.

b) Deuterium Lamps :

In these lamps deuterium is enclosed in a discharge tube. Its intensity is 3 to 5 times than that of hydrogen lamp.

It is used to produce high intensity.

c) Mercury arc lamp :

They are two types.

i) **Low pressure mercury arc :** It contain mercury droplets and a mixture of inert gases (helium, neon, argon).

It cover the wavelength range 1800Å to 10,000 Å.

They are useful for calibration and in liquid chromatography.

ii) **High pressure mercury arc :** It consists mercury vapour at a pressure of 80 atmosphere. Electric discharge excite the mercury atoms in the lamp.

They produce sharp lines or bands.

d) Xenon discharge lamps : It consists of of xenon gas filled tube at a pressure of 10-30 atmosphere with two tungsten electrodes separated by 8 mm.

These lamps produce ultraviolet light with more intensity than hydrogen lamp.

e) Tungsten / Halogen lamps : These lamps are called as quartz / halogen lamps. It consists of Iodine with quartz envelope.

The life time of quartz / halogen lamp is double that of ordinary tungsten lamp.

These lamps are used in modern spectroscopic instruments due to extended wavelength range, greater intensity and longer life.

4.4 SOURCES OF EXCITATION FOR VISIBLE RADIATONS

Its wavelength range lies in between 4000Å to 8000 Å.

Incandescent tungsten filament lamp is a common source of visible radiations.

It consists of tungsten wire sealed in a bulb.

Carbon arc is another source of visible radiation and it is used as more intense source for visible region.

4.5 SOURCE OF EXCITATION FOR INFRARED RADIATION :

a) Incandescent lamp : A tungsten lamp with silica envelope is used for near IR.

A coil of nichrome wire is another soruce for IR radiation. This coil is raised to incandescent by heating upto 1100^{0}C. It provide long service and more reliability.

b) Nernst Glower : It consists of fused mixture of oxide of zirconium, yittrium and Thorium in the form of hollow rods of 1-3 mm diameter, 2-5cm in length. The rods has a negative temperature coefficients of resistance.

The glower is electrically heated to a range of temperature 1000^0 to 1800^{0}C to provide IR radiation of 7100 cm^{-1}.

c) Globar source : It is a rod of sintered silicon carbide of 50 mm in length and 4mm in diameter.

It emit the radiations in IR region, when the rod is heated between 1300^{0}C to 1700^{0}C. It emit maximum raidation of 5200 cm^{-1}.

d) Mercury arc : It is a high pressure mercury arc with an extra quartz jocket ot reduce thermal loss.

It gives intense radiation for IR region.

At shorter wavelengths, the heated quartz envelope emits the radiation.

At longer wavelengths, the mercury plasma provides radiation through quartz.

4.6 PRISM AND GRATING SPECTROGRAPH FOR VISIBLE ULTRAVIOLET AND INFRARED REGIONS :

Prism and Gratings are devices for wavelength electron. The selection of wavelength can be done by two resolving devices. namely,

i) Filters ii) Monochromator

Filters : Filters are of two types

a) Absorption Filter : It works on the principle of absorption. They transmit a limited wavelength region and absorb the other wavelengths.

It transmit a bandwidth of wavelengths from 20nm to 50 nm.

b) Interference Filter : It works on the principle of interference. They are used for absorption measurments.

Figure (4.6.1) shows the interference filter

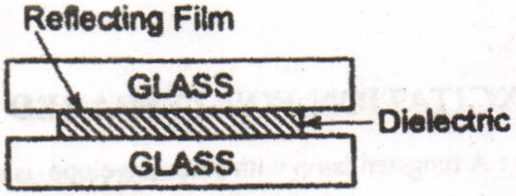


FIG 4.6.1

A glass plate is coated with reflecting metal film. A thin film of dielectric metal like quartz or MgF_2 coated on top of reflecting metal film. The dielectric layer is coated with film of reflecting metal and placed a glass plate on layer for protection.

When a beam of light is incident normally on this filter, transmits a band of order n at wavelength λ.

These are used in UV, visible regions and upto 14 μm wavelength in IR region.

They doesnot absorb energy and hence they are free from over heating.

c) Monochromator : Prism and grating form the components of monochromator. It separate out a narrow range of spectrum for intensity measurements in spectra.

Figure (4.6.2) shows the different parts of monochromator.

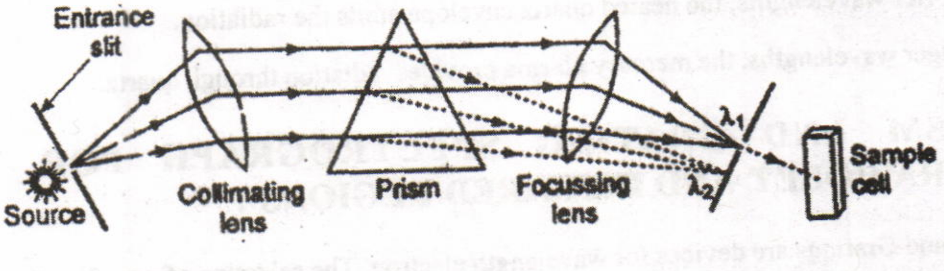


FIG. 4.6.2

Monochromator conists of following parts :

i) **Entrance slit :** It admits a narrow part of Polychromatic radiation from the source.

ii) **Collimating device :** It tenders the beam parallel by using a lens or mirror.

iii) **Dispersing device :** It resolves the radiation into component wavelengths by using a prism or grating.

iv) **Focusing lens or mirror :** It focusses the different wavelengths at different places.

v) **Exit slit :** It allows a narrow band of wavelength.

Figure (4.6.3) shows two monochromator using Littrow arrangement.

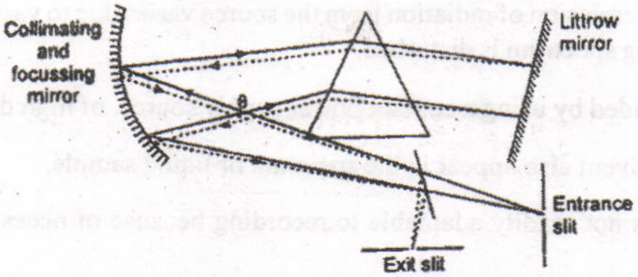


FIG. 4.6.3

In this monochromator, the collination and focussing are done by a front-silvered concave mirror. This can be used for visible with glass prism, for ultraviolet with quartz prism and for far IR with prism of NaC*l* or KC*l* or KBr etc.

It increases the dispersion of radiation to double. In this monochromator, the prism and mirror is on a single platform which may be turn by a drum and screw to change the mean λ of exit beam.

4.7 SINGLE BEAM AND DOUBLE BEAM INSTRUMENTS FOR ABSORPTION SPECTRA:

1. **Single beam spectrophotometer :** The block diagram of arrnagement used to observe absorption spectra is shown in figure 4.7.1.

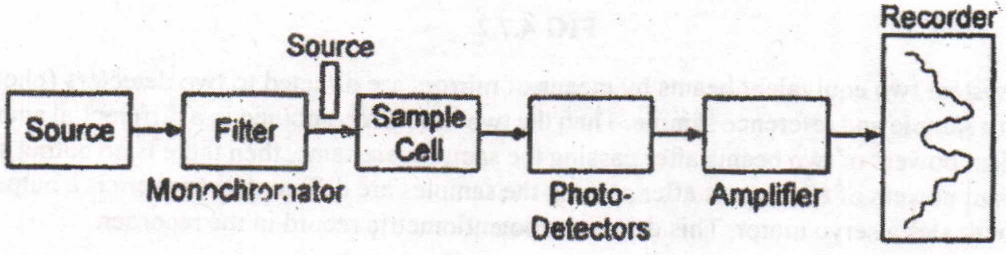


FIG. 4.7.1

In this system the radiation emitted by source enters the filter or monochromator to isolate a paritcular narrow band of wavelength. In monochromator, the radiation is dispersed by prism or grating. When prism or grating is rotated, various resolved bands of radiations are focussed at the exist slit. Then the radiation passes through the sample cell and enter the detector. The detector maybe thermopiles, voltmeters. The detector measures the intensity of radiation. By measuring the degree of absorption at a given wavelength, the absorption spectrum of sample can be recorded with a recorder.

Disadvantages of single beam spectrometer :

1. The intensity of emission of radiation from the source varies due to variation in power supply and then the resulting spectrum is disturbed.

   This can be avoided by using a contant power supply source. of high degree stabilization.

2. The bands of solvent also appear in the spectrum of liquid sample.
3. The spectrum is not readily adaptable to recording because of necessity of calibration at each wavelength.

2. Double beam spectrophotometer :

The block diagram of arrangements used to observe absorption spectra is shown in figure.

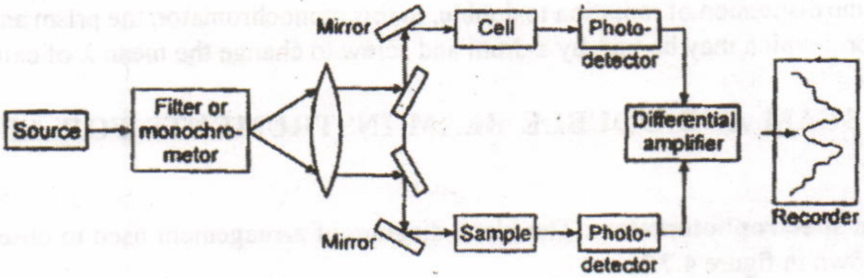


FIG 4.7.2

In this system two equivalent beams by means of mirrors are directed to two detectors (photo cells) through a sample and reference sample. Then the two beams recombined in a differential amplifier. If the radiant powers of two beams after passing the samples are same, then there is no output signal. If the radiant powers of two beams after passing the samples are different, then there is a output signal which activates a servo motor. This drives the potentiometric record in the recorder.

Advantages of Double beam Spectrometer :

1. Any error due to variation in the intensity of source and fluctuations in the detector is minimized.

2. The calibration at each wavelength is not necessary as in case of single beam spectrophotometer.
3. This system lends itself to rapid scanning over a wide wavelength region.

4.8 RECORDING SYSTEMS OR DETECTORS :

Detector : An instrument which record or measure the variation of intensity of electromagnetic radiation of intensity of electromagnetic radiation as function of wavelength is known as detector.

A detector absorbs the energy photons that strike it. The detectors generate an electrical signal to activate recorder.

Important requirements for detectors :

i) high sensitivity with low noise level.

ii) generated electrical signal canbe easily amplified for recorder.

iii) long term stability to ensure qualitative response.

4.9 ULTRAVIOLET AND VISIBLE RADIATION DETECTORS :

The electric current generated in case of photoelectric effect or absorption of photon by semiconductor is directly proportional to the radiant power of absorbed photons. The device used for this purpose are called photoelectric detectors.

The photoelectric detectors are two types, namely (i) photo tubes, (ii) semiconductor photodetector (photo voltaic cell).

a) Photo Tubes : It consists of three parts.

i) An evacuated glass envelope haing a quartz window to allow the ultraviolet radiation.

ii) A semi-cylindrical cathode whose inner surface is coated with alkali and alkaline earth oxide.

iii) A central wire serves as anode.

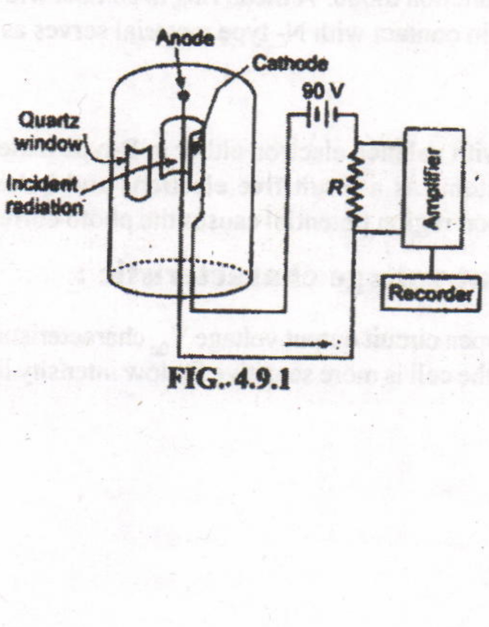


FIG..4.9.1

Figure (4.9.1) shows the photo tube circuit. The radiation enters through quartz and strike the photoemissive surface. The electrons escaped from the surface are collected by anode then a current (i) flows in the circuit.

At a given radiant power, photo current increases with applied voltage. At a particular voltage, the current is maximum. The maximum voltage is called as saturation voltage.

Photo tube currents are small and require amplification. A high resistance connected in circuit and P.D developed across R is connected to amplifier circuit and then to a recorder.

2. Semicondcutor photodetector (Photovoltaic cell) :

It is used for detection and measurement of radiation in visible region.

In solar cells the generated electrical voltage is proportional to the intensity of incident light. Hence they are called photovoltaic cells.

Construction : Fig. 4.9.2 shows the construction of Photo voltaic cell.

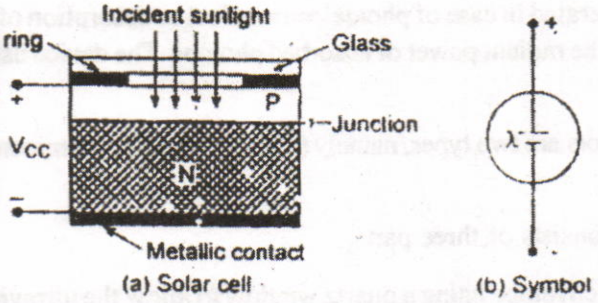


FIG 4.9.2

The cells consists of P-N junction diode. A metal ring in contact with P type material serves as positive terminal and a metal ring in contact with N- type material serves as negative terminal of cell.

Working :

When a photon collides with valence electron either in P-type material or N-type material, electrons are ejected from purest atoms as a result free electrons and holes are generated on either side of junction. Then the depletion region potential causes the photo current across the external load.

Open-Circuit output voltage characteristic :

Figure(4.9.3a) shows the open circuit output voltage V_{0c} characteristic of a typical photovoltaic cell.The graph (4.9.3b) shows that the cell is more sensitive for low intensity light levels than high intensity light levels.

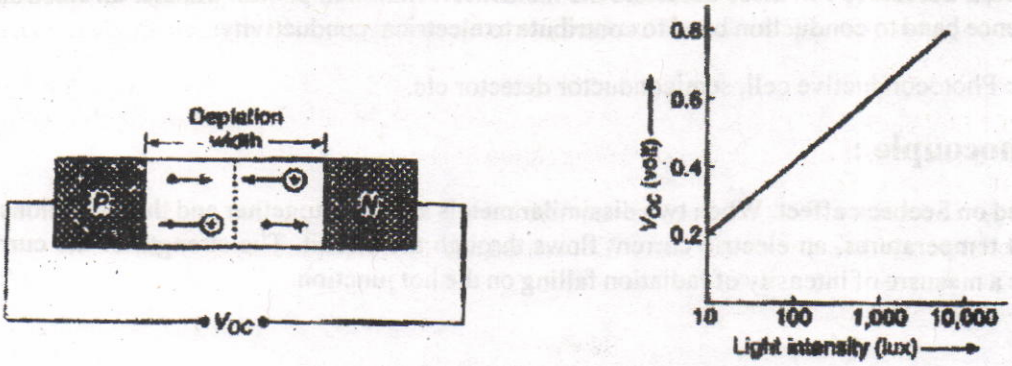


FIG 4.9.3(a),(b)

Output current - characteristics ;

Figure(4.9.4) shows the output characteristics of a typical photovoltaic cell for various load resistances.

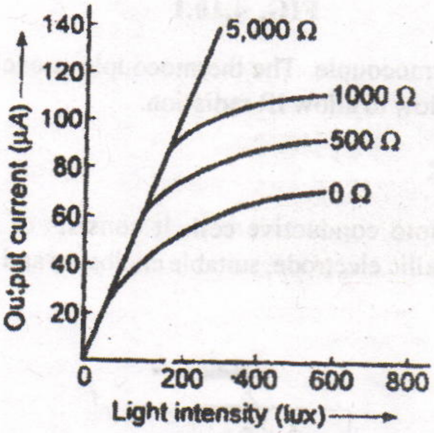


FIG 4.9.4

The graph shows that the output current of cell increases with increase in light intensity.

4.10 INFRARED DETECTOR :

IR detectors are suitable for absorption spectroscopy.

They are classified into two broad groups.

i) **Thermal detectors :** They depend on integrated energy of number of photons to produce measurable heating effects. These are used in middle and far infrared region.

Ex : Bolometer, thermocouple etc.

ii) Photon detectors : In these detectors the incident IR radiation photon transfer an electron from valence band to conduction band to contribute to electrical conductivity.

Ex : Photoconductive cell, semiconductor detector etc.

Thermocouple :

It is based on Seebeck effect. When two dissimilar metals are fixed together and their junctions are at different temperatures, an electric current flows through the circuit. The strength of the current in circuit is a meausre of intensity of radiation falling on the hot junction.

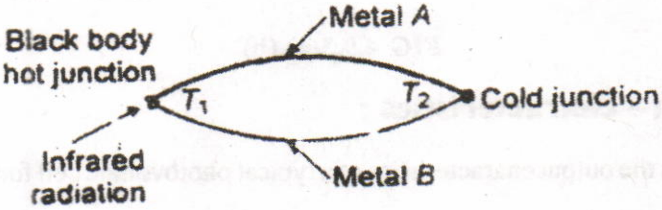


FIG. 4.10.1

Figure (4.10.1) shows the thermocouple. The thermocouple is enclosed in an evacuated steel case provided with KBr to CSi window to allow IR radiation.

Photoconductive Cell :

Figure(4.10.2) shows the photo conductive cell. It consists of ceramic substance coated with photoconductive material, metallic electrode, suitable enclosure and window.

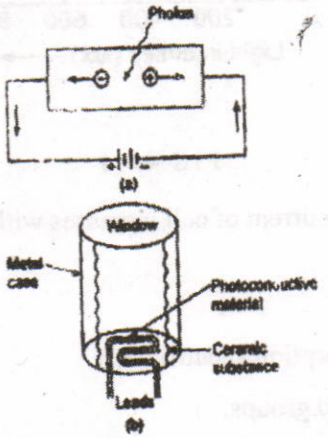


FIG.4.10.2

The necessary energy for valence electrons to become free current carriers is varies from 0.2 to 3 eV. This is basis for the operation of photo conductive cell. The decrease in the resistance of layer of photoconductive material is proportional to the intensity of light required. External field is necessary for electrons flow through the detector and external circuit.

4.11 SUMMARY :

1. Spectrophotometer is used to study the absorption or emission of electromagnetic radiation intensity as a function of wavelength.
2. Hydrogen discharge lamps, deuterium lams, mercury arc lamps, xenon discharge lamps, tungsten lamps are sources of excitation for ultra violet radiation.
3. Incandescent tungsten filament lamp is a common source of excitation for visible radiation.
4. Incandescent lamp, Nernst Glower, Globar source and Mercury arc are sources of excitation for infrared radiation.
5. Single beam and double beam instruments.
6. Ultraviolet and visible radiation detectors : 1) Photo tubes, 2) Photovoltaic cell
7. Infrared detectors : 1) Thermocouple, 2) Photoconductive cell.

4.12 KEY WORDS :

Spectrometers, Spectrophotometer, excitation sources, prism and grating spectrographs, single and double beam instruments, detectors.

4.13 SELF-ASSESSMENT QUESTIONS :

1. Describe in detail the different sources of excitation in ultraviolet, visible and infrared regions.
2. What is monochromator ? Explain the working of prism monochromator.
3. Describe single beam spectrophotometer and give its disadvantages.
4. Describe double beam spectrophotometer and gives it advantages.
5. Describe and explain the ultraviolet and visible radiation detectors.
6. Describe and explain two infrared detectors.

4.14 REFERENCE BOOKS :

1. Spectroscopy	Straughen and Walker
2. Physics of Atom	Wher and Richards
3. Modern Physics	S.L. Gupta, Sanjeev Gupta
4. Introduction to Atomic Spectra	H.F White

UNIT-2

LESSON-5

ORIGIN OF QUANTUM MECHANICS AND PHOTOELECTRIC EFFECT

OBJECTIVES:

After the completion of this lesson the student will be able to

1) Understand the Bohr's Atom Model.
2) **Understand the Bohr's theory of hydrogen atom and energy levels.**
3) **Understand the limitationsof Bohr's theory.**
4) **Understand the photo-electric effect and laws of photoelectric emission.**
5) **Understand the Einsteins's photoelectric equation and Millikan's experimental verification.**

STRUCTURE:

5.1 INTRODUCTION:

To overcome the instability of Rutherford's model of an atom, Bohr proposed the new revolutionary idea that an electron revolving in an orbit does not radiate energy and its angular momentum is quantized. So its orbit will be stationary and stable. Further, to explain the line spectrum of hydrogen atom, he postulated that an electron absorbs or emits radiation only when it moves from one stationary orbit to another stationary orbit. Using these quantum concepts, Bohr successfully explained the stability of hydrogen atom and its line spectrum.

The classical concepts cannot be applied to atomic phenomenon and it is failed to explain the stability of the atom. The classical theory failed to explain the spectrum of hydrogen atom. Thus the classical mechanics does not hold in the region of atomic dimensions.

In order to explain the shape of black body radiation curves, Max Plank in 1900 proposed quantum theory. According to this theory, matter is composed of a large number of oscillating particles which vibrate with different frequecies. Planck concluded that the emission absorption of thermal energy is not a continuous process but it takes place in dicrete amounts. The phenomenon of photoelectric effect was discovered by Hertz. Millikan investigated this effect with a number of alkali metals over a wide range of light frequencies.

5.2 BOHR'S THEORY OF HYDROGEN ATOM:

Bohr explained the atomic structure of atom on the basis of quantum theory.

1. Electron revolves round the nucleus in a circular orbit the electrostatic force of attraction between the nucleus and $\bar{e}$ gives necessary centripetal force i.e.,

$$\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0} \cdot \frac{ze.e}{r^2} \text{ (neglecting - ve sign)}$$

$$mv^2 = \frac{1}{4\pi\varepsilon_0} \cdot \frac{ze^2}{r} \longrightarrow ①$$

2. The angular momentum of $\bar{e}$ in a stationary orbit is quantised and is equal to integral multipe of $\frac{h}{2\pi}$

$$L = mvr = \frac{nh}{2\pi}$$

$$r = \frac{nh}{2\pi mv} \longrightarrow ②$$

Similary, $$v = \frac{nh}{2\pi mr} \longrightarrow ③$$

3. When $\bar{e}$ jumps from one orbit to another orbit the energy is released or absorbed and is equal to difference between the energies of the two orbits i.e.,

$$E_2 - E_1 = h\nu \xrightarrow{\qquad} ④$$

Bohr applied these postulates to the hydrogen atom in which z = 1.

a) Radius of the Bohr orbit (or) First orbit :

Substituting the eq (3) in eq (1) we get,

$$m\left(\frac{nh}{2\pi mr}\right)^2 = \frac{1}{4\pi\epsilon_0}\cdot\frac{e^2}{r}$$

$$m\left(\frac{n^2h^2}{2\pi^2 m^2 r^2}\right) = \frac{1}{4\pi\epsilon_0}\cdot\frac{e^2}{r}$$

For n^{th} orbit, $r = r_n$.

$$r_n = \frac{\epsilon_0 n^2 h^2}{\pi m e^2} \xrightarrow{\qquad} ⑤$$

or $$r_n = \left(\frac{\epsilon_0 h^2}{\pi m e^2}\right) n^2$$

$$r_n = \frac{8.85\times10^{-12}\times\left(6.62\times10^{-34}\right)^2}{3.14\times9.1\times10^{-31}\times\left(1.6\times10^{-19}\right)^2} n^2 = 0.53\times10^{-10} n^2 \text{ meter}$$

$$= 0.53 n^2 \overset{0}{A}$$

If n = 1, radius of Bohr orbit, $r_1 = 0.53\times1^2\,A^0 \Rightarrow r_1 = 0.53A^0$

$n = 2, \quad r_2 = 0.53\times2^2A^0$

$n = 3, \quad r_3 = 0.53\times3^2A^0$

$r_1 : r_2 : r_3$ -------------- $= 1 : 2^2 3^2 :$ --------------

= 1 : 4 : 9 ---------------

b) Velocity of the electron :

Substituting eq ②in ①we get,

$$mv^2 = \frac{1}{4\pi\epsilon_0}.\frac{1.e^2}{n.\dfrac{h}{2\pi mv}}$$

$$mv^2 = \frac{1}{2\epsilon_0}.\frac{mve^2}{nh}$$

$$v = \left(\frac{e^2}{2\epsilon_0 h}\right).\frac{1}{n}$$

By substituting all the values.

$$v = \frac{2.175\times10^6}{n} ms^{-1} \longrightarrow \text{⑥}$$

c) Energy of the electron :

$$\text{The K.E of the } \overset{-}{e}\text{ , K.E} = \frac{1}{2}mv^2 = \frac{1}{2}.\frac{1}{4\pi\varepsilon_0}.\frac{e^2}{r}$$

$$\therefore \text{K. E} = \frac{1}{8\pi\varepsilon_0}.\frac{e^2}{r} \longrightarrow \text{⑦}$$

We know that potential energy P.E = work done in bringing the $\overset{-}{e}$ from ∞ to the orbit of radius r.

$$\text{P.E.} = \int_\infty^r F dr = \int_\infty^r \frac{1}{4\pi\epsilon_0}.\frac{e^2}{r^2}dr = \frac{e^2}{4\pi\epsilon_0}\int_\infty^r \frac{1}{r^2}dr = \frac{e_2}{4\pi\varepsilon_0}\left[\frac{-1}{r}\right]_\infty^r$$

$$= \frac{e^2}{4\pi\epsilon_0}\left[\frac{-1}{r}+\frac{1}{\infty}\right]$$

$$\therefore \text{PE} = \frac{1}{4\pi\epsilon_0}.\frac{-e^2}{r} \longrightarrow \text{⑧}$$

∴ Total energy of the $\overset{-}{e}$, E = P.E + K.E

$$E = -\frac{1}{4\pi\epsilon_0}.\frac{e^2}{r} + \frac{1}{8\pi\epsilon_0}.\frac{e^2}{r}$$

$$E = -\frac{1}{8\pi\epsilon_0}.\frac{e^2}{r}$$

For nth orbit, $E_n = -\frac{1}{8\pi\epsilon_0}.\frac{e^2}{r_n}$

Using the equation (5)

$$E_n = -\frac{1}{8\pi\epsilon_0}.\frac{e^2}{\left(\frac{n^2\epsilon_0 h^2}{\pi m e^2}\right)}$$

$$E_n = \frac{-me^4}{8\epsilon_0^2 h^2}.\frac{1}{n^2} \longrightarrow ⑨$$

By substituting all there values

$$E_n = \frac{-13.6}{n^2} ev \longrightarrow ⑩$$

For the first orbit, $n = 1$, $E_1 = -13.6ev$

2nd orbit, $n = 2$, $E_2 = \frac{-13.6}{4} = -3.4ev$

3rd orbit $n = 3$, $E_3 = \frac{-13.6}{9} = -1.51ev$

$n = \infty$, $E_\infty = \frac{-13.6}{\infty^2} = 0$

Ionisation Energy :

It is the amount of energy supplied to send an $\bar{e}$ from first orbit to infinity is called ionisation energy. For the hydrogen atom, ionisation energy $E = E_\infty - E_1$

$$\therefore E = 0 - (-13.6) = 13.6 \text{ ev}$$

According to Bohr's 3rd postulate, e jumps from n_2 to n_1 orbit, the difference of energy levels radiated in the form of light of frequency ν

i.e., $En_2 - En_1 = h\nu$

$$h\nu = \frac{-me^4}{8\in_0^2 h^2}\cdot\frac{1}{n_2^2} - \left(\frac{-me^4}{8\in_0^2 h^2}\cdot\frac{1}{n_1^2}\right)$$

$$h\nu = \frac{me^4}{8\in_2^0 h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_1^2}\right]$$

$$\frac{hc}{\lambda} = \frac{me^4}{8\in_0^2 h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_1^2}\right]\left[\therefore \nu = \frac{c}{\lambda}\right]$$

$$\frac{1}{\lambda} = \frac{me^4}{8\in_o^2 h^3 c}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\because \frac{1}{\lambda} = \bar{\nu}$$, **wave number and**

$$\frac{me^4}{8\in_0^2 ch^3} = R$$, **Rydberg constant. Its value is $1.09677 \times 10^7 m^{-1}$**

$$\nu = R\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

R is the Rydberg constant for hydrogen when nucleus mass is not considered

5.3 SPECTRAL SERIES OF HYDROGEN ATOM:

S.No	Series	n_1	n_2	Position in spectrum	Wave length
1	Lyman	1	2, 3, 4 ...... ∝	Ultraviolet	
2	Balmer	2	3, 4, 5 ...... ∝	Visible region	6, 564 Å-3,647 Å 3 →2 ∝ →2
3	Paschen	3	4, 5, 6 ..... ∝	Infra red	
4	Bracket	4	5, 6, 7 ...... ∝	Infra red	
5	P fund	5	6, 7, 8 ...... ∝	Infra red	

5.4 LIMITATIONS OF BOHR'S THEORY:

1. It could not explain the complicated spectra of atoms except hydrogen.
2. It could not explain the relative intensities of spectral lines.
3. This theory could not explain the zeeman & start effect.
4. If could not explain the chemical bonding
5. If could not explain the distribution of e in the atom

5.5 EFFECT OF NUCLEAR MOTION ON ATOMIC SPECTRA:

By taking the mass of the nucleus into account the wave number $\vec{\nu}_H = \frac{1}{\lambda_H} = \frac{\mu e^4}{8 \epsilon_0^2 ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$.

μ is called reduced mass

$$\text{i.e., } \mu = \frac{Mm}{M+m}$$

M= mass of the Nucleous

m= mass of the electron

$$\therefore \vec{\nu}_H = \frac{1}{\lambda_H} = \frac{\frac{Mm}{M+m}.e^4}{8 \epsilon_0^2 ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\vec{\nu}_H = \frac{1}{\lambda_H} = \frac{M}{M+m}.\frac{me^4}{8 \epsilon_0^2 ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\frac{1}{\lambda_H} = \frac{M}{M+m}.\frac{1}{\lambda\infty}$$

$$\lambda_H = \frac{M+m}{M}.\lambda\infty$$

$$\frac{\lambda_H}{\lambda_\infty} = \frac{M+m}{M} > 1$$

$\lambda_H > \lambda_\infty$

The wavelength slighthy greater than the wavelength corresponding to infinitely heavy nucleus i.e., the spectral lines shifts towards the highr wavelength side.

5.6 RITZ- COMBINATION PRINCIPLE:

By combination of terms that occur in Balmer formula, other relations can be obtained which shows new lines and new series. From the Balmer series for H_α line $n_1 = 2, n_2 = 3$

$$\vec{\nu}_\alpha = R\left[\frac{1}{2^2} - \frac{1}{3^2}\right] \longrightarrow ①$$

For the second member i.e., for H_β line $n_1 = 2, n_2 = 4$

$$\vec{\nu}_\beta = R\left[\frac{1}{2^2} - \frac{1}{4^2}\right] \longrightarrow ②$$

subtract eq ① from eq ② $\vec{\nu}_\beta - \vec{\nu}_\alpha = R\left[\frac{1}{3^2} - \frac{1}{4^2}\right] \longrightarrow ③$

Similarly H_γ line, $n_1 = 2, n_2 = 5$

$$\vec{\nu}_\gamma = R\left[\frac{1}{2^2} - \frac{1}{5^2}\right] \longrightarrow ④$$

subtract eq ① from eq④ $\Rightarrow \vec{\nu}_\gamma - \vec{\nu}_\alpha = R\left[\frac{1}{3^2} - \frac{1}{5^2}\right] \longrightarrow ⑤$

This series was later discovered by paschen and it is known as paschen series

For H_δ line, $n_1 = 2, n_2 = 6$

$$\vec{\nu}_\delta = R\left[\frac{1}{2^2} - \frac{1}{6^2}\right] \longrightarrow ⑥$$

subtract eq ② from eq ④ $\Rightarrow \vec{\nu}_\gamma - \vec{\nu}_\beta = R\left[\frac{1}{4^2} - \frac{1}{5^2}\right]$

subtract eq ② from eq ⑥ $\Rightarrow \vec{\nu}_\delta - \vec{\nu}_\gamma = R\left[\frac{1}{4^2} - \frac{1}{6^2}\right]$

Later this series was discovered by Brackett in IR region and named as Brackett series

subtract eq ⑤ from eq ⑥ $\Rightarrow \vec{\nu}_6 - \vec{\nu}_r = R\left[\frac{1}{5^2}-\frac{1}{6^2}\right]$ which is the first line of p-fund series

5.7 PHOTOELECTRIC EFFECT:

When light of sufficient energy incident on photosensitive metal (alkali metal) such as k, Zn, Li, Na, Mg, etc. $\bar{e}$ emitted from the metal surface .These $\bar{e}$ are called photo electrons and the phenomenon is called photo electric effect. The metal used is called photo metal

Hallawack first invented this effect and Hertz conducted number of experiments on this effect

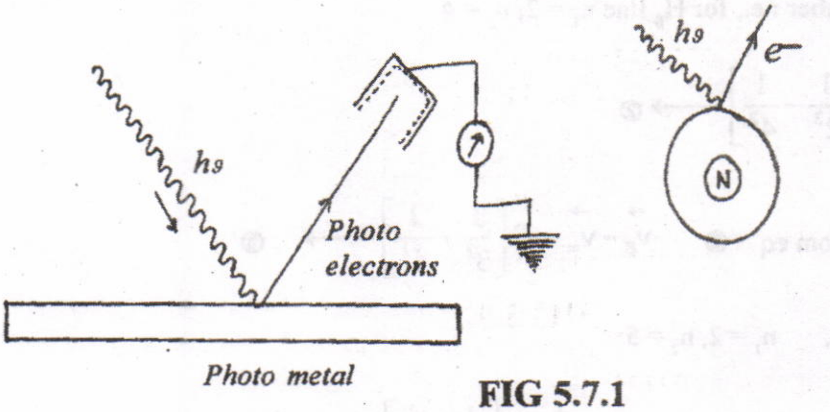


FIG 5.7.1

5.8 LAWS OF PHOTOELECTRIE EFFECT:

1. The strength of photo electric current is proportional to intensity of incident light
2. The K.E of emitted electrons is directly proportional to the frequency of incident radiation
3. The K.E. of emitted $\bar{e}$ is independent on intensity of incident light
4. There exists a critical frequency ν_0 called threshold frequency above which only $\bar{e}$ liberated from the metal surface. This frequency varies from metal to metal.
5. There is no time lag between the incident photon and emitted electron
6. The rate of emission of photo $\bar{e}$ is independent on raise of temperature

5.9 EXPERIMENTAL STUDY OF PHOTOELECTRIC EFFECT AND CHARACTERISTICS OF PHOTOELECTRONS:

It consists of an evacuated glass tube made of glass containing photo sensitive metal plate C(cathode and another metal plate A (Anode) as shown in figure(5.9.1). The window W allows the UV radiatior through it and then incident on the plate C.The photo $_e$ are emitted by cathode and collected by the plate A called collector. The P.D between A and C can be varied with the help of rheostat Rh and can be measured by voltmeter.The potential of C relative to A can be varied with commutator then micrometer measures the photo electric current.

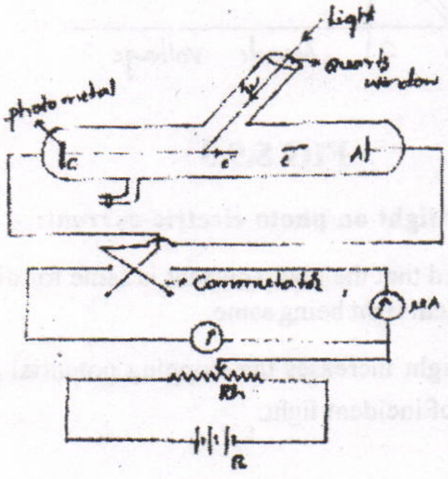


FIG 5.9.1

The experimental findings can be classified as follows.

1. Effect of intensity of incident light on photo electric current:

By adjusting the distance between the source and the emitter the intensity of incident light can be changed. Then the photo electric current changes linearly with intensity of light. The number of photo $\bar{e}$ (photo current) emitted per second depends on the intensity of incident light as shown in the figure(5.9.2).

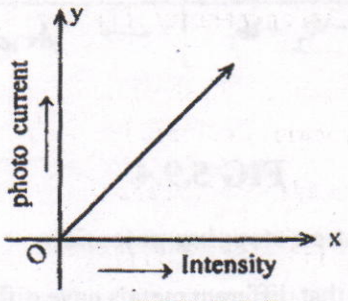


FIG 5.9.2

2.Effect of anode potential (voltage) for different intensities of incident light on photo current :

As the frequency of incident light remains same at different intensities across the different vol of emitter as shown in figure(5.9.3).It is found that the stopping potential V_0 remains same for dif

intensities i.e., the stopping potential does not depends on intensity of incident light.

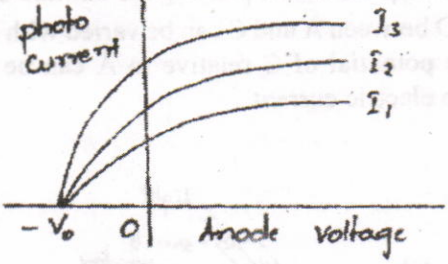


FIG 5.9.3

3.Effect of frequency of incident light on photo electric current:

1. **From the graph(5.9.4) it is noted that the photo current is same for different frequencies of incident light when the intensity of incident light being same.**

. **As the frequency of incident light increases the stopping potential also increases i.e., the K.E. of photo $\bar{e}$ depends in frequency of incident light.**

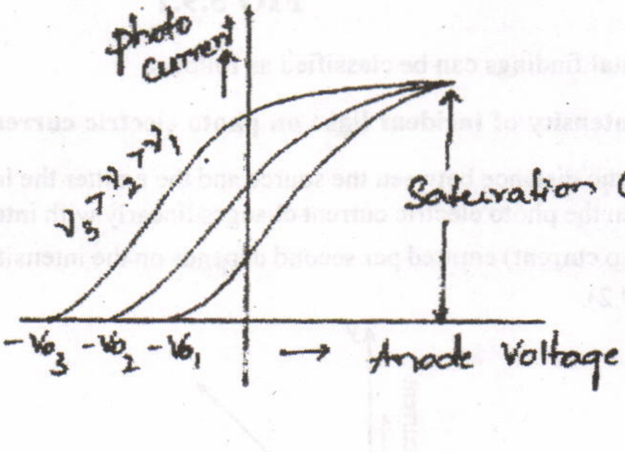


FIG 5.9.4

4.Effect of frequency of incident light on stopping potential:

From the graph(5.9.5) it is observed that different metals have different work functions i.e., different threshold frequencies which shown in the following graph

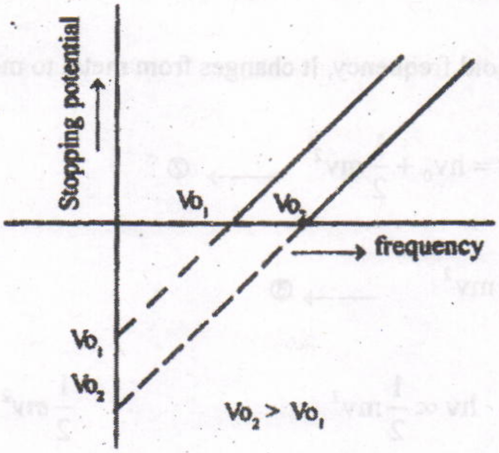


FIG 5.9.5

5.10 EINSTEIN'S PHOTOELECTRIC EQUATION:

The laws of photo electric effect explained by Einstein on the basis of quantum theory.

According to quantum theory the radiation consists of shower of photons and each photon has energy $h\nu$. When photon collides the atom in a metal surface, the energy is completely absorbed by single $\bar{e}$. This energy is utilized into two ways.

1. **A part of energy is utilized to liberate the $\bar{e}$ from the surface of the metal. This energy is called work function W.**
2. **The remaining energy $h\nu$-W is given to the liberated $\bar{e}$ as K.E ($\frac{1}{2}mv^2$)**

∴ from the above two laws,

$$h\vartheta - w = \frac{1}{2} mv2$$

$$h\nu = W + \frac{1}{2}mv^2 \longrightarrow ①$$

This equation is called Einstein's photo electric equation.

Work function W :-It is the minimum energy required to liberate the $\bar{e}$ from the from the surface of metal i.e.,

$W = h\nu_0$

where ν_0 is called threshold frequency, It changes from metal to metal

from eq^n ① $\Rightarrow$ $h\nu = h\nu_0 + \frac{1}{2}mv^2 \longrightarrow$ ②

$$h(\nu - \nu_0) = \frac{1}{2}mv^2 \longrightarrow ③$$

$\because$ $h\nu_0$ is constant $h\nu \propto \frac{1}{2}mv^2$ $\therefore$ $\frac{1}{2}mv^2 \propto \nu_0$

kinetic energy of $\bar{e}$ proportional to frequency of incident photon.

Stopping Potential V_0: It is the minimum -ve voltage given to the collector such that the photo current is zero. If V_0 is the stopping potential, the K.E. of the $\bar{e}$

$$\frac{1}{2}mv^2 = eV_0$$

$\therefore$ eq ③ $\Rightarrow h(\nu - \nu_0) = eV_0 \longrightarrow$ ④

$$V_0 = \frac{h}{e}(\nu - \nu_0) \longrightarrow ⑤$$

These [illegible] modified from of photo electric equation.

To plot the graph(5.10.1) between frequency of spectral line and stopping potential we got a straight line with intercept on x – axis (threshold frequency). The slope of the graph $= \frac{h}{e}$, Then $h = \text{slope} \times e$

Basing on this equation Millikan experimentally showed that the value of $h = 6.625 \times 10^{-34}$ J-S which is exactly coincide with the values from other various methods. Hence Einstein's photo elcectric equation was proved.

Slope $= \frac{h}{e}$

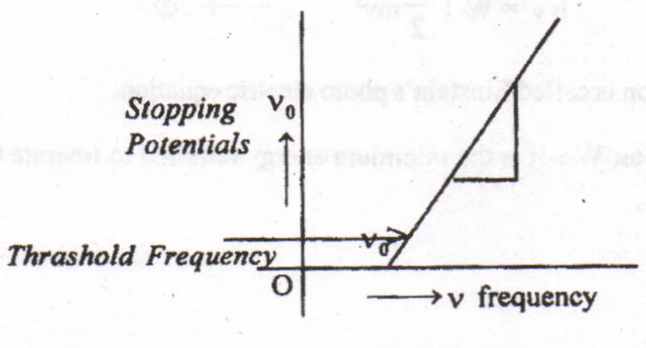


FIG 5.10.1

.11 SOLVED PROBLEMS:

1.The wave length of H_β line is 4861 A°. Find the Rydberg constant. [Ans:$1.097\times10^7 m^{-1}$]

ol : For H_β line in Balmer series, $n_1 = 2, n_2 = 4$

Given $\lambda_\beta = 4861\,\overset{\circ}{A} = 4861\times10^{-10}m$

we know that $\vec{\nu}_\beta = \frac{1}{\lambda_\beta} = R\left[\frac{1}{2^2}-\frac{1}{4^2}\right]$

$$\frac{1}{4861\times10^{-10}} = R\left[\frac{1}{4}-\frac{1}{16}\right] = R\left[\frac{3}{16}\right]$$

$$R = \frac{16\times10^{10}}{3\times4861} = 1.097\times10^7 m^{-1}$$

2. The wavelength of first line of Paschen series in hydrogen spetrum is 1.875×10^{-6}m. Find the Rydberg constant. [Ans:$1.09714\times10^7\ m^{-1}$.]

Sol : For 1st line of Paschen series $n_1 = 3, n_2 = 4$

$\lambda = 1.875\times10^{-6}m$

But $\vec{\nu} = \frac{1}{\lambda} = R\left[\frac{1}{n_1^2}-\frac{1}{n_2^2}\right]$

$$\frac{1}{1.875\times10^{-6}} = R\left[\frac{1}{3^2}-\frac{1}{4^2}\right] = R\left[\frac{1}{9}-\frac{1}{16}\right]$$

$$\frac{1}{1.875\times10^{-6}} = R\left[\frac{7}{9\times16}\right]$$

$$R = \frac{9\times16}{7\times1.875\times10^{-6}} = 1.09714\times10^7\ m^{-1}.$$

3. The wavelength of First line of Balmer series is 6563 $\overset{\circ}{A}$. Calculate the wavelength of second line [Ans:4861 $\overset{\circ}{A}$]

Sol : For the first line of the Balmer series $n_1 = 2, n_2 = 3.$

For H_α line, $\lambda = 6563\,\overset{\circ}{A} = 6563\times10^{-10}m$

$$\nu_\alpha = \frac{1}{\lambda_\alpha} = R\left[\frac{1}{2^2}-\frac{1}{3^2}\right] = R\left[\frac{5}{36}\right]$$

$$\frac{1}{6563\times10^{-10}} = \frac{5R}{36}$$

$$R = \frac{36\times10^{10}}{6563\times5} = 1.097\times10^{7}\,m^{-1}$$

For the second member $n_1 = 2$, $n_2 = 4$

$$\vec{\nu}_\beta = \frac{1}{\lambda_\beta} = R\left[\frac{1}{2^2} = \frac{1}{4^2}\right] = R\left[\frac{3}{16}\right]$$

$$\frac{1}{\lambda_\beta} = \frac{1.097\times10^{7}\times3}{16} \qquad \lambda_\beta = \frac{16}{3\times1.097\times10^{7}} = 4861\overset{0}{A}$$

4.The threshold wavelength for Na metal is 6800A°. Calculate the work function of Na metal in electron volt. **[Ans:1.818 eV]**

Sol : Work function $W = h\nu_0 = \frac{hc}{\lambda}$

Given threshold wavelength $\lambda_0 = 6800\,\overset{0}{A} = 6800\times10^{-10}$m

velocity of light $c = 3\times10^{8}\,ms^{-1}$

Planck's constant $h = 6.62\times10^{-34}$ J–S

$$W = \frac{hc}{\lambda_0} = \frac{6.62\times10^{-34}\times3\times10^{8}}{6800\times10^{-10}}$$

$$W = 2.91\times10^{-19}J$$

But $1ev = 1.6\times10^{-19}J$

$$\therefore 1\,J = \frac{1}{1.6\times10^{19}}\,eV$$

$$W = \frac{2.91\times10^{-19}}{1.6\times10^{-19}}$$

$$W = 1.818\ eV$$

5. Calculate the work function for Na metal when threshold frequency $\nu_0 = 4.39 \times 10^{14}$Hz

[Ans:1.818 eV]

Sol : Work function $W = h\nu_0 = \dfrac{hc}{\lambda_0}$

Given threshold frequency $\nu_0 = 4.39 \times 10^{14}$Hz

Planck's constant $h = 6.62 \times 10^{-34}$J–S

$$W = h\nu = 6.62 \times 10^{-34} \times 4.39 \times 10^{14}$$

$$= 39.06 \times 10^{-20}\text{J}$$

$$W = \frac{29.06 \times 10^{-20}}{1.6 \times 10^{-19}} = 18.162 \times 10^{-1}\text{eV}$$

$$= 1.8162 \text{ eV}$$

6. Calculate the work function of photo electric surface in which longest wavelenth of radiation to emit $\bar{e}$ from the surface is 6000 A°? **[Ans:2.0915 eV]**

Sol : From the given problem, threshold wavelength $\lambda_0 = 6000\ \overset{0}{A}$

$$\lambda = 6000 \times 10^{-10}\text{m} = 6 \times 10^{-7}\text{m}$$

$$\text{Threshold frequency } \nu_0 = \frac{c}{\lambda_0} = \frac{3 \times 10^{8}}{6 \times 10^{-7}} = 0.5 \times 10^{15}$$

$$\nu_0 = 5 \times 10^{14}\text{Hz}$$

$$W = h\nu_0 = 6.625 \times 10^{-34} \times 5 \times 10^{14}$$

$$= 33.125 \times 10^{-20}\text{J}$$

$$\therefore W = \frac{33.125 \times 10^{-20}}{1.6 \times 10^{-19}} \text{ eV}$$

$$= \frac{33.125 \times 10^{-1}}{1.6} = \frac{3.3125}{1.6} = 2.0915 \text{ eV.}$$

7. Radiation of wavelength 4000A° falls on a surface whose work function is 2eV. Calculate the maximum velocity of ejected $\bar{e}$. **[Ans:6.2282×10^5 ms^{-1}]**

Sol : From the given problem,

work function W $= 2\ eV = 2\times1.6\times10^{-19}J$

$= 3.2\times10^{-19}J$

Planck's constant, h $= 6.62\times10^{-34}J\text{–}S$

$$\lambda = 4000\ \overset{0}{A} = 4000\times10^{-10}m = 4\times10^{-7}m$$

$$\nu = \frac{C}{\lambda} = \frac{3\times10^{8}}{4\times10^{-7}} = 0.75\times10^{15}Hz$$

Mass of the $\bar{e}$, $m = 9.1\times10^{15}kg$

$$h\nu = W + \frac{1}{2}mV^2$$

$$\frac{1}{2}mV^2 = h\nu - W$$

$$V^2 = \frac{2(h\nu - W)}{m}$$

$$V = \sqrt{\frac{2(h\nu - W)}{m}}$$

$$= \sqrt{\frac{2\times\left(6.62\times10^{-34}\times0.75\times^{15} - 3.2\times10^{-19}\right)}{9.1\times10^{-31}}} = 6.2282\times10^{5}\ ms^{-1}$$

8. The photo electric surface of the work function is 4eV. What is the maximum velocity of photo $\bar{e}$ emitted by the light of frequency 3 × 10^{15}Hz **[Ans:1.7198 × 10^6 m/s]**

Sol : Work function $W = 4eV = 4\times1.6\times10^{-19}J$

Planck's constant $h = 6.62\times10^{-34}J\text{–}S$

frequency $= 3\times10^{15}H_2$

mall $m = 9.1\times10^{-31}kg$

$$V^2 = \frac{2(h\nu - W)}{m}$$

$$v = \sqrt{\frac{2\times\left(6.62\times10^{-34}\times3\times10^{15}-6.4\times10^{-19}\right)}{9.1\times10^{-31}}}$$

$= 1.7198 \times 10^{6}$ m/s

9.Calculate the work function of a metal in eV when its threshold frequency is 4.4×10^{14} Hz

Sol : Given $\nu_0 = 4.4 \times 10^{14}$ Hz **[Ans:1.8205 eV]**

$W = h\,\nu_0$

$= 6.62 \times 10^{-34} \times 4.4 \times 10^{14}$

$= 29.128 \times 10^{-20}\,J = \dfrac{29.128\times10^{-20}}{1.6\times10^{-19}}\,eV$

$= 18.205 \times 10^{-1}$ eV

$= 1.8205$ eV

10. Light of wavelength 800 Å and 700 Å incident on a metal surface is found to emit photo $\bar{e}$ K.E 1.8 eV and 4.5 eV respectively. Find the planck's constant [Ans:6.625×10^{-34}J-S]

Sol : Since work function is same in two cases.

According to Einstein's Photo electric equation

In case (i)	In case (ii)
$h\nu_1 = W + KE_1$	$h\nu_2 = W + KE_2$
$h\dfrac{c}{\lambda_1} = W + KE_1$	$h\dfrac{c}{\lambda_2} = W + KE_2$
$h\dfrac{3\times10^{8}}{800\times10^{-10}} = W+1.8\times1.6\times10^{-19}J \rightarrow$ ①	$h\dfrac{3\times10^{8}}{700\times10^{-10}} = W+4.5\times1.6\times10^{-19}J \rightarrow$ ②

Subtract eq ① from eq ②

$$\Rightarrow h.\frac{3\times10^{8}}{10^{-8}}\left[\frac{1}{7}-\frac{1}{8}\right]=1.6\times10^{-19}(4.5-1.8)$$

$h = 6.625\times10^{-34}$ J-S

5.12 SUMMARY:

1.Bohr postulates state that

electron revlove around the nuclues in circular orbit

centripetal force $= \frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0}.\frac{ze.e}{r^2}$ (neglecting - ve sign)

$$m\,v^2 = \frac{1}{4\pi\varepsilon_0}.\frac{ze^2}{r} \longrightarrow ①$$

In a stationary orbit, the orbital angular momemtum of electron ie equal to an integral multiple of $\frac{h}{2\pi}$

$$L = mvr = \frac{nh}{2\pi}$$

$$r = \frac{nh}{2\pi mv} \longrightarrow ②$$

When $\bar{e}$ jumps from one orbit to another orbit the energy is released or absorbed and is equal to difference between the energies of the two orbits i.e.,

$$E_2 - E_1 = h\nu \longrightarrow ④$$

2.Radius of the Bohr orbit : $r_n = \frac{\epsilon_0 n^2 h^2}{\pi m e^2} \longrightarrow ⑤$

$r_n = 0.53n^2 \overset{0}{A}$

3.Velocity of the $\bar{e}$: $v = \left(\frac{e^2}{2\,\epsilon_0 h}\right).\frac{1}{n}$

$$v = \frac{2.175\times10^6}{n} ms^{-1} \longrightarrow ⑥$$

4. Energy of the $\bar{e}$: $\therefore K.E = \frac{1}{8\pi\varepsilon_0}.\frac{e^2}{r} \longrightarrow ⑦$

$$\therefore PE = \frac{1}{4\pi\epsilon_0}.\frac{-e^2}{r} \longrightarrow ⑧$$

$$E_n = \frac{-me^4}{8\epsilon_0^2 h^2} \cdot \frac{1}{n^2} \longrightarrow ⑨$$

By substituting all there values $E_n = \frac{-13.6}{n^2} ev \longrightarrow ⑩$

5. Wave number: $\vec{\nu} = R\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$

6. Einstein's photo electric equation: $h\nu = W + \frac{1}{2}mv^2$

$$h(\nu - \nu_0) = \frac{1}{2}mv^2$$

7. Work function W :-It is the minimum energy required to liberate the $\bar{e}$ from the from the surface of me

$$W = h\nu_0$$

8. Stopping Potential V_0: It is the minimum -ve voltage given to the collector such thatthe photo curren zero. If V_0 is the stopping potential, the K.E. of the $\bar{e}$

$$\frac{1}{2}mv^2 = eV_0 \qquad \text{and} \qquad h(\nu - \nu_0) = eV_0$$

$$V_0 = \frac{h}{e}(\nu - \nu_0)$$

5.13 KEY WORDS:

Atom. hydrogen atom,. Bohr's theory,atomic spectra,spectral series,wave length, Rydberg constant, Photoelectric effect,Einstein's equation, Threshold frequency, Limitting wave length

5.13 SELF-ASSESSMENT QUESTIONS:

1. Using Bohr's theory, obtain the expression for radius of orbit, velocity of electron in a orbit energy of electron in any orbit.

2.State and explain the fundamental postulates of Bohr's theory of hydrogen atom and derive expressions for various hydrogen spectral lines.

3. What is Photoelectric effect .Describe an experimental set up with which the Photoelectric effect has been investigated.

4. State fundamental laws of Photoelectric emission.

5. Mention the limitations of Bhor's theory

6. Explain the following terms.

a) Stopping potential b) Threshold frequency c) Work function d) Long wave length limit

7. What is the effect of nuclear motion on atomic spectra.

8. Explain Ritz combination principle in spectra.

9. State and explain Einstein's Photoelectric equation.

EXERCISE:

1.Calculate the frequency of $\bar{e}$ in Bohr orbit of hydrogen **[Ans:6.534×10^{15}Hz]**

Hint : For Bohr orbit n = 1, radius = $r_1 = 0.53n^2$ Å

$$= 0.53 \times 10^{-10}\text{m}$$

from the Bohr second postulate, $mvr = \frac{nh}{2\pi}$

$$v = n\frac{h}{2\pi mr} = 1.\frac{6.62 \times 10^{-34}}{2 \times 3.14 \times 9.1 \times 10^{-31} \times 0.53 \times 10^{-10}} = 2.175 \times 10^{6}\text{m}$$

But $V = r\omega \Rightarrow V = r2\pi\nu$ $\nu = \frac{V}{2\pi r} = \frac{2.175 \times 10^{6}}{2 \times 3.14 \times 0.53 \times 10^{-10}}$]

.Calculate the stopping potential for photo $\bar{e}$ emitted by gold cathode. If the wavelength of incident radiation is 2.5×10^{-7}m and workfunction 4.8 eV. **[Ans: 0.16875 volt]**

Hint : Given work function $W = hV_0 = 4.8\text{ eV} = 4.8 \times 1.6 \times 10^{-19}\text{J}$

$$E = h\nu = \frac{hc}{\lambda} = \frac{6.62 \times 10^{-34} \times 3 \times 10^{8}}{2.5 \times 10^{-7}} = 7.95 \times 10^{-19}\text{J}$$

K.E $\frac{1}{2}mv^2 = eV$ $V_0 = ?$

∴ From Einstein's photo electric equation $h\nu = W + eV_0$

$$eV_0 = h\nu - W = E - W = 7.95 \times 10^{-19} - 7.68 \times 10^{-19} = 0.27 \times 10^{-19}$$

$$\therefore 1.6 \times 10^{-19} \times V_0 = 0.27 \times 10^{-19}$$

$$V_0 = \frac{0.27 \times 10^{-19}}{1.6 \times 10^{-19}}\,]$$

3. If the minimum wavelength recorded on the x–ray spectrum of 50KV tube is 0.257 Å Calculate the Planck's constant. **[Ans: 6.67×10^{-34} J-S**

[Hint :Maximum energy of the x – rays emitted is $h\nu = \frac{hc}{\lambda}$

= maximum energy of $\bar{e}$ emitted from the x – ray tube = eV

$$\frac{hc}{\lambda} = eV \qquad h = \frac{eV}{c} = \frac{1.6\times10^{-19} \times 50 \times 1000 \times 0.25 \times 10^{-10}}{3\times10^{8}}\,]$$

5.14 REFERENCE BOOKS:

1. Introductory of Atomic Spectra	H.F. White
2. Spectroscopy	Stranghen and Walker
3. Physics of atom	Wher and Richards
4. Prospective of Modern Physics	A.Beiser
5. Quantum Mechanics	Mathaws and Venkatesan
6. Introduction to Quantum Mechanics	Pauling and Wilson
7. Unified Physics Vol-IV	Jai Prakash & Co

UNIT-2

LESSON-6

MATTER WAVES AND de- BROGLIE'S HYPOTHESIS

OBJECTIVES:

After the completion of this lesson the student will be able to

1) Understand the de Broglie's concept of matter waves
2) Understand the expressions for de Broglie wave length
3) Understand the Davisson and Germer's electron diffraction experiment.
4) Understand the G.P. Thomson Experiment - Electron diffraction
5) Understand the Phase velocity or Wave velocity (V_p) and Group velocity (V_g)

STRUCTURE:

6.1 INTRODUCTION:

Particle is specified by its mass,velocity, momentum and energy. A wave is specified by its frequency, wavelength,phase of wave velocity, amplitude and intensity.Radiation some times behave as a wave and at some other time as a particle, i.e., it has a wave particle duality. But the radiation can not exhibit its particle and wave properties simultaneously.Light has a dual nature.

Louis de-Broglie in 1924 extended the wave particle duality of optics to all fundamental particles such as electron, protons, neutrons,atoms and molecules. He suggested that like radiation, matter also has a dual characteristic.A moving particle has always got a wave associated with it. and the particle is controlled by the wave in a manner similar to the photon is controlled by the wave. a wave associated with a moving particle is known as de-Broglie wave.

6.2 de BROGLIE'S CONCEPT OF MATTER WAVES AND EXPRESSION FOR THE de BROGLIE WAVELENGTH:

Radiation including ultra violet, infra red, visible light etc. behaves as waves from experments based on interference, diffraction, polarisation etc. Thus we conclude that radiation behaves as waves.

According to photo electric effect, comption effect, radiation behaves as particles called photon's. Thus sometimes radiation behaves as waves and some other times radiation behaves as particles i.e., radiation has dual property. But the radiation cannot exhibit dual nature simultaneously.

de Broglie extended this phenomenon to all material particles such as $\bar{e}$, neutron, proton, atoms, molecules etc. he concluded that matter also exhibits the dual characteristic property like radiation. A moving particle also associated a wave and the wavelength is called de Broglie wavelength.

Expression for deBroglie wavelength

1. For radiation :

According to Einstein's mass energy relation,

$$E = mc^2 \longrightarrow ①$$

From Planck's quantum theory $E = h\nu \longrightarrow ②$

From ① & ② $mc^2 = h\nu$

$$mc^2 = \frac{hc}{\lambda} \qquad \because c = \nu\lambda$$

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

$\because$ mc is the momentum of the photon p.

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

$\therefore$ de Broglie wavelength $\lambda = \frac{h}{p}$

2. For material particle :

Consider a particle of mass 'm' moving with a relocity v, its momentum p = mv

$\therefore$ wavelength associated with the particle $\lambda = \frac{h}{p} = \frac{h}{mv}$

K.E of the particle $E = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$

$$p^2 = 2mE$$

$$p = \sqrt{2mE}$$

$\therefore$ de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

3. For Electron :

Consider an $\bar{e}$ of mass m and charge 'e' is accelerated by a potential V volt from rest to velocity v then work done on $\bar{e}$,

$$W = \text{change in K.E}$$

$$W = \frac{1}{2}mv^2$$

$$eV = \frac{p^2}{2m} \qquad \because K.E = \frac{1}{2}mv^2 = \frac{p}{2m}$$

$$P^2 = 2meV$$

$$P = \sqrt{2meV}$$

∴ de Broglie wavelength associated with an $\bar{e}$,

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{h}{\sqrt{2me}} \cdot \frac{1}{\sqrt{V}}$$

Since $h = 6.62 \times 10^{-34}$ J. sec, $m = 9.1 \times 10^{-31}$kg, $\bar{e} = 1.6 \times 10^{-19}$col.

∴ By substituting these values,

$$\lambda = \frac{6.62 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}} \cdot \frac{1}{\sqrt{V}} = \frac{12.26}{\sqrt{V}} \overset{0}{A}$$

If V = 100 volt, $\lambda = \frac{12.26}{\sqrt{V}} \overset{0}{A} = \frac{12.26}{\sqrt{100}} \overset{0}{A} = \frac{12.26}{\sqrt{10}} \overset{0}{A} = 1.226 \overset{0}{A}$

4. de Broglie wavelength associated with material particle (molecule) with temperature :

When a material particle (molecule) is in thermal equilibrium at temperature T then the K.E. = E = $\frac{3}{2}$KT where K is Bottzmann's constant 1.38×10^{-23}J/K.

de Broglie wavelength associated with particle.

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2m.\frac{3}{2}KT}}$$

$$\lambda = \frac{h}{\sqrt{3mKT}}$$

6.3 DAVISSON AND GERMER'S ELECTRON DIFFRACTION EXPERIMENT:

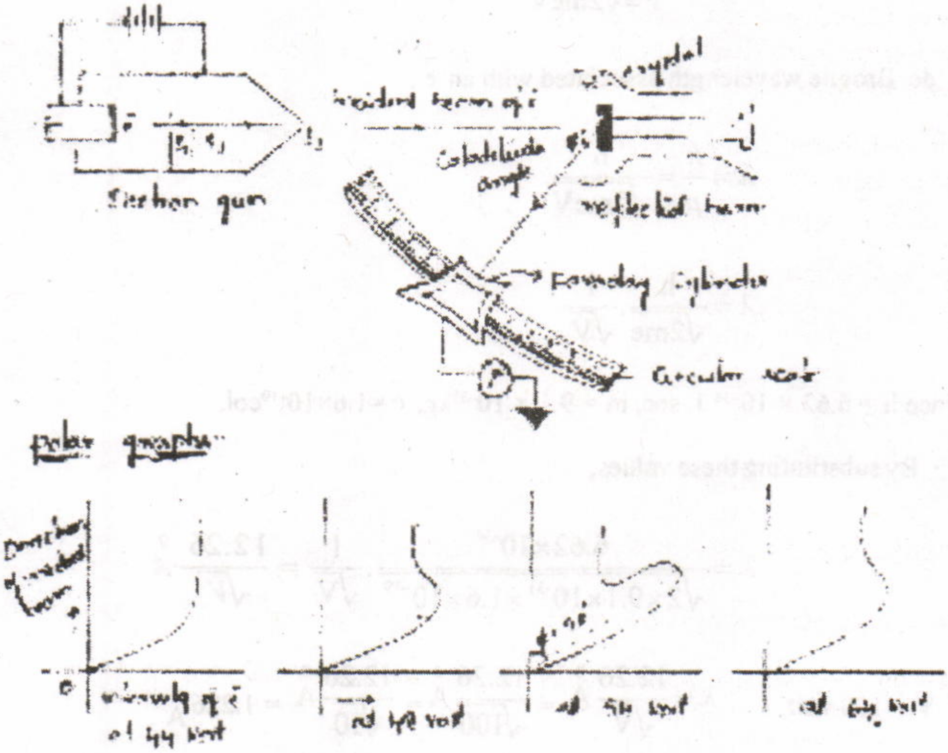


FIG 6.3.1

The $\bar{e}$ waves are experimentally determined by Davission and Germer. It is proved that the intensity of reflected electrons varies between max & min. from Ni target.Thus they conclude that the electrons diffracted like x rays i.e., $\bar{e}$ posses wave nature. The expermental arrangement is as shown in the figure. The apparatus consists of 3 steps.

1. **Electron Gun :** It is a tungsten filament 'f' heated to dull red, electrons emitted due to thermionic emission.
2. A variable electrons field of known p.d is applied to accelerate electrons.
3. The electrons collimated by two slits s_1 and s_2 produces fine beam, this fine beam of $\bar{e}$ s fall on the Ni

crystal. The refleted $\overline{e}$ s from the atoms of the crystal can be detected by faraday cylinder. The cylinder c can be moved on a circular scale, so that the reflected $\overline{e}$ s can be collected at angles 29° & 90°. This cylinder is connected to sensitive galvanometer G. The entire apparatus is enclosed in a evacuated chamber.

The cylinder is moved to various positions on the circular scale and the galvanometer reflections are noted in each position. The observations are taken as curves (polar graphs) for different voltages shown above.

It is seen that this spur (bump) begins to appear at 44V. The maximum. development of spur is obtained at colatitude $\phi = 50^0$ and potential at 54V. i.e., this spur gives that information about the wave nature of $\overline{e}$. At this position the reflected $\overline{e}$ from the atomic planes interfere constructively. According to de Broglie the wavelength of $\overline{e}$ at 54V is given by

$$\lambda = \frac{12.26}{\sqrt{V}} = \frac{12.26}{\sqrt{54}} \overset{0}{A}$$

$$\lambda = 1.668 \overset{0}{A}$$

Prediction of wavelength of $\overline{e}$ from Bragg's law.

The wavelength of $\overline{e}$ can be determined by Bragg's law i.e., $2d \sin\theta = n\lambda$

$\because \theta = 90 - \alpha$, d = interplanar distance

$$2d \sin(90 - \alpha) = n\lambda$$

$\because n = 1$, i. e., for first irder $2_{\infty} \cos\alpha = \lambda$ $(\because \sin(90 - \alpha) = \cos\alpha)$

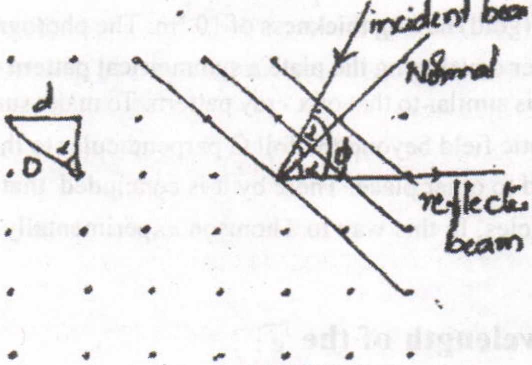


FIG 6.3.2

from figure(6.3.2) $\because d = D\cos\alpha$ $\cos\alpha = \frac{d}{D}$

$$2D \sin\alpha \cos\alpha = \lambda$$

$$\Rightarrow D \sin 2\alpha = \lambda$$

For Ni crystal $D = 2.15\ \overset{0}{A}$ and $\phi = 50^0$

$$\therefore \lambda = 2.15 \sin 50 = 1.647\ \overset{0}{A}.$$

As the two values are nearly equal it shows that the beam of $\bar{e}$ deffracted from the surface of the Ni crystal posses wavelength characteristics.

Hence de Broglie concept is verified from Davisson and Germer experiment.

6.4 G.P. THOMSON EXPERIMENT- ELECTRON DIFFRACTION:

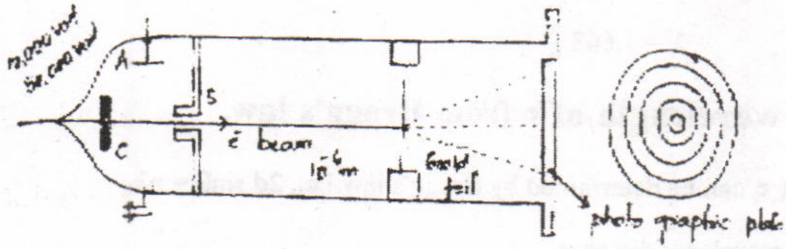


FIG 6.4.1

G.P Thomson experimentally showed that $\bar{e}$ are diffracted when passed through thin metal foils. In this experiment, the diffraction pattern of $\bar{e}$ is similar to that of x – ray pattern. $\bar{e}$ beam with high energy produced by cathode is made to pass through narrow slit S, a fine pencil beam is obtained as shown in figure(6.4.1). This fine beam is excited by potential from 10,000 to 50,000 volt. This accelerated fine beam of $\bar{e}$ fall on the thin film (gold) having thickness of 10^{-8}m. The photograph of beam is recorded on the photographic plate. After developing the plate a symmetrical pattern consisting of concentric rings is obtained. This pattern is similar to that of x - ray pattern. To make sure that this pattern is due to $\bar{e}$, Thomson applied magnetic field beyond the foil G parpendicular to the beam. It was observed that the entire pattern is shifted to other place. There by it is concluded that the pattern is due to the waves but not due to the particles. In this way to Thomson experimentally proved that the $\bar{e}$ beam behaves as waves.

Determination of the wavelength of the $\bar{e}$:

In poly crystalline film (gold film) there will be certain crystals set at correct angle θ to give Bragg's reflection.

As a result series of rings formed on the photographic plate. Let AB be the incident beam which suffered Bragg's reflection in the film.

Let $OP = R$, radius of the ring and $\angle PBO = 2\theta$

According to Bragg's law $2d \sin\theta = n\lambda$

$\because$ θ is very small, $\sin\theta \approx \theta$ and for first order $n = 1$

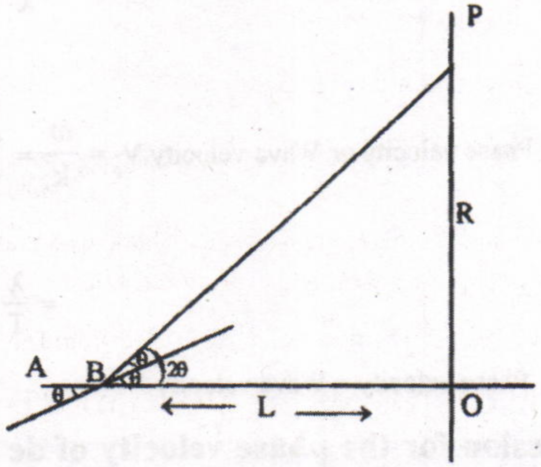
$$\therefore 2d.\theta = 1.\lambda$$

$$\lambda = 2d.\theta \longrightarrow \text{①}$$

from the figure(6.4.2), $\tan 2\theta \approx 2\theta = \frac{R}{L}$

$$2\theta = \frac{R}{L}$$

$$\Rightarrow \theta = \frac{R}{2L} \longrightarrow \text{②}$$



from ①&② $\lambda = 2.d.\frac{R}{2L}$

$$\lambda = Rd/L$$

FIG 6.4.2

By knowing all the terms, wavelength of the $\bar{e}$ can be calculated i.e., from this experiment, λ value is found that 1.669A°. It is completely aggred with the theoretical value 1.66A°.

$\therefore$ It gives the information for the wave nature of e .

Uses of $\bar{e}$ diffraction :

1. The $\bar{e}$ diffraction is used to determine the internal structure of the matter such as the surface structure of the thin film.
2. The diffraction pattern obtained with $\bar{e}$ is stronger than that obtained with x – rays and there by it requires less exposure time.

6.5 PHASE VELOCITY or WAVE VELOCITY (V_p) AND GROUP VELOCITY (V_g) :

The speed at which the wavefront of the wave travels is called phase velocity or wave velocity.

Angular frequency of each wave $\omega = \frac{2\pi}{T}$ and

Propagation constant or Wave number $k = \frac{2\pi}{\lambda}$

$\therefore$ Phase velocity or Wave velocity $V_p = \frac{\omega}{k} = \frac{\frac{2\pi}{T}}{\frac{2\pi}{\lambda}}$

$= \frac{\lambda}{T}$

$\therefore$ Phase velocity = Wave velocity

Expression for the phase velocity of de Broglie Wave :

We know that de Broglie wavelength $\lambda = \frac{h}{mv} \longrightarrow$ ①

$E = mc^2 = h\nu \Rightarrow \nu = \frac{mc^2}{h}$

Angular frequency w $= 2\pi\nu = 2\pi\frac{mc^2}{h} \longrightarrow$ ②

from theory of relativity mass $m = \frac{m_0}{\sqrt{1 - v^2/c^2}}$

$\therefore$ eq ② $\Rightarrow = \frac{2\pi m_0}{\sqrt{1-v^2/c^2}}.\frac{c^2}{h} \longrightarrow$ ③

Wave number $k = \frac{2\pi}{\lambda} = \frac{2\pi}{\frac{h}{mv}} = \frac{2\pi mv}{h}$

$\therefore k = \frac{2\pi m_0}{\sqrt{1-v^2/c^2}}.\frac{v}{h} \longrightarrow$ ④

$$\therefore \text{Phase velocity } V_p = \frac{\omega}{k} = \frac{\frac{2\pi m_0}{\sqrt{1-v^2/c^2}}.\frac{c^2}{h}}{\frac{2\pi m_0}{\sqrt{1-v^2/c^2}}.\frac{v}{h}}$$

$$v_p = \frac{c^2}{v} \qquad \text{i.e., } v_p > c$$

Phase velocity is greater than velocity of light. But it is impossible.

Group velocity (V_g) : The velocity with which the group of waves or wavepacket travels is called group velocity.

$$\therefore \text{Group velocity } V_g = \frac{d\omega}{dk} = \frac{\left(\frac{d\omega}{dv}\right)}{\left(\frac{dk}{dv}\right)} \longrightarrow ⑤$$

Diffraction eq ③ with respect to V

$$\left(\frac{d\omega}{dv}\right) = \frac{2\pi m_0 c^2}{h}.\frac{-1}{2}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\left(-\frac{2v}{c^2}\right)$$

$$\left(\frac{d\omega}{dv}\right) = \frac{2\pi m_0 v}{h\left(1-\frac{v^2}{c^2}\right)^{3/2}} \longrightarrow ⑥$$

Diffraction eq ③ eith respect to v

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left[V\left\{-\frac{1}{2}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\left(\frac{-2v}{c^2}\right)\right\} + \left(1=\frac{v^2}{c^2}\right)^{-1/2}.1\right]$$

$$= \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-1/2}\left[\frac{v^2}{c^2}\left(1-\frac{v^2}{c^2}\right)^{-1}+1\right]$$

$$= \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-1/2}\left[\frac{\frac{v^2}{c^2}}{1-\frac{v^2}{c^2}}+1\right] = \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-1/2}\left[\frac{\frac{v^2}{c^2}+1-\frac{v^2}{c^2}}{\left(1-\frac{v^2}{c^2}\right)}\right]$$

$$\frac{dK}{dV} = \frac{2\pi m_0}{h}\cdot\frac{1}{\left(1-\frac{v^2}{c^2}\right)^{3/2}} \longrightarrow ⑦$$

Substitute eq ⑥ & eq ⑦ in eq ⑤

$$V_g = \frac{d\omega}{dk} = \frac{\dfrac{2\pi m_0 v}{h\left(1-\frac{v^2}{c^2}\right)^{-3/2}}}{\dfrac{2\pi m_0}{h}\cdot\dfrac{1}{\left(1-\frac{v^2}{c^2}\right)^{3/2}}} = V$$

$$V_g = V$$

∴ Group velocity = Particle velocity. Thus the de Brogalie wave group associated with moving particle travels with the same velocity as that of the particle.

Wave packet :

A localised wave function is called wave packet or wave group. It consists of group of waves of slight different wavelengths with different phases and amplitudes, in which they interfere constructively over a small region of space and destructively else where.

6.6 CONSEQUENCES OF de BROGLIE CONCEPT:

1. de Broglie explained the quantisation of angulär momentum being takes place interms of wave nature of moving $\bar{e}$ around the nucleus.
2. From neutron diffraction the wave nature is used to investigate the structure of matter and arrangement of nucleus.
3. de Broglie concept leads to uncertainity principal. A material particle exhibits wave like nature but these two natures cannot be exhibited simultaneoushy.

e hypothesis explains the Bohr's principle of complementarity.

6.7 SOLVED PROBLEMS:

1.Find the de-Broglie wavelength of an $\bar{e}$ accelerated by the P.D of 6400V.

Sol : Planck's constant $h = 6.62 \times 10^{-34}$J [Ans: 0.153 Å]

Given p.d, V = 6400 voits

Mass of $\bar{e}$, $m = 9.1 \times 10^{-31}$ kg

charge of $\bar{e}$, $e = 1.6 \times 10^{-19}$ col

de Broglie wavelength associated with $\bar{e}$, $\lambda = \frac{h}{\sqrt{2meV}}$

$$\lambda = \frac{6.62 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}} . \frac{1}{\sqrt{6400}}$$

$$= \frac{12.24 \times 10^{-10}}{80}$$

$$= \frac{1.53 \text{Å}}{10}$$

$\lambda = 0.153$ Å

2.Calculate the de - Broglie wavelength associated by the $\bar{e}$ having the K.E. of 0.1512MeV and rest mass energy E_0 = 0.51 MeV. [Ans: 0.006 Å]

Sol : According to Einstein's theory of relativity,

Total Energy E = Rest mass energy + K.E

E = 0.51 MeV + 0.1512 MeV

E = 06612 MeV =0.6612MeV

$\because$ 1 MeV $= 1.6 \times 10^{-13}$J

E $= 0.6612 \times 1.6 \times 10^{-13}$J

$\because E = mc^2$

$m \times (3 \times 10^8)^2 = 0.6612 \times 1.6 \times 10^{-13}$

$$m = \frac{0.6612\times1.6\times10^{-13}}{\left(3\times10^{8}\right)^{2}} = 3.6\times10^{-30}\text{kg}$$

$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$\sqrt{1-\frac{v^2}{c^2}} = \frac{m_0}{m}$$

$$\sqrt{1-\frac{v^2}{c^2}} = \frac{m_0}{m}$$

$$\frac{v^2}{c^2} = 1-\frac{m_0^2}{m^2} \qquad v = \sqrt{c^2\left(1-\frac{m_0^2}{m^2}\right)}$$

$$\Rightarrow v = \sqrt{\left(3\times10^{8}\right)^{2}\left[1-\frac{\left(9.1\times10^{-31}\right)^{2}}{\left(3.6\times10^{-30}\right)^{2}}\right]}$$

$$v = 2.9\times10^{8}\ \text{ms}^{-1}$$

∴ wavelength associated with $\bar{e}$ is $\lambda = \frac{h}{mv}$

$$= \frac{6.62\times10^{-31}}{3.6\times10^{-30}\times2.9\times10^{8}}$$

$$= 0.006\times10^{-10}\text{m} = 0.006\ \mathring{A}$$

3.Find the de Broglie wavelength of neutron having the K.E of 28.8 MeV and mass of neutron is $m = 1.67\times10^{-27}$kg. **[Ans: 0.0000533 $\mathring{A}$]**

Sol : Given $m = 1.67\times10^{27}$kg

$\lambda = ?$

$E = 28.8\ \text{MeV} = 28.8\times1.6\times10^{-13}\text{J}$

de-Broglie wavelength associated with neutron $\lambda = \frac{h}{\sqrt{2mE}}$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{6.62\times10^{-34}}{\sqrt{2\times1.67\times10^{-27}\times28.8\times1.6\times10^{-13}}}$$

$$\lambda = 5.33\times10^{-15}\text{m} = 5.33\times10^{-5}\,\overset{0}{\text{A}} = 0.0000533\,\overset{0}{\text{A}}$$

4. Find the de Broglie wavelength of neutron having the K.E of 12.8 MeV & mass of neutron is a m = 1.67 ×10⁻²⁷kg. [Ans: 0.00008 $\overset{0}{\text{A}}$]

Sol : Given $m = 1.67\times10^{-27}$kg

$E = 12.8$ MeV $= 12.8\times1.6\times10^{-13}$J

de-Broglie wavelength associated with neutron $\lambda = \frac{h}{\sqrt{2mE}}$

$$\lambda = \frac{6.62\times10^{-34}}{\sqrt{2\times1.67\times10^{-27}\times12.8\times1.6\times10^{-13}}}$$

$$= \frac{6.62\times10^{-34}}{\sqrt{68.40\times10^{-40}}} = \frac{6.62\times10^{-34}}{8.270\times10^{-20}}$$

$$= 8.00\times10^{-15}\text{m} = 0.00008\,\overset{0}{\text{A}}$$

5.Calculate the wavelength associated with a particle of mass 1gm moving with velocity of 2000ms⁻¹

Sol : $\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}}{1\times10^{-3}\times2000} = 3.31\times10^{-34}\text{m}$ [Ans: $3.31\times10^{-24}\,\overset{0}{\text{A}}$]

$$\lambda = 3.31\times10^{-24}\,\overset{0}{\text{A}}$$

6. Find the energy of neutron in eV whose de Broglie wave length is 1 $\overset{0}{\text{A}}$

Sol : Mass of neutron $m = 1.67\times10^{-27}$kg [Ans: 0.8 eV]

Planck's constant, $h = 6.62\times10^{-34}$ J–S

$\lambda = 1\,\overset{0}{\text{A}} = 1\times10^{-10}\text{m}$, $E = ?$

de Broglie wavelength, $\lambda = \frac{h}{\sqrt{2mE}}$

$$\sqrt{2mE} = \frac{h}{\lambda}$$

$$= \frac{6.62\times10^{-34}}{1\times10^{-10}} = 6.62\times10^{-24}$$

$$\sqrt{2\times1.67\times10^{-27}E} = 6.62\times10^{-24}$$

$$3.34\times10^{-27}E = (6.62\times10^{-24})^2$$

$$E = \frac{(6.62\times10^{-34})^2}{3.34\times10^{-27}} = 13.1\times10^{-21}J$$

But $1eV = 1.6\times10^{-19}J \Rightarrow 1J = \frac{1}{1.6\times10^{-19}} eV$

$$E = \frac{13.1\times10^{-21}ev}{1.6\times10^{-19}} = 0.8\ eV$$

7. Determine the velocity and K.E of neutron having de–Broglie wavelength of 1 Å

Sol : $\lambda = \frac{h}{\sqrt{2mE}} \Rightarrow 2mE = \frac{h^2}{\lambda^2}$ **[Ans: 3963 m/s]**

$$2\times1.67\times10^{-27}\times E = \left(\frac{6.62\times10^{-34}}{1\times10^{-10}}\right)^2$$

$$= (6.62\times10^{-24})^2$$

$$E = \frac{43.82\times10^{-48}}{3.34\times10^{-27}} = 13.12\times10^{-21}J$$

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

$$\Rightarrow v^2 = \frac{2E}{m}$$

$$V = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2\times13.12\times10^{-21}}{1.67\times10^{-27}}} = 3.9639\times10^3\ m/s = 3963\ m/s$$

:.Calculate the wavelength associated with an $\bar{e}$ subjected to p.d of 1.25 KV

[Ans: 0.34 Å]

Sol : $V = 1.25\times10^3$ Volt $\Rightarrow$ 1250 Volt

$$\lambda = \frac{12.24}{\sqrt{V}}\mathring{A}$$

$$\lambda = \frac{12.24\times10^{-10}}{\sqrt{1250}} = \frac{12.24\times10^{-10}}{35.35}$$

$$= 0.34\times10^{-10}\text{m} = 0.34\,\mathring{A}$$

9.Calculate the de-Broglie wavelength associted with proton moving with a velocity equal to $\frac{1}{20}$ th velocity of light **[Ans: $2.64\times10^{-4}\,\mathring{A}$]**

Sol : Given velocity of proton $V = \frac{1}{20}C$

$$= \frac{1}{20}\times3\times10^{8}$$

$$= \frac{3}{20}\times10^{8}\text{ms}^{-1}$$

$$m = 1.67\times10^{-27}\text{kg}$$

$$h = 6.62\times10^{-34}\text{ J-S}$$

$$\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}}{1.67\times10^{-27}\times\frac{3}{20}\times10^{8}} = 2.64\times10^{-14}\text{ m} = 2.64\times10^{-4}\,\mathring{A}$$

10.What would be the wavelength of the quantum of radiant energy emitted. If an $\overset{-}{e}$ transmitted into radiation and converted into 1 quantum. **[Ans: 0.0245 $\mathring{A}$]**

Sol: According to Planck'e energy associated with 1 quantum

$$E = h\nu = \frac{hc}{\lambda}$$

when the energy of $\overset{-}{e}$ transmitted into radiation

$$E = mc^{2} = \frac{hc}{\lambda} \qquad \lambda = \frac{h}{mc} = \frac{6.62\times10^{-34}}{9.1\times10^{-31}\times3\times10^{8}} = 0.0245\,\mathring{A}$$

6.8 SUMMARY:

1. Particle is specified by its mass, velocity, momentum and energy. A wave is specified by its frequency, wavelength, phase of wave velocity, amplitude and intensity.

2. Radiation some times behave as a wave and at some other time as a particle, i.e., it has a wave particle duality. Light has a dual nature.

3. Radiation can not exhibit its particle and wave properties simultaneously.

4. Louis de-Broglie in 1924 extended the wave particle duality of optics to all fundamental particles such as electron, protons, neutrons, atoms and molecules.

5. Louis de-Broglie in 1924 extended the wave particle duality of optics to all fundamental particles such as electron, protons, neutrons, atoms and molecules.

6. Expressions for deBroglie wavelength

For radiation : de Broglie wavelength $\lambda = \frac{h}{p}$

For material particle :de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$

For Electron : de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}$

with temperature :de Broglie wavelength $\lambda = \frac{h}{\sqrt{3mKT}}$

7. Wavelength of $\bar{e}$ from Bragg's law: $\lambda = D \sin 2\alpha$

For Ni crystal $D = 2.15\ \overset{0}{A}$ and $\phi = 50^0$ $\therefore \lambda = 2.15 \sin 50 = 1.647\ \overset{0}{A}$

8. G.P. Thomson Experiment - Electron Diffraction:

$\lambda = Rd/L$

9. Phase velocity or Wave velocity (V_p):The speed at which the wavefront of the wave fravels is called phase velocity or wave velocity. $\therefore$ Phase velocity $V_p = \frac{c^2}{v}$

10. Group velocity (V_g) : The velocity with which the group of waves or wavepacket travels is called group velocity. $\therefore$ Group velocity $V_g = \frac{d\omega}{dk}$

6.9 KEY WORDS:

Wave particle duality, Radiation, de Broglie's concept, Wavelength, Momentum, Bottzmann's constant, Bragg's law, Electron, Diffraction, Phase velocity, Group velocity.

6.10 SELF-ASSESSMENT QUESTIONS:

1. Describe the experiment of Davisson and Germer to demonstrate the wave character of electrons. What are the important conclusions that could be drawn from it.
2. Describe G.P.Thomson's experiment on electron diffraction and explain the important conclusions.
3. Describe the de Broglie thory of matter waves.
4. What is de Broglie hypothesis. Obtain an expression for the wavelength associated with matter waves..
5. Write short notes on 1) matter waves 2) properties of matter waves 3) wave velocity and group velocity
6. Show that the phase velocity of de Broglie wave is greater than the velocity of light
7. Show that the group velocity of de Broglie wave is equal to the velocity of the particle with which the waves are associated.

EXERCISE:

1. An $\bar{e}$ is accelerated by p.d of 54 volt. Calculate the velocity of $\bar{e}$ and de-Broglie wavelength

[Ans: 4.371 × 10^6 ms^{-1}]

[Hint: : Wavelength associted with $\bar{e}$, $\lambda = \frac{12.24}{\sqrt{v}} \overset{0}{A}$

$$\lambda = \frac{12.24}{\sqrt{5v}} \overset{0}{A} \qquad \text{and} \qquad \lambda = 1.667 \overset{0}{A}$$

$$\lambda = \frac{h}{mv} \Rightarrow v = \frac{h}{m\lambda} = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 1.667 \times 10^{-10}}] = 4.371 \text{ X } 10^6 ms^{-1}$$

2. The energy of a neutron at absolute temperature 7 is KT then find the wavelength associ- ated by the therm alneutrons at 27^0**c (Mass of neutron = 1.67 × 10^{-27}kg) and Boltzmann constant K = 8.6 × 10^{-5} eV ?** **[Ans: 1.78A°]**

[Hint: Wavelength $\lambda = \frac{h}{\sqrt{2mE}}$

energy of the neutron E = KT

$K = 8.6 \times 10^{-5} \times 1.6\times10^{-19}$ J/S/K $\qquad T = 27 + 273 = 300k$

$E = KT = 8.6 \times 1.6 \times 10^{-24}\times300$

$m = 1.67 \times 10^{-27}kg \qquad h = 6.62 \times 10^{-34}J–S$

Wavelength associated with neutron $\lambda = \frac{h}{\sqrt{2mE}}$

$$\lambda = \frac{6.62\times10^{-34}}{\sqrt{2\times1.67\times10^{-27}\times8.6\times1.6\times300\times10^{-24}}}$$

$\lambda = 1.78\times10^{-10}m$]

3.Find the wavelength associated with the electron travelling with a velocity equal to 0.01 times the velocity of light. **[Ans: 2537 $\overset{0}{A}$]**

[Hint: Velocity of the electron, $v = 0.01c = 1.10\times3\times10^{8} = 3\times10^{6}\ ms^{-1}$

$m = 9.1 \times 10^{-31}kg \qquad h = 6.62 \times 10^{-34}J–S$

$\therefore$ wavelangth associated with electron, $\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}}{9.1\times10^{-31}\times3\times10^{6}}$] $= 2537\ \overset{0}{A}$

6.11 REFERENCE BOOKS:

1. Spectroscopy	Straughen and Walker
2. Physics of Atom	Wher and Richards
3. Elements of Modern Physics	Patil
4. Prospective of Modern Physics	A.Beiser
5. Unified Physics Vol-IV	Jai Prakash & Co
6. Quantum Mechanics	Mathaws and Venkatesan
7. Introduction to Quantum Mechanics	Pauling and Wilson

UNIT -2

LESSON-7

UNCERTAINTY PRINCIPLE AND QUANTIZATION

OBJECTIVES:

After the completion of this lesson the student will be able to

1) Understand the Heisenberg's uncertainty principle and quantization.

2) Know about the time- energy uncertainty principle.

3) Understand the Gamma ray microscope

4) Understand the determination of electron in Bohr orbit using uncertainty principle.

5) Understand the diffraction of electron at a slit

STRUCTURE:

7.1 INTRODUCTION:

de Broglie concept leads to uncertainty principle.The material particle exhibits particle nature as well as wave nature.In 1927 Heigenburg uncertainty principle which is a direct consequence of the dual nature of matter. In classical mechanics a moving particle at any instant has a fixed position in space and a finite momentum.In wave mechanics the particle is described in terms of a wave packet.According to Bohr probability interpretation, the particle may be found anywhere witnin the wave packet.When the wave packet is small, the position of particle may be fixed but velocity becomes indeterminate.When the wave packet is large, the velocity of particle may be fixed but position becomes indeterminate.In this way uncertainty in position or momentum.

7.2 HEISENBERG'S PRINCIPLE AND QUANTIZATION

According to uncertainty principle, "it is impossible for both position and momentum of particle can be measured simultaneously at any desired degree of accuracy".

In general this principal states that the product of magnitudes of uncertainity is equal to Palnck's constant h.

i.e., $\Delta P \times \Delta x \cong h$

where ΔP = uncertanity in finding the momentum of the particle.

and Δx = uncertanity in finding the position of the particle. This relation also hold good for energy and time

i.e.. $\Delta E \times \Delta x \cong h$

where ΔE = uncertanity in determining the energy of the particle in the interval Δt.

This relation also hold good for angular momentum and angular displacement.

i.e., $\Delta J \times \Delta\theta \cong h$

Different forms of uncertainty principls as follows

$$\Delta P \times \Delta x \geq \frac{h}{4\pi} \text{ or } \frac{\hbar}{2} \quad = \quad 0.527 \times 10^{-34} \text{ J-S}$$

$$\text{(or)} \quad \Delta P \times \Delta x \geq \hbar \text{ or } \frac{h}{2\pi} \quad = \quad 1.054 \times 10^{-34} \text{ J-S}$$

7.3 EXTENSION OF UNCERTAINTY PRINCIPLE TO TIME-ENERGY:

Consider a free particle of rest mass m_0 moving along x– axis with velocity V_x^2, the k.E

$$E = \frac{1}{2} m_0 Vx^2 = \frac{P_x^2}{2m_0} \longrightarrow ①$$

If ΔP_x and ΔE be the uncertainities in determining the energy and momentum of the particle.

differntiate eq ① $\Delta E = \frac{2P_x \times \Delta P_x}{2m_0}$

$$\Delta E = \frac{P_x \Delta P_x}{m_0}$$

$$\Delta P_x = \frac{m_0 \times \Delta E}{P_x} \longrightarrow ②$$

Since $P_x = m_0 V_x$

eq ② becomes $\Delta P_x = \frac{m_0 \times \Delta E}{m_0 V_x} = \frac{\Delta E}{V_x} \longrightarrow ③$

But $V_x = \frac{\Delta x}{\Delta t}$

where Δx is the uncertainity in determining the position of the particle during the interval Δt.

$\therefore$ eq ③ $\Rightarrow$ $\Delta P_x = \frac{\Delta E}{\left(\frac{\Delta x}{\Delta t}\right)} = \frac{\Delta E \times \Delta t}{\Delta x}$

$$\Delta E \times \Delta t = \Delta Px \times \Delta x$$

$$\Delta E \times \Delta t \cong h \qquad \therefore \Delta P_x \times \Delta x \cong h$$

This is the uncertainty in energy and time

7.4 GAMMA RAT MICROSCOPE:

Gamma ray microscope is used to locate the position of the particle ($\bar{e}$) more accurately. To observe the position of the $\bar{e}$ atleast one photon must strike the $\bar{e}$ in the scatterer in the field of view of microscope. Then the $\bar{e}$ position can be observed.

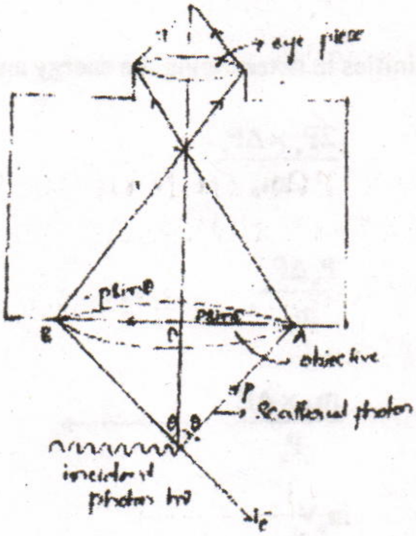


FIG 7.4.1

∴ resolving power of gamma ray micrscope is

$$\Delta x = \frac{\lambda}{2\sin\theta} \longrightarrow ①$$

where λ = wavelength of the light used and θ is the semi Vertical angle of cone of light

Initial moment of photon $P = \frac{h}{\lambda}$

After scattering enters the field of view of microscope, the maximum viewing angle by the cone of rays in the field is θ. The uncertainty in measurement of x – component of momentum.

$$\Delta P_x = P\sin\theta - (-P\sin\theta)$$

$$\Delta P_x = 2P\sin\theta$$

$$\lambda = \frac{h}{P}$$

$$\Delta P_x = \frac{2h}{\lambda} \sin\theta \xrightarrow{} ② \qquad \because P = \frac{h}{\lambda}$$

$$① \ \& \ ② \qquad \Delta P_x \times \Delta x = \frac{2h}{\lambda} \sin\theta \times \frac{\lambda}{2\sin\theta} = h$$

$$\Delta P_x \times \Delta x = h$$

If represents the Heisenberg uncertainity priciple.

7.5 DETERMINATION OF POSITION OF ELECTRON IN BOHR ORBIT USING UNCERTAINTY CONDITION(for hydrogen atom):

Let E be the total energy of the $\bar{e}$, when an $\bar{e}$ in hydrogen atom revolves in the first orbit i.e., Bohr orbit, total energy of $\bar{e}$, E = P.E + K.E

$$E = K.E. + P.E$$

$$= \frac{P^2}{2m} - \frac{1}{4\pi \epsilon_0} \cdot \frac{e^2}{r} \xrightarrow{} ①$$

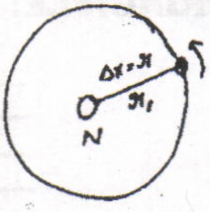


FIG 7.5.1

From uncertainity priciple, $\Delta P \times \Delta x = \hbar$

$$\Delta P \times \Delta x = \frac{h}{2\pi}$$

$$\Delta P = \frac{h}{2\pi \times \Delta x} \xrightarrow{} ②$$

By putting $\Delta P = P$, $\Delta x = r$ radius of Orbit

$$\therefore \text{eq (2)} \Rightarrow P = \frac{h}{2\pi r} \xrightarrow{} ③$$

Substituting ③ in ① $\Rightarrow E = \frac{h^2}{2m \times 4\pi^2 r^2} - \frac{1}{4\pi \epsilon_0} \cdot \frac{e^2}{r}$

$$E = \frac{h^2}{8\pi^2 m r^2} - \frac{e^2}{4\pi \epsilon_0 r} \xrightarrow{} ④$$

For the most stable state energy of $\bar{e}$ is almost constant differntiate eq ④

$$0=\frac{h^2}{8\pi^2 m}\left\{\left[\frac{-2}{r^3}\right]dr\right\}-\frac{e^2}{4\pi\in_0}\left[-\frac{1}{r^2}dr\right]=0$$

$$\frac{-2h^2}{8\pi^2 mr^3}dr=\frac{-e^2}{4\pi\in_0 r^2}dr$$

$$\frac{h^2}{\pi mr}=\frac{e^2}{\in_0}$$

$$r=\frac{h^2\in_0}{\pi me^2}\approx 0.53\overset{o}{A}$$

This is expression for the radius of Bohr Orbit.

7.6 DIFFRACTION OF ELECTRON AT A SLIT- VERIFICATION UN CE TAINTY PRINCIPLE:

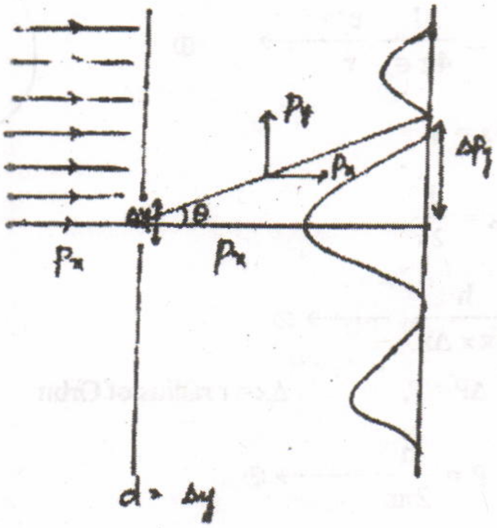


FIG 7.6.1

Consider b ng same energy incident on the slit of width Δy. The slit width Δy is th

uncertainity he position of the $\bar{e}$ in y–direction Sin

According to diffraction condition $n\lambda = d\sin\theta$ for the first order $n = 1$, $d = \Delta y$

$$\therefore 1 \times \lambda = \Delta y \sin\theta$$

$$\sin\theta = \frac{\lambda}{\Delta y}$$

Since θ is very small, $\sin\theta \approx \theta = \dfrac{\lambda}{\Delta y} \longrightarrow$ ①

Due to the wave particle duality the $\bar{e}$ are considered as waves and producing diffraction pattern on the screen while passing through the slit. After diffraction ΔPy be the uncertainity in determining the momentum of the $\bar{e}$ along y – axis.

$$\therefore \tan\theta \approx \theta = \frac{\Delta Py}{P_x} \longrightarrow ② \qquad (\because P_x \text{ is the initial momentum of } \bar{e})$$

from ① & ② $\dfrac{\lambda}{\Delta y} = \dfrac{\Delta Py}{Px}$

$$\Delta Py \times \Delta y = \lambda P_x = \lambda = \frac{h}{P_x} \qquad \left[\because \lambda = \frac{h}{P_x}\right]$$

$$\Delta Py \times \Delta y = \frac{h}{P_x} P_x$$

$$\Delta Py \times \Delta y = h$$

Which is Heisenberg's uncertainty principal

7.7 USING UNCERTAINTY PRINCIPE TO SHOW THAT ELECTRON CAN NOT EXIST INSIDE THE NUCLEUS:

The diameter of the nucleus is 10^{-14}m

If $\bar{e}$ lies inside the nucleus the uncertainity in the position of $\bar{e}$ = Δx = diameter of the nucleus.

i.e., $\Delta x = 10^{-14}$m

Then, the uncertainity in momentum will be least.

i.e., $\Delta P \approx P$

From uncertainity principle, $\Delta P \times \Delta x \approx h$

7.8 SOLVED PROBLEMS:

1.What potential must be applied to the electron microscope to produce electron of wavelength 0.8 A° [Ans:234.09 Volts]

Sol : Given wavelength of emitted electron $\lambda = 0.8 = 0.8\times10^{-10}$m

$v = ?,\ h = 6.62\times10^{-34}$J–S

$$\lambda = \text{wavelength of electron emitted} = \frac{12.24}{\sqrt{v}}\overset{0}{\text{A}}$$

$$= \frac{12.24\times10^{-10}}{\sqrt{v}}m$$

$$\sqrt{v} = \frac{12.24\times10^{-10}}{\lambda}$$

$$V = \left(\frac{12.24\times10^{-10}}{\lambda}\right)^2 = \left(\frac{12.24\times10^{-10}}{0.8\times10^{-10}}\right)^2$$

$$V = \left(\frac{122.4}{8}\right)^2 = (15.3)^2 = 234.09 \text{ Volts}$$

2. What voltage must be applied to electron microscope to produceelectron of wavelength 0.5A° [Ans:599.2 V]

Sol : $\lambda = 0.5A^0 = 0.5\times10^{-10}$m, $V = ?$, $h = 6.62\times10^{-34}$J–S

$$\lambda = \frac{12.24}{\sqrt{V}}\overset{0}{\text{A}} = \frac{12.24\times10^{-10}}{\sqrt{V}}\text{m}$$

$$\sqrt{V} = \frac{12.24\times10^{-10}}{0.5\times10^{-10}}$$

$$V = \left(\frac{12.24}{0.5}\right)^2 = (24.48)^2$$

$$V = 599.2 \text{ V}$$

3.Using the formula $m = \frac{m_0}{\sqrt{1-v^2/c^2}}$ (where m_0 is the rest mass of the particle, Show that the velocity of the particle is 0.707 times the velocity of light (C) when the de-Broglie wavelength is equal to compton wavelength. **[Ans:0.707 C]**

Sol : de - Broglie wavelength associted with the particle $\lambda = \frac{h}{mv}$

$$\lambda = \frac{h}{mv}, \qquad \left(\because m = \frac{m_0}{\sqrt{1-\frac{v^2}{cH2}}} \right)$$

$$\lambda = \frac{h}{\frac{m_0}{\sqrt{1-v^2/c^2}}.v}$$

$$\lambda_d = \frac{h\sqrt{1-v^2/c^2}}{m_0 v} \longrightarrow ①$$

compton wavelength, $\lambda_c = \frac{h}{m_0 c} \longrightarrow ②$

from the given problem, de - Broglie wavelength = compton wavelength

$$\lambda_d = \lambda_c$$

$$\frac{h\sqrt{1-\frac{v^2}{c^2}}}{m_0 v} = \frac{h}{m.c}$$

$$\sqrt{1-\frac{v^2}{c^2}} = \frac{h}{c}$$

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

$$2\frac{v^2}{c^2} = 1 \Rightarrow \frac{v^2}{c^2} = \frac{1}{2} \Rightarrow \frac{v}{c} = \frac{1}{\sqrt{2}}$$

$$V \Rightarrow \frac{c}{\sqrt{2}} = \frac{c}{1.414} = 0.707\,C$$

4. What voltage must be applied to an electron microscope to produce electron of wavelengt 0.4A°. [Ans:936.36 Volts]

Sol : $\lambda = 0.4\text{A}^0 = 0.4 \times 10^{-10}$m, V = ?, $h = 6.62 \times 10^{-34}$J–S

$$\lambda = \frac{12.24}{\sqrt{V}}\overset{0}{A} = \frac{12.24\times10^{-10}}{\sqrt{V}}m$$

$$\sqrt{V} = \frac{12.24\times10^{-10}}{0.4\times10^{-10}}$$

$$V = \left(\frac{12.24}{0.4}\right)^2 = (30.6)^2 = 936.36 \text{ Volts}$$

5. 10 KV electron passed through thin film of metal for which plane spacing is 5.5×10^{-11}**m. What is the angle of deviation of the first order diffraction of maxima.** [Ans:12°48']

Sol : Given p.d = 10 kV = 1000V

plane spacing $d = 5.5 \times 10^{-11}$ m

for the first order n = 1

wavelength associated by the electron $\lambda = \frac{12.24}{\sqrt{V}}\overset{0}{A}$

$$= \frac{12.24}{\sqrt{10000}} = \frac{12.24}{100}$$

$$= 0.1224\ \overset{0}{A}$$

$$2d \sin\theta = n\lambda$$

$$\sin\theta = \frac{n\lambda}{2d} = \frac{1\times0.1224\times10^{-10}}{2\times5.5\times10^{-11}} = 0.1115$$

$$\theta = 6^0 24^1$$

Angle of deviation produced by electron beam $\delta = 2\theta$

$$= 2\times6^0 24^1 = 12^0 48^1$$

6. A microscope is used to locate the electron in an atom with in a distance of 0.2A°. Calcuate the uncertainity in the velocity of electron? [Ans: $3.64\times 10^7 ms^{-1}$]

Sol : Uncertainity in the position of electron, $\Delta x = 0.2\,\overset{0}{A}$

$$= 0.2\times10^{-10}m$$

Mass of the electron, $m = 9.1 \times 10^{-31}kg$

$$h = 6.62 \times 10^{-34}\,J.sec.$$

Uncertainity in the velocity of electron, $\Delta v = ?$

From uncertainity principle $\Delta x \times \Delta P = h$

$$\Delta x \times \Delta(mv) = h$$

$$\Delta x \times m\Delta v = h \Rightarrow \Delta v = \frac{h}{m \times Dx}$$

$$\therefore \Delta v = \frac{6.62\times10^{-34}}{9.1\times10^{-31}\times0.2\times10^{10}} = 3.64\times 10^7 ms^{-1}$$

7. If the uncertainity in the location of the particle is equal to de - Broglie wavelength Show the uncertainity in its velocityis equal to velocity of the particle. [Ans: $\Delta v = v$]

Sol : Given uncertainity in the position of particle,

$\Delta\lambda$ = de - Broglie wavelength λ

$$\Delta x = \frac{h}{mv}$$

From uncertainity principle, $\Delta x \times \Delta P = h$

$$\frac{h}{mv} \times (\Delta mv) = h$$

$$\frac{1}{mv} m\Delta v = 1$$

$$\frac{\Delta v}{v} = 1$$

$$\Delta v = v$$

8.Compare the uncertainities in the velocity of proton and electron confined in one nanometer box. **[Ans: 1837]**

Sol: Both the electron and proton are taken in nanometer box, the uncertainity in their position being equal.

$$(\Delta x)_e = (\Delta x)_p = 10^{-9}\text{ m}$$

from uncertainity principle, for electron

$$\Delta x_e \times \Delta P_e = h$$

$$\Delta x_e \times m_e \Delta v_e = h$$

$$m_e \Delta v_e = \frac{h}{\Delta x_e} \longrightarrow ①$$

for proton

$$\Delta x_p \times \Delta P_p = h$$

$$m_p \Delta v_p = \frac{h}{\Delta x_p} \longrightarrow ②$$

$$\frac{eq①}{eq②} \Rightarrow \frac{m_e}{m_p}\frac{\Delta V_e}{\Delta v_p} = \frac{\frac{h}{\Delta x_e}}{\frac{h}{\Delta x_p}}$$

$$\frac{\Delta v_e}{\Delta v_p} . \frac{m_p}{m_e} = \frac{1837 m_e}{m_e}$$

$$\frac{\Delta v_e}{\Delta v_p} = 1837$$

9.Find the min uncertainity in the position of electron when it is moving with a velocity of $6 \times 10^7\ ms^{-1}$ **[Ans: 0.121245×10^{-10}m]**

Sol : If the uncertainity in position of electron is minimum, the uncertainity in the momentum will be maximum from uncertainity priciple, $(\Delta x)_{min} \times (\Delta p)_{max} = h$

$$(\Delta x)_{min} \times m(\Delta v)_{max} = h$$

$$(\Delta x)_{min} = \frac{h}{m(\Delta v)_{max}} = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 6 \times 10^7}$$

$$= 0.121245 \times 10^{-10}\text{m}$$

7.9 SUMMARY:

1. de Broglie concept leads to uncertainty principle.The material particle exhibits particle nature as well a wave nature.

2. In 1927 Heigenburg uncertainty principle which is a direct consequence of the dual nature of matter.

3. According to uncertainity principle, "it is impossible for both position and momentum of particle can b measured simultaneously at anydesired degree of accuracy".

4. $\Delta P \times \Delta x \cong h$ where ΔP = uncertaity in finding the momentum of the particle.

   and Δx = uncertainity in finding the position of the particle.

5. . $\Delta E \times \Delta x \cong h$

   where ΔE = uncertainity in determining the energy of the particle in the interval.

6. $\Delta J \times \Delta \theta \cong h$

7. .Different forms of uncertainity principls as follows

$$\Delta P \times \Delta x \geq \frac{h}{4\pi} \text{ or } \frac{\hbar}{2} \quad = \quad 0.527 \times 10^{-34} \text{ J-S}$$

$$\text{(or)} \quad \Delta P \times \Delta x \geq \hbar \text{ or } \frac{h}{2\pi} \quad = \quad 1.054 \times 10^{-34} \text{ J-S}$$

7.10 KEY WORDS:

de Broglie concept, uncertainity principle, accuracy, gamma ray micrscope, hydrogen atom, diffraction.

7.11 SELF-ASSENESSMENT QUESTIONS:

1. State Heisenberg's uncertainty principle for i) position and momentum and ii) energy and time.

2. Explain the consequencies of uncertainty principle with regard to diffraction at a slit with regard to particle in a box.

3. Explain the consequencies of uncertainty relation and the gamma ray microscope experiment.

4. Starting from de Broglie wave concept, obtain Heisenberg's uncertainty principle

5. Explain the consequencies of uncertainty principle and its importance.

6. Explain theposition of electron in Bohr's orbit as a consequencies of uncertainty principle

EXCERCISE:

1.An electron has a speed of 4×10^5 with in the accuracy of 0.01%. Calculate the uncertainty in the position of electron? [Ans: 1.8186×1^{-5} m]

[Hint: Uncertainty in the velocity $\Delta v = \dfrac{0.01}{100} \times 4 \times 10^5$

$$\Delta v = 40\ \text{ms}^{-1}$$

$$\Delta P = m(\Delta v) \quad = 9.1 \times 10^{-31} \times 40\ \text{kg ms}^{-1}$$

$$\Delta P \times \Delta x = h \qquad \Delta x = \frac{6.62 \times 10^{-34}}{9.1 \times 40 \times 10^{-31}}\ ]$$

2. An electron of speed of 600ms^{-1} with an accuracy of 0.005%. Caculatethe uncertainty in position $\bar{e}$ [Ans:24.249×10^{-3}m]

[Hint: uncertainty in velocity $\Delta v = \dfrac{0.005}{100} \times 600 \quad = 0.030\ \text{ms}^{-1}$

$$\Delta P = m(\Delta v) \quad = 9.1 \times 10^{-31} \times 0.030\ \text{kg ms}^{-1}$$

$$\Delta P \times \Delta X = h \qquad \Delta x = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 0.030}\ ]$$

7.12 REFERENCE BOOKS:

1. Physics of Atom	Wher and Richards
2. Elements of Modern Physics	Patil
3. Unified Physics Vol-IV	Jai Prakash & Co
4. Quantum Mechanics	Mathaws and Venkatesan
5. Introduction to Quantum Mechanics	Pauling and Wilson

/*/*/*/

UNIT -2

LESSON-8

SCHROEDINGER WAVE MECHANICS

OBJECTIVES:

After the completion of this lesson the student will be able to

1) **Know about the Schroedinger's time independent & dependent wave equations.**
2) **Know about the significance of ψ ,Characteristics of a wavefunction & Postulates of Quantum mechanics**
3) **Know the energy levels of particle enclosed in one dimensional potential well of infinite height & three dimensional box**
4) **Understand the descrete enerfy levels of Quantum Harmonic Oscillator.**
5) **Know the Reflection at the step potential.**

STRUCTURE:

8.1 INTRODUCTION:

Sound waves, waves in strings are described by equations of Newtonian mechanics.The classical mechanics provides the correct explanation for the behaviour of macroscopic system.Light waves are described by the Maxwell's equations.In atomic systems , the classical mechanics fails to explain the microscopic system of particles due to uncertainty principle.Bohr's model failed to give a complex explanation of the behaviour of atomic system. A mathematical reformation using a wave function associated with matter waves was developed by Schrodinger. Schrodinger described the amplitude of matter waves by a complex quantity ψ (x,y,z,t) known as wave function. There are two types of wave equations namely,

1. Time independent wave equation
2. Time dependent wave equation

To describe the wave nature of the particle, a mathematical wave equations required called wave function ψ

8.2 SCHROEDINGER TIME INDEPENDENT WAVE EQUATION:

According to de-Broglie, a particle of mass m always associated with a wave of wavelength $\lambda=\frac{h}{mv}$

If the particle have wave properties, it is expected that there must be some sort of wave equation which describes the behaviour of the particle.

Let ψ be the wave displacement for the de-Broglie wave at any instant t, the differential equation for simple harmonic wave is represented as

$$\frac{\partial^2\psi}{\partial t^2} = V^2\left(\frac{\partial^2\psi}{\partial x^2}\right)(\text{along } x-\text{axis})$$

In three dimensional space

$$\frac{\partial^2\psi}{\partial t^2} = V^2\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right] \longrightarrow ①$$

It can be written as $\frac{\partial^2\psi}{\partial t^2} = V^2\nabla^2\psi \longrightarrow ②$

The solution of eq^n ② is given by

$$\psi = \psi_0 \sin \omega t \longrightarrow ③$$

where ψ_0 is the amplitude

Differentiating eqⁿ ③ we get,

$$\frac{\partial \psi}{\partial t} = \omega^2 \psi_0 \cos \omega t$$

$$\frac{\partial \psi^2}{\partial t^2} = -w^2 \psi_0 Sin \omega t$$

$$\frac{\partial \psi^2}{\partial t^2} = -w^2 \psi \longrightarrow ④$$

$$\therefore \omega = 2\pi\nu \quad \Rightarrow \quad 2\pi\frac{v}{\lambda} \quad (\because v = \nu\lambda \Rightarrow \nu = \frac{v}{\lambda})$$

$$④ \quad \Rightarrow \quad \frac{\partial^2 \psi}{\partial t^2} = -\left(2\pi\frac{v}{\lambda}\right)^2 \psi$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\frac{4\pi^2 v^2}{\lambda^2} \psi \longrightarrow ⑤$$

From ② & ⑤, $v^2 \nabla^2 \psi = \frac{-4\pi^2 v^2}{\lambda^2} \cdot \psi$

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0 \longrightarrow ⑥$$

$\because$ de-Broglie wavelength $\lambda = \frac{h}{mv}$

$$⑥ \quad \Rightarrow \quad \nabla^2 \psi + \frac{4\pi^2}{\left(\frac{h}{mv}\right)^2} \psi = 0$$

$$\nabla^2 \psi + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \longrightarrow ⑦$$

$\therefore$ Total energy of the particle E = PE + KE

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

$$\frac{1}{2}mv^2 = E - V \longrightarrow ⑧$$

$$mv^2 = 2(E-V) \Rightarrow m^2v^2 = 2m(E-V)$$

Substituting ⑧ in ⑦ $\Rightarrow \nabla^2\psi + \frac{4\pi^2 2m(E-v)}{h^2}.\psi = 0$

$$\nabla^2\psi + \frac{8\pi^2 m(E-v)}{h^2}\psi = 0 \longrightarrow ⑨$$

This is schroedinger's time independent wave equation

In quantum mechanics, $\hbar = \frac{h}{2\pi}$

$$⑨ \Rightarrow \nabla^2\psi + \frac{\frac{2m}{\left(\frac{h}{2\pi}\right)^2}(E-V)\psi}{} = 0$$

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \longrightarrow ⑩$$

For free particle in space, V = 0

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0 \longrightarrow ⑪$$

This is modified form of schroedinger's time independent wave equation. These equation are called study state schroedinger's equations. i.e., the state of a system doesnot change with time. Hence these are called time independent wave equation.

Multiplying eq. (10) by $\frac{\hbar^2}{2m} \Rightarrow \frac{\hbar^2}{2m}\nabla^2\psi + (E-V)\psi = 0$

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

$$\left(\frac{\hbar^2}{2m}\nabla^2 - V\right)\psi - E\psi$$

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi \longrightarrow ⑫$$

$\because \frac{-\hbar^2}{2m}\nabla^2 + V = H$, Hamiltonion operator

equation⑫ becomes as $H\psi = E\psi$

where E is the total energy of the system, and energy operator is H. Hence ψ is called wave function, E is called eigen value of energy, H is called eigen operator

8.3 SCHROEDINGER TIME DEPENDENT WAVE EQUATION:

Time dependent wave eq^n is used for describing the progessive waves applicable to the motion of free particles.

$\psi_r = \psi_0 e^{-i\omega t}$ where r is the position co-ordinate and t is the time co-ordinate

differenting equation ① with respect to t

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

$$\frac{\psi}{\partial t} = -i\omega\psi \qquad \because \omega = 2\pi\nu$$

$$\frac{\partial\psi}{\partial t} = -i2\pi\nu\psi \longrightarrow ② \qquad \because E = h\nu$$

$$\frac{\partial\psi}{\partial t} = -i2\pi\frac{E}{h}\psi \qquad \nu = \frac{E}{h}$$

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

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

$$\frac{\partial\psi}{\partial t} = -i\ \frac{E}{i^2\hbar}\psi$$

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

$$E\Psi = i\hbar\left(\frac{\partial\psi}{\partial t}\right) \longrightarrow ③$$

the time independent wave eqⁿ,

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

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E\Psi - V\Psi) = 0 \longrightarrow ④$$

From ③ & ④, $\nabla^2\psi + \frac{2m}{\hbar^2}\left(i\hbar\left(\frac{\partial\psi}{\partial t}\right) - v\psi\right) = 0$

$$\nabla^2\psi + \frac{-2m}{\hbar^2}\left(i\hbar\left(\frac{\partial\psi}{\partial t}\right) - v\psi\right) = 0$$

$$\frac{-\hbar^2}{2m}\nabla^2\psi = i\hbar\left(\frac{\partial\psi}{\partial t}\right) - v\psi$$

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

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + v\right)\psi = i\hbar\left(\frac{\partial\psi}{\partial t}\right) \longrightarrow ⑤$$

This is schroedinger's time dependent wave equation

$$\left(\frac{-\hbar^2}{2m}\nabla^2\psi + v\right) = \hat{H}$$, Hamiltonion operator

$$i\hbar\frac{\partial}{\partial t} = \hat{E}$$, energy value

eq^n ⑤ $\Rightarrow \hat{H}\ \psi = \hat{E}\ \psi$

8.4 SIGNIFICANCE OF ψ :

1) **In quantum mechanics, every physical state of the system must be described with a mathematical equation. This orbitary mathematical equation is called wavefunction ψ of the system.**

2) ψ has no direct physical meaning. According to max born, the paricle density $\psi\ \psi^* = |\psi|^2$

($\because \psi$ is imaginary, $\psi = x + iy$, $\psi^* = x - iy$, $\psi\ \psi^* = x^2 + y^2$)

which gives the propability in finding the particle in in unit volume

$\therefore$ The propability in finding particle in the volume

dx dy dz = $\psi\ \psi^*$dx dy dz

If the particle is somewhere in the space, the propability in finding the particle is unity.

i.e, $\iiint_v \psi\psi^* d\tau = 1$ i.e, $\int|\psi|^2 d\tau = 1$

This is called normalising condition

8.5 CHARACTERISTICS OF WAVE FUNCTION:

1) ψ must be finite for all values of x, y, z of the region.

2) ψ must be single valued at any instant

i.e, ψ (x, y, z) must have only one value at particular instant.

3) ψ must be continuous everywhere

4) The first derivative of the wave function w.r.t space i.e., $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ should also be continuous and single value.

5) **The wave function ψ must be normalizable**

i.e, $x, y, z \longrightarrow \pm\infty$, then $\psi = 0$

8.6 Postulates of Quantum mechanics :

1) **State of the system :-** Any physical system is completely described by mathematical wave function called ψ. The wave function ψ should be continuous, finite and sigle valued.

The wavefunction must vanish where the potential $V(x, y, z)$ is infinite

2) **Operators :-** It is a mathematical operation (differentiation, integration etc) applied to a function $f(x)$ or ψ when changes one function into another function i.e. $\hat{o}\, f(x) = g(x)$. here $\hat{o}$ is the operator.

3) **Eigen values of operator :-** When an operator operates an wave function ψ we can get real physical values. i.e, $\hat{o}\,\psi = a\,\psi$

Here $\hat{o}$ is an eigen operator. ψ is eigen function, a is eigen value.

Ex :-

$$\frac{d^2}{dx^2}(\sin x) = \frac{d}{dx}\cos x = -\sin x$$

$$\frac{d^2}{dx^2}(\sin x) = (-1)\sin x$$

$$\hat{o}(\sin x) = a \sin x \qquad \therefore a = -1 \text{ eigen value}$$

$$\hat{o} = \frac{d^2}{dx^2} = \text{Eigen operator}$$

4) **Propablistic outcome of measurments :**

If G is the physical quantity or operator, then its exceptation value

$$\langle G \rangle = \frac{\int_{-\infty}^{+\infty} \psi^* G \psi d\tau}{\int_{-\infty}^{+\infty} \psi\psi^* d\tau} \qquad \because \int_{-\infty}^{+\infty} \psi\psi^* d\tau = 1 \Rightarrow \langle G \rangle = \int_{-\infty}^{+\infty} \psi^* G \psi d\tau$$

8.7 Types of operators : It is a mathematical operation applied to a function $f(x)$ or ψ which changes the function into another function $g(x)$

a) Energy Operator :-Schroedinger's time independent wave equation $\left(-\frac{\hbar^2}{2m}\nabla^2+V\right)\psi=E\psi \longrightarrow$ ①

$H\psi = E\psi$ where the operator corresponding to the energy is called Hamiltonion operator H.

$$\text{i.e., } H = \left(-\frac{\hbar^2}{2m}\nabla^2+V\right) \longrightarrow ②$$

time dependent wave equation $\left(-\frac{\hbar^2}{2m}\nabla^2+V\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$

$$\Rightarrow H\psi = \left(i\hbar\frac{\partial\psi}{\partial t}\right)$$

$$\text{Energy operator } H = \hat{E} = i\hbar\frac{\partial}{\partial t} \longrightarrow ③$$

b) Momentum Operator $\hat{p}$**:** K.E operator $= \frac{-\hbar^2}{2m}\nabla^2\psi$

$$\text{K.E} = \frac{P^2}{2m}\psi \Rightarrow \frac{-\hbar^2}{2m}\nabla^2\psi$$

$$P^2 = -\hbar^2\nabla^2$$

$$P^2 = \frac{\hbar^2}{i^2}\nabla^2$$

$$\hat{P} = \frac{\hbar}{i}\nabla \longrightarrow ④$$

$$\hat{P} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\hat{P}_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad \hat{P}_y = \frac{\hbar}{i}\frac{\partial}{\partial y} \qquad \hat{P}z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

c) Velocity operator :- $\hat{P} = \frac{\hbar}{i}\nabla$

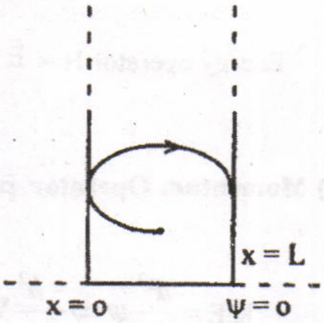
$$m\bar{v} = \frac{\hbar}{i}\nabla \qquad \hat{v} = \frac{\hbar}{mi}\nabla$$

8.8 Particle in one dimensional box or energy levels of particle enclosed in one dimensional potential well of infinite height :-

Condider a particle of mass m moving between two rigid walls of one dimensional box of infinite height. Due to the collision between the walls, the force on the particle changes.

The P.E. assumed to be zero between the limits O & L and $x \le 0$ and $x \ge 0$ The schrodinger's equation for the particle along x - axis

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E-V)\,\psi = 0$$



For a free particle V=0

$$\therefore \frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}E\,\psi = 0 \longrightarrow ①$$

$$\text{Put } \frac{8\pi^2 m}{h^2}E = K^2 \longrightarrow ②$$

$$\text{From ① \& ②} \quad \frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0 \longrightarrow ③$$

It is the differential equation of the particle executing SHM. The solution of ③ is

$$\psi = A\sin kx + B\cos kx \longrightarrow ④$$

where A & B are boundary constants

From boundary conditions, at $x = 0,\ \psi = 0 \longrightarrow$ ⑤a

at $x = L,\ \psi = 0 \longrightarrow$ ⑤b

Substitute ⑤a in eqⁿ ④ $\Rightarrow 0 = A\sin k(o) + B\cos k(o)$

$$= A(o) + B(1)$$

$$B = 0$$

Substitute these value in ④ $\Rightarrow \psi = A \sin kx$ $\longrightarrow$ ⑥

Substitute ⑤b in ⑥ $\Rightarrow 0 = A \sin kL$

$\because A \neq 0 \ \text{Sin}\, kL = 0$

$$kL = n\pi \Rightarrow k\frac{n\pi}{L} \longrightarrow ⑦$$

where n = 1, 2, 3 ----------

$\therefore$ equation ⑥ $\Rightarrow \psi = A \sin \frac{n\pi}{L} x$ $\longrightarrow$ ⑧

Substitute equation ⑦ in ② $\Rightarrow$ $\frac{8\pi^2 m}{h^2} E = \frac{n^2\pi^2}{L^2}$

$$E_n = \frac{n^2h^2}{8mL^2} \longrightarrow ⑨$$

$$E_n = \frac{n^2 4\pi^2\left(\frac{h}{2\pi}\right)^2}{8mL^2}$$

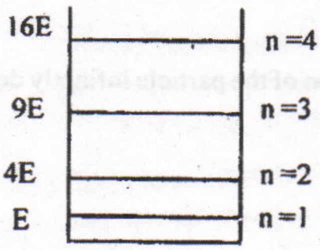
$$E_n = \frac{\pi^2\hbar^2}{2mL^2} n^2 \longrightarrow ⑩$$

If $n = 1$, $E_1 = \frac{\pi^2\hbar^2}{2mL^2} . 1 = E$

If $n = 2$, $E_2 = 4\left(\frac{\pi^2\hbar^2}{2mL^2}\right) = 4E$

If $n = 3$, $E_3 = 9E =$ -------------------------

Energylevel Diagram : In one dimensional box, the energies of a particle is in ratio 1:4:9 i.e, the energies are quantised and energy levels are shown below.



From the equation ⑧, $\psi = A \sin \frac{n\pi}{L} x$

By appling normalising condition, the value of A can be calculated. i.e, $\int_0^L |\psi(x)|^2 dx = 1$

$$\int_0^L A^2 \text{Sin}^2 \frac{n\pi}{L} x \, dx = 1$$

$$\frac{A^2}{2} \int_0^L 2\text{Sin}^2 \frac{n\pi}{L} x \, dx = 1$$

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

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

$$\frac{A^2}{2}\left[\left((x)_0^L\right) - 0\right] = 1$$

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

$$A = \sqrt{\frac{2}{L}}$$

∴ equation ⑧ $\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$

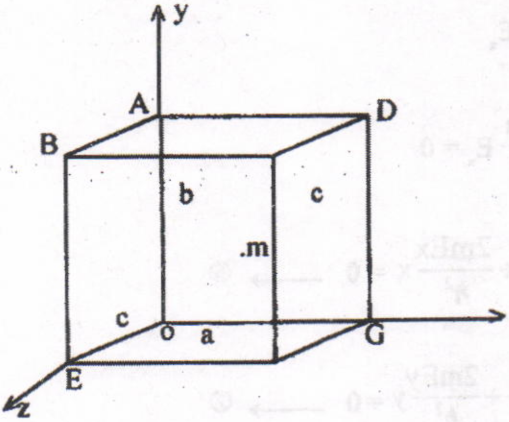
∴ The wavefunction $\psi = \sqrt{\frac{2}{L}} \text{Sin} \frac{n\pi}{L} x$

This equation represents the wavefunction of the particle infinetly deep potential well

8.9 PARTICLE IN THREE DIMENSIONAL BOX:

Consider a particle of mass m enclosed in a rectangular box of sides a, b, c respectively parallel to x, y, z axis as shown in the figure.

The particle can move freely with the region $o<x<a$, $o<y<b$, $o<z<c$ i.e, the particle can move freely inside the box.



∵ The potential V = 0 inside the box, the schroedinger's equation for a particle is given by

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2mE}{\hbar^2}\psi=0 \longrightarrow ①$$

$$\because \psi(x,y,z)=X(x),Y(y),Z(z)=xyz \longrightarrow ②$$

where X(x), Y(y), Z(z) are functions of their respective coordinates alone.

From equation ① and ②, $\frac{\partial^2}{\partial x^2}(XYZ)+\frac{\partial^2}{\partial y^2}(XYZ)+\frac{\partial^2}{\partial z^2}(XYZ)+\frac{2mE}{\hbar^2}\psi=0$

($\therefore \psi = xyz$)

$$YZ\frac{\partial^2 x}{\partial x^2}+XZ\frac{\partial^2 y}{\partial y^2}+XY\frac{\partial^2 z}{\partial z^2}+\frac{2mE}{\hbar^2}XYZ=0$$

Divide by XYZ $\Rightarrow \frac{1}{X}\frac{\partial^2 x}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 z}{\partial z^2}+\frac{2mE}{\hbar^2}=0$

Put $\frac{1}{X}\frac{\partial^2 x}{\partial x^2} = K_x, \ \frac{1}{Y}\frac{\partial^2 y}{\partial y^2} = K_y, \ \frac{1}{Z}\frac{\partial^2 z}{\partial z^2} = K_z$.

and $E = E_x + E_y + E_z$

Substitute equation ④ in ② $\Rightarrow K_x + K_y + K_z + \frac{2m}{\hbar^2}(E_x + E_y + E_z) \longrightarrow$ ⑤

Along X – axis, $K_x = \frac{-2m}{\hbar^2}E_x$

$$K_x + \frac{2m}{\hbar^2}E_x = 0$$

$$\frac{1}{X}\frac{\partial^2 x}{\partial^2 x^2} + \frac{2mEx}{\hbar^2}x = 0 \longrightarrow \text{⑥}$$

Similarly along y axis, $\frac{\partial^2 y}{\partial y^2} + \frac{2mEy}{\hbar^2}y = 0 \longrightarrow$ ⑦

Similarly along Z- axis, $\frac{\partial^2 z}{\partial z^2} + \frac{2mEz}{\hbar^2}z = 0 \longrightarrow$ ⑧

The solution for the eq^n ⑥ is obtained by

$$x = A\sin(Bx + C) \longrightarrow \text{⑨}$$

where A, B and C are boundary constants.

Now, the boundary conditions are at $x = 0, x = 0 \longrightarrow$ ⑩a

at $x = a, x = 0 \longrightarrow$ ⑩b

Applying equation ⑩a to equation ⑨

$$0 = A\sin[B(0) + C]$$

$$0 = A\sin C$$

$$A \neq o, \text{ i.e, } \sin C = 0 \quad \Rightarrow \quad C = 0$$

equation ⑨ $\Rightarrow$ $x = A\sin Bx \longrightarrow$ ⑪

Applying boundary condition ⑪b to the above equation ⑨b

$$0 = A \sin Ba$$

$$\because A \neq o, \sin Ba = 0$$

$$Ba = n\pi \Rightarrow B = \frac{n\pi}{a}$$

Sub these value in equation ⑨ we get

$$x = A \sin \frac{n\pi}{a} x \longrightarrow ⑫$$

According to Born approximation, the propability in finding the particle along x - axis at any point is $X\times|^2$

By applying the normalising condition,

$$\int_0^a |X\times|^2 dx = 1$$

$$\int_0^a A^2 \text{Sin}^2 \frac{n\pi}{a} x dx = 1$$

$$\frac{A^2}{2} \int_0^a 2\text{Sin}^2 \frac{n\pi}{a} x.dx = 1$$

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

$$\frac{A^2}{2}[a - 0] = 1 \Rightarrow \frac{A^2}{2} a = 1 \qquad A^2 = \frac{2}{a} \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\therefore \text{eq}^n ⑨ \Rightarrow \qquad X = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$

Similarly $$Y = \sqrt{\frac{2}{b}} \sin \frac{n\pi}{b} y \longrightarrow ⑬$$

$$Z=\sqrt{\frac{2}{c}}\ \sin\ \frac{n\pi}{c}z$$

The complete wave function is obtained by

$$\psi = XYZ = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}}\sqrt{\frac{2}{c}}\ \text{Sin}\ \frac{n_x\pi}{a}x.\ \text{Sin}\ \frac{n_y\pi}{b}y.\ \text{Sin}\ \frac{n_z\pi}{c}z$$

$$\psi = \frac{2^{3/2}}{\sqrt{abc}}\text{Sin}\ \frac{n_x\pi}{a}x.\ \text{Sin}\ \frac{n_y\pi}{b}y.\ \text{Sin}\ \frac{n_z\pi}{c}z \qquad \longrightarrow ⑭$$

Substitute the value of x of equation ⑬ we get

$$\frac{\partial^2 x}{\partial x^2}+\frac{2mE_x}{\hbar^2}x=0\ (\text{from ⑥})$$

$$\frac{\partial^2}{\partial x^2}\left(\sqrt{\frac{2}{a}}\sin\frac{n_x\pi}{a}x\right)+\frac{2mE_x}{\hbar^2}x=0$$

$$-\left(\frac{n_x\pi}{a}\right)^2\left(\sqrt{\frac{2}{a}}\sin\frac{n_x\pi}{a}x\right)+\frac{2mE_x}{\hbar^2}x=0$$

$$-\left(\frac{n_x\pi}{a}\right)^2x+\frac{2mE_x}{\hbar^2}x=0$$

$$\frac{2mE_x}{\hbar^2}x=\left(\frac{n_x\pi^2}{a}\right)x$$

$$E_x=\frac{\pi^2\hbar^2}{2ma^2}n_x^2=\frac{\pi^2h^2}{8\pi^2ma^2}n_x^2=\frac{h^2}{8ma^2}n_x^2$$

Similarly $E_y=\frac{h^2}{8mb^2}n_y^2$ and $E_z=\frac{h^2}{8mc^2}n_z^2$ ----------⑮

Adding $$E = E_x + E_y + E_z = \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right]$$

$$E = \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right] \text{ ----------------------------- ⑯}$$

In case of simple cube, $a = b = c$

$$E = \frac{h^2}{8m}\left(n_x^2 + n_y^2 + n_z^2\right) \longrightarrow ⑰$$

Degeneracy : When there is only one wave function (Eigen function) corresponding to a particular eigen value, the level is known as nondegenegrate.

But there are number of wavefunctions corresponing to single eigen value, the level is known as degenerate.

For non-degenerate levels $n_x = n_y = n_z = 1$ or 2 or 3 ...... etc

∴ The energy levels of two states of particle in cubical box is shown in the fingure(8.8.1)

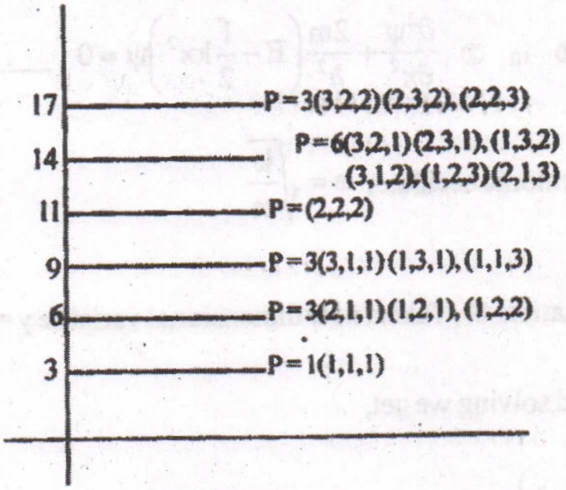


FIG 8.9.1

8.10 QUANTUM HARMONIC OSCILLATOR:

When a body (Oscillator) like atom of mass m is set into motion subjected to restoring force F

Then $F \propto x$

$F = -Kx$

Then the P.E of the oscillator = workdone in displacing from 0 to x is given by

$$V(x) = -\int_0^x F dx = -\int_0^x -kx dx$$

$$V(x) = \frac{kx^2}{2} = \frac{1}{2}Kx^2$$

$$V(x) = \frac{1}{2}Kx^2 \longrightarrow ①$$

If 'a' is the amplitude of the oscillator. Since the dimension of the oscillator is very small, the oscillator assumed to posses wave properties. From the wave mechanics, Schoedinger's equation for the harmonic oscillator is given by

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

Substitute equation ① in ② $\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0 \longrightarrow ③$

The frequency of the harmonic oscillator $\omega = \sqrt{\frac{k}{m}}$

Inorder to solve the equation ③, Take a new dimensional variable $y = \sqrt{\frac{m\omega}{\hbar}}\,x \longrightarrow ④$

Sub these value in ③ and solving we get,

$$\frac{\partial^2\psi}{\partial y^2} + \left(\frac{2E}{\hbar\omega} - y^2\right)\psi = 0 \longrightarrow ⑤$$

Put $\frac{2E}{\hbar\omega} = \alpha \longrightarrow ⑥$

$$\frac{\partial^2\psi}{\partial y^2}+\left(\propto -y^2\right)\psi=0 \longrightarrow ⑦$$

This is generalised differential wave equation of harmonic oscillator and also it is in the form of differential equation of Hermite polynomial $H_n(y)$

The soluction of the equation ⑦ is given by

$$\psi_n = A_n\, e^{y^2/2}\; H_n(y) \longrightarrow ⑧$$

Then the wavefunction ψ_n corresponding to harmonic oscillator must also satisfy the above condition for the values

$$\propto = 2n+1 \longrightarrow ⑨ \text{ where } n = 0, 1, 2 \text{----}$$

$\therefore$ From eq^n ⑥ and⑨, $\frac{2E}{\hbar\omega} = 2n+1$

$$E = \frac{\hbar\omega}{2} = 2n+1$$

$$\therefore\ E = E_n \Rightarrow \quad E_n = \frac{\hbar\omega}{2} = (2n+1) \longrightarrow ⑩$$

$$E_n = \frac{h}{2\pi}\,\frac{2\pi\nu}{2}\,(2n+1)$$

$$E_n = \frac{h\nu}{2}\,(2n+1)$$

$$E_n = h\nu\,\left(n+\frac{1}{2}\right) \longrightarrow ⑪$$

The energy levels of harmonic oscillator is given below.

If $n = 0$, $E_0 = \frac{1}{2}\hbar\omega$ or $\frac{h\nu}{2}$

If $n = 1$, $E_1 = \frac{3}{2}\hbar\omega$ or $\frac{3h\nu}{2}$

If $n = 2$, $E_2 = \frac{5}{2}\hbar\omega$ or $\frac{5h\nu}{2}$

The difference between any two sucessive energy levels is $\frac{3}{2}\hbar\omega - \frac{1}{2}\hbar\omega = \hbar\omega = h\nu$

$\therefore E_0 = \frac{1}{2}\hbar\omega$ is the energy at the lowest state which is called zero point energy. The energy levels of harmonic ascillator at different states of n, we get discrete values of energy and equal to odd multiples of $(1) \times \frac{1}{2}\hbar\omega$ or $3 \times \frac{1}{2}\hbar\omega$ or $\frac{1}{2}h\nu$

There by the energy levels are said to be quantised and shown in figure(8.9.1)

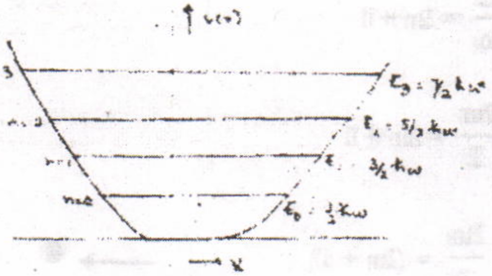


FIG 8.10.1

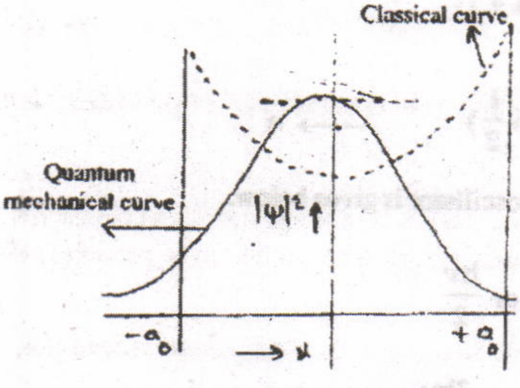


FIG 8.10.2

The propability density of the particle (oscillator) for the state n = 1 is shown in figure(8.9.2).

In case of quantum oscillator, the propanility density $|\psi|^2$ is maximum at the middle while for the classical oscillator, the propability is minimum at the middle. But there is small propability outside the classcal region for the quantum mechanical harmonic oscillator.

8.12. REFLECTION AT THE SINGLE STEP BARRIER (OR) REFLECTION AT STEP POTENTIAL:

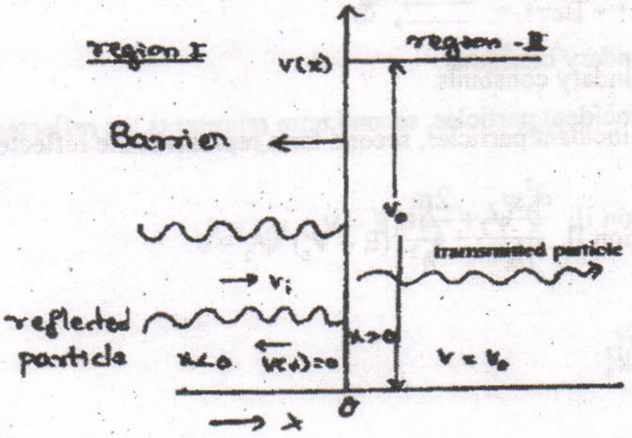


FIG 8.12.1

The step potential function can be defined as

region I, $V(x) = 0$ at $x < 0$

region II $V(x) = V_0$ at $x \geq 0$

When the beam of particles having energy E passes from region I to region II there will be

Case (i) :- When energy of the incident particles greater than potential barrier of height V_0 i.e., $E>V_0$:-

If $E>V_0$ according to classical mechanics, all the particles cross the barrier but according to quantum mechanics, due to the wave nature of particles, there are some particles reflecting from the surface of the step potential.

∴ Applying Schroedinger's wave equation to the first and second regions,

In region I :-

$$\frac{\partial^2\psi_1}{\partial x^2}+\frac{2mE}{\hbar^2}\psi_1=0$$

Put $k_1^2 = \frac{2mE}{\hbar^2}$

$$\frac{\partial^2 \psi_1}{\partial x^2} + k_1^2 \psi_1 = 0 \longrightarrow ①$$

The solution of equation ① is fiven by

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \longrightarrow ②$$

where A & B are boundary constants.

First term represents incident particles, second term represents the reflected particles.

Region II : In region II, $\frac{\partial^2 \psi_2}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi_2 = 0$

Put $\frac{2m}{\hbar^2}(E - V_0) = k_2^2$

$$\frac{\partial^2 \psi_2}{\partial x^2} + k_2 \psi_2 = 0 \longrightarrow ③$$

The solution of eq^n ③ is given by

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \longrightarrow ④$$

As t[illegible] no reflected wave in region II, the second term is neglected.

$$\therefore \psi_2 = Ce^{ik_2x} \longrightarrow ⑤$$

By applying t[illegible]y conditions, at the surface of step potential

$$(\psi_1)_{x=0} = (\psi_2)_{x=0} \longrightarrow ⑤a$$

$$\left(\frac{\partial \psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial \psi_2}{\partial x}\right)_{x=0} \longrightarrow ⑤b$$

Substitute equation ⑤a in ② & ⑤ $\Rightarrow$ $Ae^{ik_1(0)} + Be^{-ik_1(0)} = Ce^{-ik_2(0)}$

$$A + B = C \longrightarrow ⑤$$

From the equation ⑤b ⇒ $\left(\frac{\partial \psi_1}{\partial x}\right)_x = 0 \quad \left(\frac{\partial \psi_2}{\partial x}\right)_{x=0} = 0$

$$\frac{\partial}{\partial x}\left[Ae^{ik_1x} + Be^{-ik_1x}\right]_{x=0} = \frac{\partial}{\partial x}\left[Ce^{ik_2x}\right]_{x=0}$$

$$\left[ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}\right]_{x=0} = \left[ik_2Ce^{ik_2x}\right]_{x=0}$$

$$ik_1A - ik_1B = ik_2C \Rightarrow k_1(A-B) = K_2C$$

$$A - B = \frac{k_2}{k_1}C \longrightarrow ⑦$$

$$\frac{A+B = C}{}$$

From the equation⑥ and ⑦ ⇒ $2A = C\left[1 + \frac{k_2}{k_1}\right]$

$$2A = C\left[\frac{k_1+k_2}{k_1}\right]$$

$$C = \left[\frac{2k_1}{k_1+k_2}\right]A \longrightarrow ⑧$$

Substitute equation ⑧ in ⑥ ⇒ $A + B = C$

$$A + B = \left[\frac{2k_1}{k_1+k_2}\right]A$$

$$B = \left[\frac{2k_1}{k_1+k_2} - 1\right]A$$

$$B = \left[\frac{2k_1 - k_1 - k_2}{k_1+k_2}\right]A$$

$$B = \left[\frac{k_1 - k_2}{k_1 + k_2}\right]A \longrightarrow ⑨$$

where B and C are amplitudes of reflected and transmitted waves and A is the amplitude of the incident wave.

in equation ②, $e^{iK_1x} = \psi_{1i}$ represent the incident wave

$e^{iK_1x} = \psi_{1r}$ represent the reflected wave

∴ Propability density of the incident particles $|\psi_1 i^2|\, V_{1i}$ = Group velocity of incident particles

∴ Flux of incident particles $S_i = |\psi_1 i|\, V_{1i}$

Since $\psi_1 i = Ae^{ikx}$, $|\psi_1 i^2| = |\psi_1 i\ \psi_1 i^*| = |A^2 e^{ikx} X A^2 e^{-ikx}| = A^2$

$S_i = A^2 V_{1i}$

$$\because \frac{\lambda}{2\pi} = \frac{\hbar}{\sqrt{2mE}}$$

$$k_1 = \frac{2\pi}{\lambda}, \frac{\lambda}{2\pi} = \frac{\hbar}{\sqrt{2mE}}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2m - \frac{1}{2}mv_1 i^2}}{\hbar^2}$$

$$k_1 = \frac{\sqrt{mv_1 i^2}}{\hbar} = \frac{mv_1 i}{\hbar}$$

$$v_1 i = \frac{k_1\hbar}{m}$$

$$S_i = A^2 k_1 \frac{\hbar}{m} \longrightarrow ⑩$$

Reflected flux $S_r = |B|^2 V_1 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 A^2 \frac{k_1\hbar}{m}$

$$S_r = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 S_i \longrightarrow ①$$

Similarly transmitted flux, $S_t = |C^2|V_t = \left|\frac{2k_1}{k_1 + k_2}\right|^2 \left[|A|^2 \frac{k_1\hbar}{m}\right]$

$$S_t = \frac{4k_1k_2}{(k_1 + k_2)^2}|A|^2\left(\frac{k_1\hbar}{m}\right)$$

$$S_t = \frac{4k_1k_2}{(k_1 + k_2)^2} S_i$$

Adding ① & ② $S_r + S_t = \left[\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 + \frac{4k_1k_2}{(k_1 + k_2)^2}\right] S_i$

$$S_r + S_t = \left[\frac{k_1^2 + k_2^2 - 2k_1k_2 + 4k_1k_2}{(k_1 + k_2)^2}\right] S_i$$

$$S_r + S_t = \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2} S_i$$

$$S_r + S_t = S_i \longrightarrow ③$$

If $E > E_0$, Some particles are reflected and remaining are transmitted

(∴ no reflected particles in the region II)

$$\psi_2 = Ce^{k_2x}$$

Applying boundary conditions, ψ_1 at $x = 0$; ψ_2 at $x = 0$

$$AB^0 + Be^0 = Ce^0$$

$$A + B = C \longrightarrow ③$$

From second bocmdary condition, $\left(\frac{\partial\psi_2}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{x=0}$

$$ik_1Ae^0{}_1 - ik_1Be^0 = k_2Ce^0$$

$$ik_1(A-B) = K_2C$$

$$(A-B) = \frac{k_2}{ik_1}C \longrightarrow ④$$

$$A+B=C$$

Sub ③ in ④ $\Rightarrow \frac{k_1}{ik_2}(A+B)$

$$ik_1(A-B) = k_2A + k_2B$$

$$ik_1A - ik_1B = k_2A + k_2B$$

$$ik_1A - k_2A = ik_1B + k_2B$$

$$(ik_1 - k_2)A = (ik_1 + k_2)B$$

$$B = \left(\frac{ik_1-k_2}{ik_1+k_2}\right)A \longrightarrow ⑤$$

by solving $C = \left(\frac{2ik_1}{ik_1+k_2}\right)A \longrightarrow ⑥$

Reflected intensity $S_r = |B|^2V$

$$S_r = \left|\frac{ik_1-k_2}{ik_1+k_2}\right|^2 VA^2$$

Transmitted intensity $S_t = |C|^2V$

$$S_t = \left|\frac{2ik_1}{ik_1+k_2}\right|^2 VA^2$$

$$\text{Reflection coefficient } R = \frac{\text{Magnitude of reflected flux}}{\text{Magnitude of incident flux}} = \frac{\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 Si}{Si}$$

$$= \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \quad -$$

$$\text{Similarly transmission coefficient } T = \frac{\text{Magnitude of reflected flux}}{\text{Magnitude of incident flux}}$$

$$R = \left[\frac{\frac{4k_1k_2}{k_1+k_2}}{Si}\right] Si$$

$$R = \frac{4k_1k_2}{(k_1+k_2)^2} \quad \longrightarrow ①$$

$$\Rightarrow R + T = 1$$

This is characterstic quantum mechanical effect.

Case (ii) : When energy of incident particles less than potential barrier ($E<V_0$)

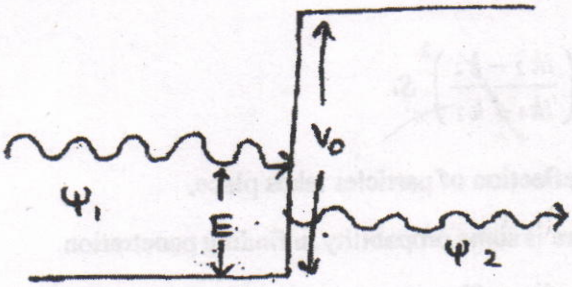


FIG 8.12.2

Acoriding to classcal mechanics, if $E<V_0$, all the particles should be refleted into the region I, But according to quantum mechanics the Schroedinger's wave equation in the first region is

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2mE}{\hbar^2}\psi=0$$

The solution of the above eq^n $\psi = Ae^{ik_1x}+Be^{-ik_1x} \longrightarrow$ ①

The Schroedinger's equation in the second region

$$\frac{\partial^2\psi_2}{\partial x^2}+\frac{2mE}{\hbar^2}(V_0-E)\psi_2=0$$

The solution is given by $\psi_2 = Ce^{k_2x}+0$

By applying boundary conditions A+B=C

ik1A - ik1B = k2C

$$\text{Solving } B=\left(\frac{ik_2-k_2}{ik_1+k_2}\right)A$$

$$C=\left(\frac{2ik_1}{ik_1+k_2}\right)A$$

$$S_i=\vartheta|A|^2$$

$$Sr=\vartheta|B|^2=\vartheta\left(\frac{ik_2-k_2}{ik_1+k_2}\right)^2|A|^2$$

$$Sr=\vartheta\left(\frac{ik_2-k_2}{ik_1\cancel{+}k_2}\right)^2 S_i$$

i.e. there is no complete reflection of particles takes place,

i.e , Eventhough E<V_0 there is some propability in finding penetration.

It is the application of tunneling effect.

8.13 SOLVED PROBLEMS:

1)The operator on the wavefunction ψ is $\frac{d^2}{dx^2}$. Find the eigen value of a function $\psi = e^{2x}$

[Ans:4]

Sol : $H\psi = E\psi$

$$H = \frac{d^2}{dx^2}; \qquad \psi = e^{2x}$$

$$\text{i.e., } \frac{d^2}{dx^2}(e^{2x}) = \frac{d}{dx}(2e^{2x})$$

$$= 4\,(e^{2x})$$

$$\frac{d^2}{dx^2}(e^{2x}) = (e^{2x})$$

$$H\psi = E\psi$$

$\therefore$ Eigen value of the function is $E = 4$

2.Find the least energy of the $\bar{e}$ moving in one dimensional infinetly high potential box of width 1A⁰ given mass of the $\bar{e}$, $m = 9.1 \times 10^{-31}$kg. [Ans:9.4056 × 10^{-4} mev]

Sol : Given $m = 9.1 \times 10^{-31}$ kg

$h = 6.62 \times 10^{-34}$J – sec

Length of the width $L = 1A^0 = 1 \times 10^{-10}$m

For the first level, $n = 1$

$\therefore$ In one dimentional potential well the energy

$$E_n = \frac{n^2h^2}{8mL^2} \Rightarrow \frac{1^2 \times (6.62\times10^{-34})^2}{8\times9.1\times10^{-31}\times(1\times10^{-10})^2} \qquad \because 1\,eV = 1.6\times10^{-19}J$$

$$E_n = \frac{0.60198\times10^{-17}}{1.6\times10^{-13}}Mev \qquad 1\,J = \frac{1}{1.6\times10^{-13}}Mev$$

$$E_n = 0.37623 \times 10^{-4}\,Mev$$

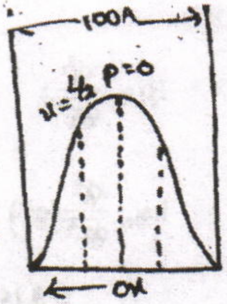
2. Calculate energy of an $\bar{e}$ moving in one dimensional infinite potential well of width of 2A⁰

Sol : Given $m = 9.1 \times 10^{-31}$ kg

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

Length of the width $L = 2A^0$

$$= 2 \times 10^{-10}m$$



$x = L/2$

$= 50A^0$

$= 5 10^{-1^0}$,

For first level n = 1

$$E_n = \frac{n^2h^2}{8mL^2} = \frac{1\times(6.62\times10^{-34})}{8\times9.1\times10^{-31}\times(2\times10^{-10})^2} = 1.5049\times10^{-17}$$

J

$$E_n = \frac{1.5049\times10^{-17}}{1.6\times10^{-13}}$$

$$E_n = 9.4056\times10^{-4}\ \text{Mev}$$

3. A particle is moving one dimensional well of infinite height of width 100A°. **Calculate the propability of finding the particle with in the interval of 10A° at the centre of the box when it is in the state of least energy.** **[Ans:0.2]**

Sol : Given length of the box $L = 100A^0$

$$= 100\times10^{-10}m$$

$$L = 10^{-8}m$$

$$\Delta x = 10A^0 = 10\times10^{-10}m = 10^{-9}m$$

wavefunction of particle enclosed in a box $\psi = \sqrt{\frac{2}{L}}\text{Sin}\left(\frac{n\pi}{L}\right)x;$ n = 1

$$= \sqrt{\frac{2}{10^{-8}}}\text{Sin}\left(\frac{1\times3.14}{10^{-8}}\right)\frac{10^{-8}}{2}$$

$$\psi = \sqrt{\frac{2}{10^{-8}}}\text{Sin}\frac{\pi}{2} = \sqrt{\frac{2}{10^{-8}}}$$

$$\psi = \frac{1.414}{10^{-4}} = 1.414\times10^{4}$$

Propability in finding the particle in the region 10A°

$$P = |\psi|^2_x$$

$$P = \left(\frac{\sqrt{2}}{10^{-4}}\right)^2 10^{-9}$$

$$P = \frac{2}{10^{-8}} \times 10^{-9} = 0.2$$

4. What is the lower energy of neutron of mass 1.67×10^{-27}kg confined to move along the edge of an infinite box of length 10^{-14}m [Ans:2.05 Mev]

Sol : Given $m = 1.67 \times 10^{-27}$ kg

$L = 10^{-14}$m

$h = 6.62 \times 10^{-34}$ J–sec

For lowest energy n = 1

$$\therefore E_n = \frac{n^2h^2}{8mL^2}$$

$$= \frac{1^2 \times (6.62 \times 10^{34})^2}{10^{-27} \times 8 \times 1.67 \times (10^{-14})^2}$$

$$E_n = 3.2802 \times 10^{-13}\,\text{J} = \frac{3.20802 \times 10^{-13}}{1.6 \times 10^{-13}} Mev = 2.05\ \text{Mev}$$

5. A particle is moving in one dimensional potential box of infinite height of width 25A°. Calculate the propability in finding the particle with in an interval of 5A° at the centre of the box when it is in the state of least energy. [Ans:2.05 Mev]

Sol : $L = 25A^0 = 25 \times 10^{-10}$m

$\Delta x = 5A^0 = 5 \times 10^{-10}$m

n = 1

w.k.t wavefunction of a particle enclosed

$$\psi = \sqrt{\frac{2}{L}} \text{Sin}\left(\frac{n\pi}{L}\right)x$$

For free particle in space, $V = 0$

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$$

$$\frac{-h}{2m}\nabla^2 + V = H$$, Hamiltonion operator

4. Schrodinger's time dependent wave equation

$$\left(\frac{-\hbar^2}{2m}\nabla_\psi^2 + v\right)\psi = i\hbar\left(\frac{\vartheta\psi}{\partial t}\right)$$

$\left(\frac{-\hbar^2}{2m}\nabla_\psi^2 + v\right) = \hat{H}$, Hamiltonion operator $\qquad i\hbar\frac{\partial}{\partial t} = \hat{E}$, energy value

5. In quantum mechanics, every physical state of the system must be described with a mathematical eq^n. This orbitary mathematical eq^n is called wavefunction ψ of the system.

6. ψ has no direct physical meaning. According to max born, the paricle density $\psi\ \psi * = |\psi|^2$

K.E operator = $\frac{-\hbar^2}{2\mu}\nabla_\psi^2$ 7.

energy operator $H = \hat{E} = i\hbar\frac{\partial}{\partial t}$

Momentum Operator $\hat{P} = \frac{\hbar^2}{i^2}\nabla$

Velocity operator $\hat{v} = \frac{\hbar}{mi}\nabla$

7. Eq^n represents the wavefunction of the particle infinetly deep potential well $\qquad \psi = \sqrt{\frac{2}{L}}$ in $\frac{n\pi}{L}x$

8. generalised differential wave equation of harmonic oscillator $\frac{\partial^2\psi}{\partial y^2} + (\propto - y^2)\psi = 0$

8.14 KEY WORDS:

wave function, wave equations, Hamiltonion operator, energy value, normalising condition, operator, three dimensional box, Degeneracy, harmonic oscillator.

8.15 SELF- ASSESSMENT QUESTIONS:

1. **Derive Schroedinger time independent and time dependent equations for matter waves.**
2. **What are the postulates of wave mechanics. Give physical significance of wave function.**
3. **Derive Schroedinger wave equation .Apply it to obtain the expression for the energy levels of a particle in one dimentional potential well of infinite height.**
4. **Derive Schroedinger wave equation .Apply it to a particle in three dimentional box.**
5. **Apply Schroedinger wave equation to harmonic oscillator.**
6. **Write a short note on i) expectation value of an operator, operator concept, eigen functions and eigen values.**

8.16 REFERENCE BOOKS:

1. Physics of Atom	Wher and Richards
2. Elements of Modern Physics	Patil
3. Unified Physics Vol-IV	Jai Prakash & Co
4. Quantum Mechanics	Mathaws and Venkatesan
5. Introduction to Quantum Mechanics	Pauling and Wilson

UNIT-3

LESSON-9

INTERACTION OF CHARGED PARTICLES AND NEUTRONS WITH MATTER AND NUCLEAR DETECTORS

OBJECTIVES :

After completing the study of this lesson the student will be able to

1. **Understand the interaction of charged particles with matter.**
2. **Understand the interaction of γ - rays with matter.**
3. **Understand the interaction of neutrons with matter.**
4. **Understand the working of nuclear detectors. i.e G.M. counter, proporitional counter, scintillations counter, Wilson – could chamber, spark chamber**
5. **Understand the photographic emulsions and their advantages and disadvantages.**

STRUCTURE :

9.1 INTRODUCTION :

Nuclear reactions are accompanied by the emission of charged particles like ∝ - Particles, protons, electrons and radiations like γ - rays. The instruments used to count these particles are known as nuclear detectors. To understand the function of these detectors. it is necessary to understand the interaction of charged particles and neutrons with matter.

In connection with the interaction of radiation with matter, it is necessary to define the following terms.

(i) Average Ionisation Energy (I) : - It is defined as the average energy used to cause excitation or ionisation of an atom of the medium through which the radiations passes.

(ii) Mean Range (R) :- It is equal to the distance traveled by particle through the medium from its source to a point at which its kinetic energy is zero.

(iii) Stopping Power (S) :- It is defined as the amount of energy lost per unit length of the medium by the incident particle in the given medium.

If depends an the initial velocity of the particle, thickness, atomic weight and density of absorbing material.

9.2 INTERACTION OF CHARGED PARTICLES WITH MATTER :

(a) Interaction of heavy charged particles with matter :

A heavy charged particle (like proton, ∝-Particle etc..... has a considerable momentum. The particle loses energy due to (i) excitation of the atoms in the medium in which it is traveling and (ii) Ionisation of the atoms on the medium in its path. The particle comes to rest after losing its energy completely.

(b) Interaction of electrons with matter : Electrons interact with matter through coulomb scattering from atomic electrons inside the matter. The interaction of electrons with matter is similar to the interaction of charged particles with matter. Very energetic electrons (>I Me V) lose an appreciable amount of energy in producing continuous X-rays.

Interaction of γ - rays with Matter :- Gamma rays are highly penetrating and uncharged quanta of energy and hence their interaction with matter is very much different from the interaction of charged particles with matter.

There are three processes which are mainly responsible for the absorption of γ - rays (0.1 Me V to 25 Me V)

(a)Photo electric absorption :- The energy of the incident photon is completely absorbed by the electron of the atom during the interaction. As a result the electron is ejected out. The ejected electron may either escape out of the matter or reabsorbed due to the collision. The kinetic energy of the electron T is given by the expression.

$$T = h\nu - W_0$$

$h\nu \rightarrow$ energy of the incident photon

$W_0 \rightarrow$ Work function

(b) Compton scattering :- A γ- ray photon interacts with an atom if low atomic number in such a way that the γ - ray is scattered by one of the free electrons. This results the emission of electron. The scattered photon loses same energy and move with less energy in a direction different from incident direction.

(c) Pair Production :- When a γ -ray photon of high energy moving in the electrostatic field of nucleon, transforms into electron, positron pair. This transformation is in accordance with Einsteins's mass energy relation.

$$\gamma \rightarrow e^- + e^+$$

(γ -photon) electron positron.

9.3 INTERACTION OF NEUTRONS WITH MATTER :

Neutrons experience a kind of force when they come very close toward the nucleus. This is called 'short range interaction'. The interaction may be regarded as a collision. The collision may be either elastic or inelastic.

i) Elastic collision : In an elastic collision, the neutrons are scattered by following the law of conservation of energy and momentum. A part of the energy of the striking neutron is transferred to the struck nucleus. Lighter is the nucleus, the greater being the energy imparted to it. Therefore, light elements are used to slow down the fast neutrons and these are called as moderators.

ii) Inelastic collision : In inelastic collisions, the laws of conservation of energy and momentum are not followed. These collisions are subdivided into the following two categories.

a) Partial inelastic collisions : In this type of collision, the neutron is scattered and the struck nucleus undergoes internal changes in energy and is raised to an excited state of higher energy.

b) **Total inelastic collisions :** In this type of collision, the neutron is captured by the nucleus. This leads to a real transformation. The capture process takes place when the energy of the neutron corresponds to the energy of an excited state of the nucleus. The capture process plays an important role in transmutations produced by neutrons, It is important to mention here that the capture process is also known as resonance capture because the neutron and nucleus are in tune with each other.

9.4 NUCLEAR DETECTORS : The instruments which are used for the detection of nuclear radiations are called nuclear detectors.

9.4.1 Geiger – Muller Counter :

This is a particle detector. It counts the number of α-particles emitted by a radioactive substance. This consists of a hollow metal cylinder enclosed in a thin glass tube, A fine wire (of tungsten) is placed along the axis of the metal cylinder. The wire is insulated from the cylinder. The cylinder is cathode and the wire is anode. The tube contains a mixture of 90% of Argon at 10 cm of pressure and 10% ethyl alcohol vapour at 1cm pressure. Different mixtures are used for different designs. At one end of the tube, a window covered with thin mica sheet for the entry of radiations. A D.C potential of about 1200 V is applied between the wire and cathode. This voltage is less than the voltage to cause the discharge in the tube. A high resistance R is connected in series with the battery as shown in Fig.9.4.1.1.

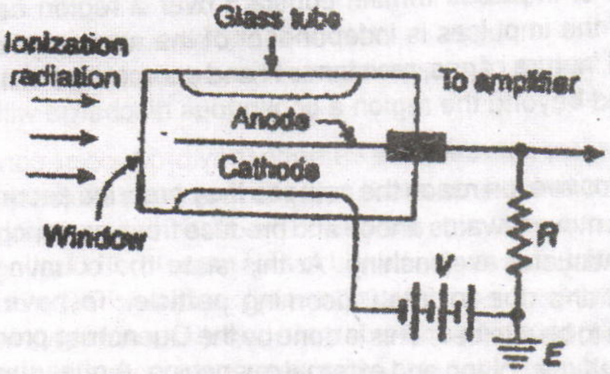


FIG 9.4.1.1

When a charged particle passes through the counter, it ionizes the gas molecules. The electrons move towards the wire and the positive ion move towards the cylinder. This causes the ionisation current. At high voltages applied to the cylinder, the electrons gain high kinetic energy and causes the further ionisation of argon atoms. Thus a large number of secondary electrons are produced. Due to the presence of large number of argon atoms and due to ionisation along the wire the number of secondary electrons produced is independent of the number of primary ions produced by the incoming particle. These avalanche of electrons quickly reach the anode causing the ionisation current. But the positive ions move more slowly away from anode forming a sheath around anode for a short while. This decreases the P.D between the electrodes, to a very low value. Hence the ionisation current stops. So a brief pulse of current flows through resistance R. This creates a p.d. across R. This P.D. is applied to a counter circuit. As each incoming particle produces a pulse the number of incoming particles is counted.

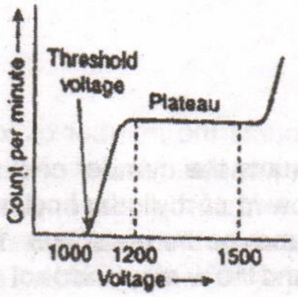


FIG 9.4.1.2

Depending on the applied voltage the counter works. Consider the graph between the applied voltage and counting rate. The counting rate increases with voltage up to 1200 volts, Beyond this voltage the number of impulses remain constant over a region called plateau. In this region the magnitude of the impulses is independent of the amount of original ionisation, It depends on the potential, nature of gas, resistance R and geometrical conditions of apparatus. If the voltage is increased beyond the region a continuous discharge will take place.

Quenching : When a positive ion reach the cathode they produce secondary electrons from cathode. These electrons move towards anode and produce fresh avalanches. Now the counter is kept in a state if continuous avalanching. At this state the counting is resulted by the continuous avalanching and due to fresh incoming particle. To have ideal counting the continuous avalanching is to be avoided. This is done by the Quenching process. The quenching process is of two types, self quenching and external quenching. A quenching agent like alcohol vapour is introduced in the tube. Alcohol is of low ionisation potential than argon. The argon ions neutralize by absorbing electrons from alcohol molecules. The alcohol ions are neutralized by reaching cathode These molecules still possess some energy. But they do not produce secondary electrons, because this energy is utilised in dissociation into alcohol atoms. Thus the continuous avalanching is avoided by connecting a large resistance in series with counting circuit. This produces a large volatage drop across R. This lowers the potential avoiding the further ionisation. Internal quenching technique is generally used.

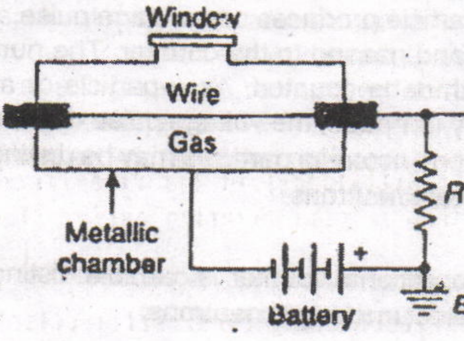
The Counting rate is controlled by paralyse time. The positive ions take 100 micro seconds to reach the cathode, this is the dead time. The tube takes 100 micro seconds to come to original working conditions. This is called delay time. The sum of dead time and recovery time is called paralyse time. So after this time only it counts the second incoming particle. So a particle is counted for every 200 micro seconds. Thus 500 particles can only be measured.

Advantages : 1) It is widely used to detect and count each individual particle separately 2) It can detect low ionising of α and β particles 3) This is very small in size and handy 4) It can also be used in cosmic rays research and mineral exploration also.

Disadvantage : 1) It cannot specify the energy of the particle. 2) It counts the number of particles, but cannot give any other information such as charge, momention, energy, range etc. 3) It has no sensitimity in the time internal of 400 μs range.

9.4.2 PROPORTIONAL COUNTER :

The proportional counter consists of a cylindrical metal chamber with a thin wire situated along its axis and insulated from it. The wire is connected to the positive pole of high tension battery and serves as collecting electrode. The negative of high tension battery is connected to the chamber as shown in Fig. (9.4.2.1) A high resistance R is connected in the battery circuit. The wire in turn is connected to pulse amplifier and counting circuit. The cylindrical tube is also provided with a mica window so, that charged particles and ionizing radiations can enter into it. The chamber is filled with a gas like methane argon, carbon dioxide or a mixture of suitable gases for a particular purpose at suitable atmospheric pressure. The proportional counter functions satisfactorily at voltages 500 to 800 volts or above at pressure of about one atmosphere.



Proportional counter

FIG 9.4.2.1

When a charged particle enters in metallic chamber, ionisation of gas takes place resulting ion pair formation. The positive ions move to the chamber while the negative ions (electrons) move towards the central wire. Now an extremely short electric flow or pulse passes through high resistance. R which develops a voltage cross it. When the applied voltage is low, many ions recombine before reaching the central wire and hence the current is small. But when the voltage is increased, more and more ions, reach the central wire and the current increases. When all the ions are collected by the central electrode, the current reaches the saturation value as shown in Fig. (2) by region (ii). When the voltage is further increased, the ions fain sufficient kinetic energy to produce secondary electrons by collisions with the atoms of the gas. In this case, the current would be very large. For a given applied voltage, the current is proportional to the number of primary ion pairs produced by incoming charged particles.

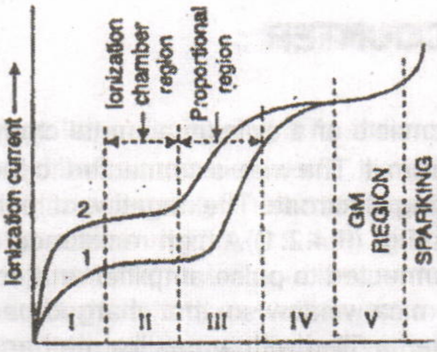


FIG 9.4.2.2

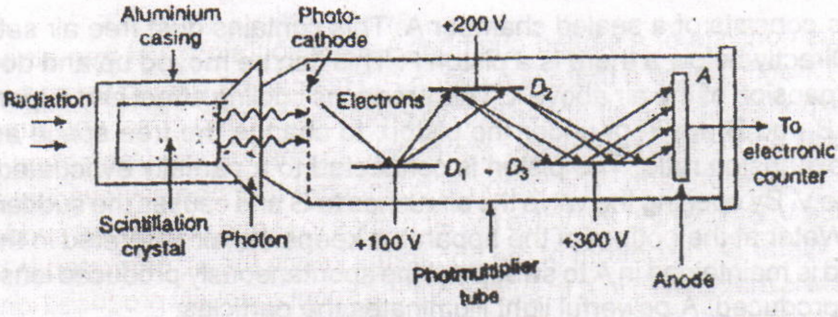
The counter now works as proportional counter. This is shown by region (III) in fig. (9.4.2.2). Every incoming charged particle produces one voltage pulse across the resistance which is amplified by the amplifier and passed to the counter. The number of particles entering the tube in a given time can thus be counted. As α-particle or a β-particle or γ-ray produces different number of primary ion-pairs, the voltage pulse developed across R will be different in these cases. Thus different incoming particles may be distinguished from each other. This counter can be used to detect neutrons.

Advantages : 1) The proportional counter is capable distinguishing between α, β and γ-particles. 2) It can also detect uncharged neutrons.

Disadvantages : The proportionality factor depends on the applied voltage and hence the applied voltage should be maintained at a constant value.

9.4.3 Scintillation counter :- The particles are detected by the scintillations produced by them, when they are incident on fluorescent substances like zinc sulphide. If the scintillations are to be visually observed, the particles must have high energy so that they produce visible photons when they strike the fluorescent material. This energy range is same that measured in ionization chambers. However very sensitive scintillation technique is used in the photo multiplier tube.

When a charged particle or radiation passes through a phosphor (the scintillating material) some of its atoms are excited. As these atoms return to the ground state photons are emitted. The photons enter the photo multiplier tube and strike a photo cathode. Photo electrons are emitted out. A number of anodes called dynodes are arranged in the tube at increasing positive potential. These dynodes have specially prepared surface (coating of CS-Sb, or Ag-Mg) so as to have high secondary emission.



Scintillation counter

FIG 9.4.3.1

The electron from photo cathode is accelerated towards the first dynode D_1Secondary electrons are emitted and they are accelerated towards the second dynode D_2Which is at higher positive potential. Secondary emission takes place from D_2 and the electrons are accelerated towards D_3. This process continues up to last but one diode, resulting in a large multiplication of the electrons. The last dynode acts as collector of electrons. The resulting current pulse produces a voltage pulse across the load resistance. This voltage pulse is amplified electronically and recorded by an electronic counter.

The electrical pulses are usually proportional to the energy of the incident gamma rays. So with this arrangement besides detecting the gamma rays, their energy is also measured. In measuring the gamma rays energy the instrument must initially be calibrated using the gamma rays of known energy.

The intensity of the light flash produced in the phosphor depends on the energy given up by the charged particle. Caesium iodide in crystalline form is very often used for the detection of protons and α-particles sodium iodide is used for the detections of gamma rays. A small impurity like Thallium is added to the scintillator to achieve optimum scintillation counter.

Advantages: It has many advantages over other detectors. They are (i) high efficiency (ii) Short times of rise and recovery (iii) large life of usage.

9.4.4 Wilson – Cloud Chamber :

In 1911, C.T.R. Wilson devised an instrument known as cloud chamber by which it is possible to detect and record the paths of charged particles (α and β rays), studying the behaviour of individual atoms etc.,

Principle : The basic principle of Wilson cloud chamber is based on the principle that super cooled vapour condensed only on charged particles and if the charged particles are not present they remain in vapour phase i.e., they do not condense.

The apparatus consists of a sealed chamber A. This contains dust free air saturated with water vapour. Directly below a there is a piston P. This can be moved up and down causing the adiabatic expansion of the air above it. This produces cooling effect and super saturation. Ebonite blocks B and B are kept under the piston, to change the free space and there by controlling the expansion ratio. The piston is connected to a partially evacuated glass bulb through the value V. By opening the valve the air rushes to G and causes the sudden expansion of air above P. Water at the bottom of the apparatus keeps the air saturated in the chamber. An electrical field is maintained in A to sweep out the spontaneously produced ions. Otherwise a diffuse fog is produced. A powerful light illuminates the particles.

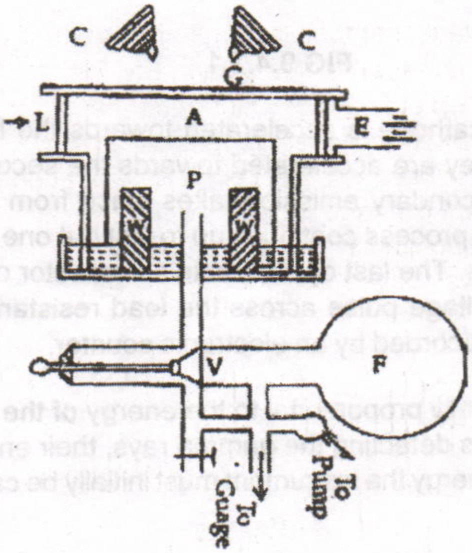


FIG 9.4.4.1

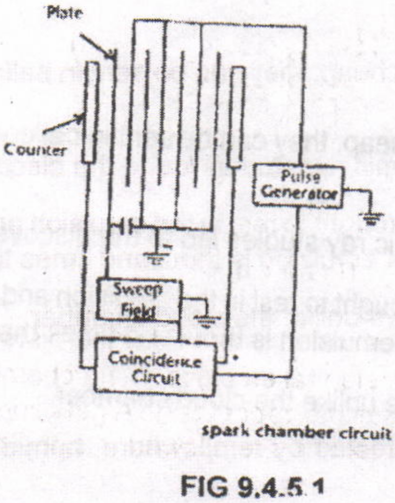
Working : When value V is opened, the air under the piston rushes into the vacuum suddenly. There by adiabatic expansion takes place in the chamber A. Due to this sudden expansion causes cooling and a result the vapor inside A gets super saturated. At this stage the ionizing charged particle or radiations are allowed into the chamber through the side window. This produces ionization of air inside A. The water vapoer condenses and forms droplets in the ions. These droplets appear as a linear cloud along the path of incident particles or radiations., When the chamber is fluorinated with light, the tracks of the ionizing particles or radiations appears as a white line of fog on a black back ground. The tracks can be photographed by means of cameras C and C.

The chamber is cleared off the ions by means of sweeping electric field applied across the chamber. The piston P is returned to the original position so that the chamber is once again ready to study the track of another ionizing particle.

Advantages : 1) Using cloud chamber, the ionizing particles can easily be identified through their paths 2) By counting drops in cloud track, the specific ionization can be determined. 3) By applying a magnetic field on the moving particle the sign of the charge, its momentum and energy can also be determined.

Disadvantages : 1) If the range of a particle exceeds the dimensions of the chamber, entire track cannot be photographed. 2) This cannot directly record the tack of electrically neutral particles like neutron. 3) One cannot be always sure often direction of the track photographed.

9.4.5 Spark Chamber : The spark chamber consists of a large no. of thin parallel metal plates of aluminum spaced about 1 cm apart inside a chamber filled with neon gas at atmospheric pressure. One set of alternate plates are grounded (connected to earth) and the other set to a high volt D.C pulse generator. (Each pulse generators a high potential in short bursts of the order of microsecond.) The visible and audible sparks produced by the ionizing particle are recorded by two cameras (at right angles to one another). A small sweep field is applied continuously in a direction opposite to the high voltage spark field so as to clear out the ion pairs produced in the chamber.



spark chamber circuit

FIG 9.4.5 1

Working : The high voltage D.C pulse applied produces a high electric field between the plates lasting per one microsecond each. Because of the ions (produced in the gas due to ionization by charged particles), sparks will be produced between the plates. When ever the ionizing particle enters into the chamber, ion pairs are produced along its path. As a result, the trajectory of an ionizing particle is observed as a series of sparks. This track is photographed and analysed. By placing the chamber in an external magnetic field, we can determine the momentum, sign of charge and energy of the particle.

Advantage : 1) The process of triggering and removal of ions using a sweep are comparatively small. 2) The individual event produced by one particle among the many particles passing through the chamber at a rate of million per second can be studied.

Disadvantages : 1) The interaction after incoming particle is not restricted in the spark chamber. 2) The coordinates of the tracks and points of intersection are observed with less accuracy than in other kinds of chambers.

9.4.6. Photo Graphic Emulsions : When an ionizing particle travels through a photographic plate emulsion, it leaves a track in the emulsion which appears when the plate is developed.

Special photographic emulsions are prepared for this purpose. They are called nuclear emulsions. They are coated on photographic plates. The thickness of the coating is more and have a large size and density of silver bromide grains than an ordinary optical emulsion. The tracks which are left by the ionizing particles passing through these emulsion are short. The tracks a measure of the number of particles entering the emulsion and the study of the structure of track gives information about the mass. charge and energy of the particle. This gives the permanent record of the events. These tracks resemble those obtained from cloud chamber or bubble chamber.

Advantages :

1. The emulsion is relatively light and cheap. they can be sent in balloons, space slips for high attitude cosmic ray experments.
2. Emulsions were widely used in cosmic ray studies led to the discovery of π and k mesons.
3. Unstable high energy particles are brought to rest in the emulsion and their decay procedures and studied. The stopping power of emulsion is thousand times that of standard air.
4. The emulion is continuously sensitive unlike the cloud chamber.

Disavantages :

1. The sensitive and thickness are affected by temperature, humidity, age of the emulsions befor development.

2. It is difficult to determine the sign of the charge and the momentum of a particle fron observaticns of the curvature of the path in a strong magnetic field. Because the autual patl in the emulsion is small compared to that in a cloud chamber.

9.5 SOLVED EXAMPLES :

1. **An uranium emitting δ - particles of 4.18 MeV is placed near Ionization chamber. Assum that only 10 particles per second enter the chamber. Calculate the current produce Given that 1 ion pair requires energy of 35ev and $e = 1.6 \times 10^{-19}$C.**

[Ans:1.904×10^{-13}A]

Sol: Given that

Charge of electron $e = 1.6 \times 10^{-19c}$

1 ion pair requise energy = 35ev

Energy emitted by δ - particle = 4.18 MeV = 4.18×10^6ev

Particle enter/second = 10

Number of ion paire produced by one δ - particle $N = \dfrac{4.18 \times 10^6}{35}$

$= 1.19 \times 10^5$ pairs

Number of Ion – pairs prodond per second

$= 1.19 \times 10^5 \times 10 = 1.19 \times 10^6$ ion - pairs/sec

Current i = (Number of ion pair produced / second) charge on each ion

$= (1.19 \times 10^6)(1.6 \times 10^{-19}) = 1.904 \times 10^{-13}$A

2. **A Geiger – Muller counter wire collects 10^8 electrous per discharge. Whar is the avarage current in circuit when the counting rate is 500 counts/minute? [$e = 1.6 \times 10^{-19}$C]**

[Ans:1.33×10^{-10} amp]

Sol: Given that

electrons collected by wire /discharge = 10^8

Counting rate = 500 counts/minute

$\therefore$ total number of electrons collected in one minute is

$n = 500 \times 10^8 = 5 \times 10^{10}$

Charge / minute = ne = $(5\times10^{10})\,(1.6\times10^{-19})$ Coul/min

$$\text{Charge/sec} = \frac{(5\times10^{10})(1.6\times10^{-19})}{60} = 1.33\times10^{10}\text{amp}$$

Charge/sec = avarage current = 1.33×10^{-10} amp

9.6 SUMMARY :

1. Arrange ionization energy (I) is defined as the average energy needed to cause ionization of an atom of medium through which the radiation passes.
2. The mean range is equal to the distance traveled by particle through the medium from its source to a point at which its kinetic energy is zero.
3. Stopping power (S) defined as the amount of energy lost per unit length of the medium by the in lid cut particle in the given medium.
4. The stopping power depends upon the initial velocity of particle, thickness atomic weight and density of absorbing material.
5. Electrons interact with matter through coulomb scattering from atomic electrons inside the matter.
6. It pair production γ - photon → electron (e^-) + positron (e^+)
7. The absorption of neutrons by matter is due to short range interactions with matter.
8. The instrument which are used for the detection of nuclear radiation are called nuclear detectors. Several detectors use the property of ionization to detect the radiation.
9. The process of preventing the continuous avalanching is known as quenching.
10. The counting rate of GM counter is about 500 particles per second are it depends upon dead time, recovery time, paralysis time.

9.7 KEYWORDS :

Mean range, stopping power, ionization energy, Interaction, absorption, detectors, chambers, emulsion.

9.8 SELF – ASSESSMENT QUESTIONS

1. Explain the interaction of γ - rays with matter.
2. Expalin the interaction of neutrons with matter.
3. Describe the corporation and explain limitations.
4. Explain the corporation and working of

   (a) Wilson cloud chamber (b) Proportional counter
5. Explain the principle and working of spoke chamber6. Write short notes on

   (a) photographic emulption(b) Stopping power

   (c) Ionization energy and mean range
6. Describe the Construction and working of scintillations counter.

Exercises :

1. G. M Counter wire collects 10^8 electrons / discharge. When the counting rate is 1000 counts/minute, what is the average current in the circuit? [Ans:2.66×10^{-10} amp]

[Hint : Count rate / scond = $\frac{1000}{60} = 50/3$

Number of electrons collected/second = $\left(\frac{50}{3}\right) \times 10^8$

charge/second = $\left(\frac{50}{3}\right) \times 10^8 \times 1.6 \times 10^{-19}$= average current]

2. α - particle of energy 5 MeV pass through an ionization chamber at the rate of 10 per second. Calculate the current produced when 35eV is required to produce ion pair [$e = 1.6 \times 10^{-19}$C] [Ans:2.287×10^{-13} amp]

[Hint : Energy of α - particle = 5×10^6eV

Energy required to produce ion pair = 35eV

$\therefore$ Number of ion pairs produced = $5 \times 10^6/35 = 1.429 \times 10^5$

Number of ion pairs produced / sec = No. of pairs $\times \alpha$ – particles /sec = $(1.429 \times 10^5) \times 10$

$\therefore$ current= ion pairs produced × charge on.one ion = $[(1.429 \times 10^5] \times 10) 1.6 \times 10^{-19})]$

9.9 REFERENCE BOOKS:

1. Unified physics vol-4	S.L. Gupta,'Sanjeev Gupta.
2.Introductory of Atomic Spectra	H.F. White
3. Physics of atom	Wher and Richards
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5. Elements of Modern Physics	Patil
6. Atext book of common core physics	Vikas publications

UNIT-3

LESSON- 10

STRUCTURE OF NUCLIE

OBJECTIVES:

After completing the study of this lesson the student will be able to

1. Understand the nuclear constituents
2. Know about the general properties of Nucleus
3. Understand the term Binding energy and obtain Deuteron Binding energy
4. Understand the proton-proton and neutron – proton scattering
5. Understand the general concepts of nuclear forces
6. Understand the β – decay and Gamow's explanation
7. Understand the α - decay, range of α –particles and Gamow's theory

STRUCTURE:

10.1 INTRODUCTION:

Rutherford concluded that atom consists of central core called nucleus.The nucleus consists electrons revolving around it. The nucleus consists of nucleons (protons, neutrons). The number of protons in nucleus is called atomic number and sum of protons and neutrons is called mass number. The stability of nucleus depends upon relative number of protons and neutrons. Artificial radioactivity shows that many particle like α particles, protons, neutrons, positrons, β-particles etc. enter into the constitution of the nucleus. Cosmic ray studies leads to the existence of mesons. Nuclear forces are short range forces and attractive in nature, keep the nucleus together in the nucleus.

10.2 GENERAL PROPERTIES OF NUCLEUS:

Some of the important properties of atomic nucleus are given below.

i) Nuclear mass: The mass of the nucleus is the sum of the masses of the neutrons and protons obtained in it. This is usually expressed in terms of atomic mass unit (amu).

$$1 \text{ amu} = 1.66 \times 10^{-27} \text{ kg}.$$

.: $_6C^{12}$ nucleus has a mass of 12 amu. So that its mass number A = 12.

Mass of the nucleus = $Zm_p + Nm_n$.

where m_p and m_n are the masses of protons and neutrons respectively. Here N is the number of neutrons.

ii) Nuclear charge : The charge on the nucleus is due to protons contained in it. The charge on each proton is 1.6×10^{-19} coulomb which is equal in magnitude to charge of an electron. Taking the charge of a proton as one unit the total charge on the nucleus is numerically equal to the number of protons.

∴ A hydrogen nucleus carries a single unit charge.

iii) Nuclear radius : The size of the nucleus is estimated by the study of proton and neutron scattering experiments.The radius of an atomic nucleus (assumed spherical) can be determined from the empirical relating

$$r = r_0 A^{1/3}.$$

where r_0 is a linear constant and has an average value of 1.4×10^{-15}m = 1.4 fermi.

A is mass number of the nucleus.

∴ For carbon (A=12), radius of an atomic nucleus $r = 1.4 \times 10^{-15} \times (12)^{1/3}$

$$= 3.21 \times 10^{-15} \text{m}$$

iv) Neclear density : The density of the nucleus can be calculated as follows.

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

where 'r' is the radius of the nucleus, $r = 1.4 \times 10^{-15} A^{1/3}$ metre.

We have volume of the nucleus $V = \frac{4}{3}\pi (1.4 \times 10^{-15})^3 = 14.15 \times 10^{-45} \text{A m}^3$

Mass of nucleus = A× Mass of protons = 1.673×10^{-27} A kg.

$$\text{Density of the nucleus} = \frac{1.673 \times 10^{-27} \text{A}}{14.15 \times 10^{-45} \text{A}} \text{ kg/m}^3$$

$$= 1.18 \times 10^{17} \text{kg/m}^3$$

v) Nuclear Spin : Like the electron, the proton and neutron each have a spin angular momentum $= \frac{1}{2}(h/2\pi)$. Each contribute a spin to the nucleus and combine to give it a spin angular momentum. Due to the spin the nucleus possesses a magnetic moment.

vi) Angular momentum and magnetic moment : The nucleus move in different orbits and they have spin. The total angular momentum is the sum of the spin and orbit angular momenta of the nucleons.

The nucleons with even A and even Z have zero angular momentum and zero magnetic moment.

Even A and odd Z nuclei have integral angular momenta and magnetic moment.

Odd A and odd Z nuclei have half integral angular momenta and magnetic moment.

The angular momenta of protons and neutrons compensate separately.

vii) Electric quadruple and shape of nucleus : The shape of the nucleus is supposed to be spherical. But the nucleus has electric quadruple moment. This shows that the shape of the nucleus is non-spherical. Depending upon the direction of the quadruple moment the nucleus may be oblate ellipsoid or prolate ellipsoid.

10.3 DEUTERON BINDING ENERGY:

The deuterium atom is approximately twice as massive as the hydrogen atom. *It consists of* one proton and one neutron in the nucleus.

Mass of proton = 1.007825 amu.

Mass of neutron = 1.008665 amu

∴ Total mass of proton and neutron = (1.007825 + 1.008665) amu

= 2.016490 amu

Actual mass of deuteron = 2.014104 amu

∴ Mass defect Δm = (2,016490 – 2.014104) amu

= 0.002386 amu

Binding energy = 0.002386 × 931= 2.23 MeV.

10.4 PROTON-PROTON SCATTERING[p-p scattering]:

The p – p scattering is the only way to get direct evidence on proton-proton interaction force inside the nucleus. p–p scattering is caused not only by the nuclear forces but also by the coulomb force. The wave function describing the two protons must change sign on the interchange of the two particles. Hence a symmetric space wave function (S,D states etc. $l = 0, 2,$ ---------- etc) can only be associated with an anti symmetric (singlet) spin wave function, where as a symmetric (triplet) spin wave function is required for an anti - symmetric space wave function. For incident protons of energy below 10 MeV, only the S-state interaction is of any importance in the scattering, since protons in higher orbital angular momentum states stay a part from each other beyond the range of the nuclear force. Experimental study of P – P scattering is more accurate than n – p scattering due to the following reasons.

1. Protons are easily available over a wide range of energies
2. Protons can be made more mono energetic
3. Protons can be produced in well collimated beam
4. Protons can be easily detected by their ionizing properties.

10.5 NEUTRON-PROTON SCATTERING(n-p Scattering) :

Since neutrons have no charge, they are undeflected by the coulomb field and their scattering will directly reflect the operation of the nuclear forces.

Two kinds of interactions may be involved, they are 1) scattering and 2) radiative captiure. In general protons are bound in molecules. The chemical banding energy of protons in a molecule is about 0.1 eV. Thus for neutron energies is less than 10 MeV only the associated S wave over laps with the nuclear potential and scattered. n-p sattering depends on relative spin orientations of the neutron and the proton. n-p scattering is also effected by the chemical binding.

10.6 GENERAL CONCEPTS OF NUCLEAR FORCES:

Gravitational and electromagnetic forces obey the inverse square law but the nuclear forces are complicated in nature and do not obey any simple law. The scattering experiments have revealed the following characteristic properties of the nuclear forces.

1. **Nuclear forces are charge independent** : The nuclear force between a neutron and a proton is identical in between two protons or two neutrons i.e., the nuclear force in between two protons or between two neutrons or between a proton and a neutron are the same. So they are nonelectric in nature and are independent of the charge on the nucleons. In protons, there is an electrostatic force of repulsion as well which is only about 1% of the nuclear force. At a distance of about 1.9×10^{-15}m this repulsive force is even less than 1% of the nuclear force between them and hence the electrostatic force is quite negligible at this distance.

2. **Nuclear forces are short range forces** : It means that nuclear forces operate only at distances between the nucleus that are comparable to size of the nucleons. These distances

are called the action radii or range R of the nuclear forces. The range of nuclear force is generally taken as 1.5×10^{-15} m where its magnitude drops off to about $\frac{1}{3}$ of its maximum value. At a distance of about 4.2×10^{-15}m the nuclear force is zero. On the other hand the gravitational and electromagnetic forces are long range forces.

3. **Nuclear forces show saturation properties :** This means that each nucleon interacts only with its immediate neighbours, rather than with all other nucleons in the nucleus.

4 **Nuclear forces are forces of attraction :** The nuclear force is generally attractive. Although it is strongly attractive at a distance of 10^{-15}m, it becomes highly repulsive at a distance of 0.4×10^{-15}m. If it were not so, under the action of strong attractive force, the nucleons would come very close together and the whole nucleus would collapse to a size equivalent to the range of nuclear forces. In such a case, the size of the nucleus becomes independent of the number of nucleons in it which is contrary to our observed results. The distance of 0.4×10^{-15}m is known as 'hard core'. However this does not imply that nuclear forces are repulsive. On the whole they are always attractive. Gravitational forces are always attractive, electrostatic forces between two charges may be attractive or repulsive depending on the nature of the charges. But nuclear force are both attractive or repulsive depending on the distance between two nucleons.

10.7 BETA DECAY:

β-decay is the process of emission of electrons from nuclear.

The electron emission takes place in the following two processes.

i) Spontaneous conversion of a neutron into a proton by ejecting π - meson.

ii) The π^- meson decays almost instantly into an electron $(\bar{e})$ and anti neutrino $(\bar{v})$

$$n \rightarrow p + \pi \ \rightarrow p + e^- + v^-$$

In the case of Beta decay the product nucleus will be having the same mass number as the parent nucleus but the atomic number will change.

In positive beta decay (β^+ emission) The atomic number will decrease by one where as in negative beta decay (β^- emission) the atomic number will increase by one.

10.8 RANGE OF α - PARTICLES:

The Distance through which an α-particle travels in a substance before coming to rest is called the range (R) of the particle in that substance.

The range of α - particle depends upon the following factors (i) Initial velocity of α-particle (ii) Nature of emitting radioactive element (iii) Nature and pressuse of the gas or nature of absorber.

The range of an α-particle can be meassed using (i) Wilson - cloud chamber (ii) By counting the number of ions produced along the path (3) By scintillations produced on a fivorescent screen.

10.9 GEIGER-NUTTAL LAW:

Geiger and Nuttal measured the range of α-particles emitted by several radioactive elements and observed that there exists a relationship between the ranges and half lives of an element.

The relationship is

$\log \lambda = A + B \log R.$

Where A and B are constants for a given radioactive serices, λ is the disintegration constant of the source and R is its range.

The graph between logarithms of range and the disintegration constant is a straight line. The figure(10.9.1) shows the graph for three main radioactive series. They are straight lines parallel to one another. This indicates that A is different for different series while B is same for all series

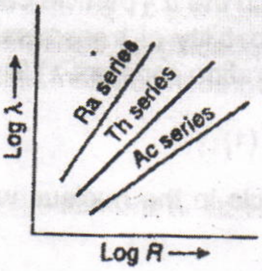


FIG 10.9.1

10.10 GAMOW'S EXPLANATION OF BETA DECAY:

For the beta transitions to occur, certain definite relations connecting the initial and final states of the nucleus must be followed. These are called the selection rules. According to Gamow and Teller the selection rules to be followed in the case of beta decay are

(i) The parity of the nucleus remain unchanged

$$\Delta p = 0$$

(ii) The angular momentem of the nuclues changes by one or remains the same.

$$\Delta I = \pm 1 \text{ or } O.$$

If electron and neutrino are emitted with their spins parallel (triplet state), ΔI may be + 1, 0, or −1.

Ex : $He^6 \rightarrow Li^6 + e^- + \bar{\nu}$

If electron and neutrino are emitted with intrinsic spins, anti parallel (singlet state), the change in nuclear spin. ΔI must be strictly zero

10.11 ALPHA DECAY: (Gamow's theory of alpha decay

According to wave mechanics, the motion of the α-particle is described by a wave function φ which obey's Schroedinger's equation.

1. An α-particle may exist as an entity within a heavy nucleus.
2. α-particle is in constant motion and bounces back and forth from the barrier walls
3. In each collision with walls there is a definite probability that the particle will leak through the potential barrier.

Let ν be the frequency with which the α - particle collides with the walls in order to escape from the nucleus. 'P' is the probability of transmission in each collision. Then the decay probability per unit time (disintegration constant λ) is given by

$$\lambda = \nu p \text{ .... (1)}$$

If there be only one of α - particle in the nucleus which moves back and forth along the nuclear diameter, then

$$\nu = \frac{V}{2r_0} \text{ .... (2)}$$

where V is the velocity of α - particle and r_0 be the nuclear redius.

$$\therefore \lambda = \left(\frac{V}{2r_0}\right)p \text{ .... (3)}$$

Figure(10.11.1) represents qualitatively approximate form of potential energy of α-particle as a function of its distance from the nucleus. The potential that exists around the nucleus is known as potential well. In the figure OA = - V_0 is potential energy of α-particle when it is inside the nucleus, CD is equal to V_C, the electrostatic potential energy of α-particle when it is just outside the range.

In quantum mechanics a moving particle is treated as a wave and there is a definite probability to leak through the barrier. The α-particle has a finite probability of being able to cross the potential hill.In quantum mechanics a moving particle is treated as a wave and there is a definite probability to leak through the barrier. The α-particle has a finite probability of being able to cross the potential hill.

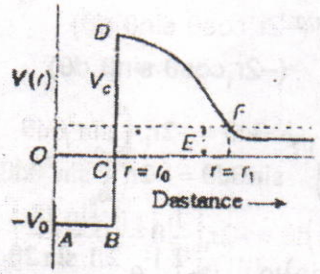


FIG 10.11.1

The probability P can be calculated by the following formula.

$$\log_e P = -\frac{2}{\hbar}\int_{r_0}^{r_1}\sqrt{\{2mv(r)-E\}}\,dr \quad \text{......................} (4)$$

where m is the mass of the particle and $\hbar = \frac{h}{2\pi}$

Further $V(r) = \frac{2ze^2}{4\pi \in_0 r}$ .... (5)

is the electrostatic potential energy of α-particle at a distance r from the nucleus of charge Ze. The charge on α-particle is 2e.

$$\therefore \log_e P = \frac{-2}{\hbar}\int_{r_0}^{r_1}\sqrt{\left\{2m\left(\frac{2ze^2}{4\pi \in_0 r}-E\right)\right\}}\,dr \quad \text{.............} (6)$$

At r = r_1, E = $2ze^2/(4\pi\varepsilon_o r_1)$

$$\therefore \log_e P = \frac{-2}{\hbar}\int_{r_0}^{r_1}\sqrt{\left\{2m\left(\frac{Er_1}{r}-E\right)\right\}}\,dr$$

or $$\therefore \log_e P = \frac{2}{\hbar}(2mE)^{1/2}\int_{r_0}^{r_1}\left(\frac{r_1}{r}-1\right)^{1/2} dr \text{ .... (7)}$$

Let us solve the integral

$$\int_{r_0}^{r_1}\left(\frac{r_1}{r}-1\right)^{1/2} dr$$

Let us substitute $r = r_1\cos^2\theta$ and $r_0 = r_1\cos^2\theta_0$

$\therefore$ $dr = -2r_1\cos\theta\,\sin\theta\,d\theta$

$$= \int_{\theta_0}^{0}\left(\frac{r_1}{r_1\cos^2\theta}-1\right)^{1/2}(-2r_1\cos\theta\,\sin\theta\,d\theta)$$

$$= -2r_1\int_{\theta_0}^{0}\left(1-\cos^2\theta\right)^{1/2}\sin\theta d\theta = -2r_1\int_{\theta_0}^{0}\sin^2\theta d\theta$$

$$= -2r_1\int_{\theta_0}^{0}\frac{1}{2}\left(1-\cos^2 2\theta\right)d\theta = -2r_1\left[\frac{1}{2}\theta-\frac{1}{2}\frac{\sin 2\theta}{2}\right]_{\theta_0}^{\theta}$$

$$= -2r_1\left[\frac{1}{2}\theta_0+\frac{1}{4}\sin 2\theta_0\right] = r_1[\theta_0-\sin\theta_0\cos\theta_0]$$

As $\quad \cos^2\theta_0 = \frac{r_0}{r_1}$ hence $\theta_0 = \cos^{-1}\sqrt{\left(\frac{r_0}{r_1}\right)}$

and $\quad \sin\theta_0 = \sqrt{\left(1-\frac{r_0}{r_1}\right)}$

$$\therefore \int_{r_0}^{r_1}\left(\frac{r_1}{r}-1\right)^{1/2} dr = r_1\left[\cos^{-1}\sqrt{\left(\frac{r_0}{r_1}\right)}-\sqrt{\left(1-\frac{r_0}{r_1}\right)}\sqrt{\left(\frac{r_0}{r_1}\right)}\right] \text{ .... (8)}$$

From equations (7) and (8), we get

$$\log_e P = -\frac{2}{\hbar}(2mE)^{1/2}r_1\left[\cos^{-1}\sqrt{\left(\frac{r_0}{r_1}\right)}-\sqrt{\left(1-\frac{r_0}{r_1}\right)}\sqrt{\left(\frac{r_0}{r_1}\right)}\right] \text{ .... (9)}$$

Because the potential barrier is relatively wide ($r>r_0$), hence

$$\cos^{-1}\left(\frac{r_0}{r_1}\right)^{1/2} = \frac{\pi}{2}-\left(\frac{r_0}{r_1}\right)^{1/2} \qquad \text{and} \qquad \left(1-\frac{r_0}{r_1}\right)^{1/2} = 1$$

Substituting these values in eq. (9), we get

$$\log_e P = -\frac{2}{\hbar}(2mE)^{1/2} r_1\left[\frac{\pi}{2} - \left(\frac{r_0}{r_1}\right)^{1/2} - \left(\frac{r_0}{r_1}\right)^{1/2}\right]$$

$$= -\frac{2}{\hbar}(2mE)^{1/2} r_1\left\{\frac{\pi}{2} - 2\left(\frac{r_0}{r_1}\right)^{1/2}\right\}$$

Here $$r_1 = \frac{2Ze^2}{4\pi\varepsilon_0 E}$$

$$\therefore \log_e P = -\frac{2}{\hbar}(2mE)^{1/2}\frac{2Ze^2}{4\pi\varepsilon_0 E}\left[\frac{4}{2} - 2\times\left(\frac{r\pi\varepsilon_0 E r_0}{2Ze^2}\right)^{1/2}\right]$$

or $$\log_e P = \frac{4e}{\hbar}\left(\frac{m}{\pi\varepsilon_0}\right)^{1/2} Z^{1/2} r_0^{\ 1/2}\ \frac{e^2}{\hbar\varepsilon_0}\left(\frac{m}{2}\right)^{1/2} ZE^{-1/2} \qquad \text{.........} (10)$$

Substituting the values of various constants in eq. (10), we have

$$\log_e P = 2.97Z^{1/2} r_0^{\ 1/2} - 3.95ZE^{-1/2} \qquad \text{...............} (11)$$

Here E = kinetic energy in MeV, r_0 = nuclear radius in fermi (1 fermi = 10^{-15}m) and Z = atomic number of nucleus – alpha particle

The decay constant is given by

$$\lambda = \nu P = \left(\frac{V}{2r_0}\right)P$$

$$\therefore \log_e \lambda = \log_e\left(\frac{V}{2r_0}\right) + \log_e P = \log_e\left(\frac{V}{2r_0}\right) + 2.97Z^{1/2} r_0^{\ 1/2} - 3.95ZE^{-1/2} \qquad \text{...........} (12)$$

Eq. (12) represents the α - decay.

When base of $\log_e$ is changed to base_{10}, we have

$$\log_{10}\lambda = \log_{10}\left(\frac{V}{2r_0}\right) + 1.29Z^{1/2} r_0^{\ 1/2} - 1.72ZE^{-1/2} \qquad \text{.....} (13)$$

Expression (13) is regarded as theoretical form of Geiger-Nuttal law. This equation tells that the decay contant veries exponentially with the energy of α - particle.

10.12 BETA RAY CONTINUOUS AND DISCRETE SPECTRUM:

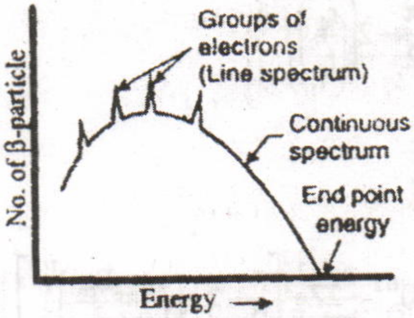


FIG 10.12.1

By using a G.M.counter the number of electrons per unit time with different velocities is counted. A graph is then plotted between number of electrons and their energy. The graph is shown in figure(10.12.1).The graph is extensive continuum upon which a few sharp lines are superposed.The graph shows that β–particles emitted by radioactive substance possess a continuous range of energies, i.e., β– ray spectrum is continuous. Aphotographic plate is used and after developing the plate with suitable exposure , a photograph is obtained with a dark back ground with several black lines. The back ground shows the presence of β–particles having a wide range of velocities and the lines signifies the groups with definite and disctrete velocities and hence energies.

Characteristics of β– ray spectra:

i). Continuous Spectrum: The β–particles have a continuous distribution of energy. The continuous spectrum energy ranging from 0 to a certain maximum value.The upper value is called the end point energy and is a characteristic of the emitter.

ii). Discrete Spectrum: Some radioactive substances can emit beta particles which produce line spectra(D isctrete spectra) superimposed on the continuous faint background. These are called secondary spectra. **Discrete Spectrum:** Some radioactive substances can emit beta particles which produce line spectra(D isctrete spectra) superimposed on the continuous faint background. These are called secondary spectra.

10.13 SOLVED EXAMPLES:

1.Calculate the total mass of particles in Li^7 nucleus. Mass of proton is 1.6725×1^{-27}kg and mass of neutron is 1.6748×1^{-27} kg **[Ans:11.7167×10^{27} kg]**

Sol : Given that Mass of proton mp $= 1.6725 \times 10^{-27}$ kg

Mass of neutron mn $= 1.6748 \times 1.0^{-27}$kgTotal mass of nucleous = 2mp + (A +Z) mr

$$= (3\times 1.6725 \times 10^{-27}) + (7-3)\,(1.6748\times 10^{-27})$$

$$= 5.0175\times 10^{-27} + 6.6992\times 10^{27} = 11.7167\times 10^{27} \text{ kg}$$

2.What is the mass number A of a nucleus whole radius r = 2.71 ferni [$r_0 = 1.3\times 10^{-15}$m]

[Ans:9]

Sol : Given that radus of nucleeus r = 2.71 fermi

$$= 2.71 \times 10^{-15}\text{m}$$

$$r_0 = 1.3 \times 10^{-15}\text{m}$$

Formula $r = r_0 A^{1/3}$

then $A^{1/3} = r/r_0$

$A = (r/r_0)^3$

$$= \left(\frac{2.71\times 10^{-15}}{1.3\times 10^{-15}}\right)^3 = \left(\frac{2.71}{1.3}\right)^3 = (2.08)^3 = 9$$

3. The radius of element HO^{165} is 7.731 fermi. find the radius of He^4 [Ans:2.238 fermi]

Sol : Given that $A_1 = 165$

$A_2 = 4$

and $r_1 = 7.731$ fer

formula $r = r_0 A^{1/3}$

$[r_2/r_1] = [A_2/A_1]^{1/3}$

$r_2 = r_1[A_2/A_1]^{1/3} = 7.731[4/165]^{1/3} = 2.238$ fermi

4.Estimate the density of nucleus of radius $r = 1.3A^{1/3}$ fermi [Ans:1.8x10^{-17}kg/m^3]

Sol: Given that $r = 1.3A^{1/3}$fermi Mass of nucleus M= A amu= Ax1.66x10^{-27} kg

Volume of nucleus $V = 4/3\,\pi r^3$

Density $d = M/V = M/4/3\,\pi r^3 = 3M/4\pi r^3$

$$= [\,3xAx1.66x10^{-27}\,]/\,[4x3.14x(1.3A^{1/3})^3\,]$$

$$= [\,3Ax1.66x10^{-27}]/[4x3.14x(1.3)^3\,A] = 1.8x10^{-17}\text{kg/m}^3$$

5.Calculated the binding energy of deutron.[Mass of proton=1.007825 amu, mass of neutron= 1.008665 amu, 1 amu=931 MeV and actual mass=2.014104]

[Ans:2.23MeV]

Sol: Given that Mass of proton mp. = 1.007825 amu

Mass of neutron mn = 1.008665 amu

actual mass of deutron= 2.014104 amu

mass of nucleus = mp + mn =1.007825 + 1.008665= 2.016490 amu

Mass defect Δm = mass of nucleons - actual mass

= 2.016490-2.014104 = 0.002386 amu

Binding energy = 0.002386 amu = 0.002386 x 931 MeV = 2.23 MeV

6. A neutron breaks into a proton and electron. Calculate the energy produced in MeV [me=9×10^{-31}kg . mp=1.6725×10^{-31}kg , mn= 1.6747×10^{-31}kg, speed of light c= 3xx10^8m/s]

[Ans:0.73MeV]

Sol: Given that me=9×10^{-31}kg
mp=1.6725×10^{-31}kg
mn= 1.6747×10^{-31}kg
speed of light c= 3×10^8m/s

Formula: mass defect Δm = mass of nucleus - (me +mp)

$= [1.6747\times10^{-31}\text{kg} - (9\times10^{-31}+1.6725\times10^{-31})]$

$= 0.0013\times10^{-27}$kg

Energy released $E= \Delta mc^2 = 0.0013\times 10^{-27}(3\times10^{8})^2$

$= 1.17\times10^{-13}\text{J} = 1.17\times10^{-13}/1.6\times10^{-13}$ MeV = 0.73MeV

10.14. SUMMARY:

1. Rutherford concluded that atom consists of central core called nucleus.The nucleus consists electrons revolving around it.
2. The nucleus consists of nucleons (protons, neutrons). The number of protons in nucleus is called atomic number and sum of protons and neutrons is called mass number.
3. Nuclear mass: The mass of the nucleus is the sum of the masses of the neutrons and protor obtained in it. This is usually expressed in terms of atomic mass unit (amu).
4. 1 amu = 1.66×10^{-27} kg
5. Nuclear charge : The charge on the nucleus is due to protons contained in it.
6. radius of an atomic nucleus $r = 1.4\times10^{-15}\times(12)^{1/3} = 3.21\times10^{-15}$m
7. Density of the nucleus $= \dfrac{1.673\times10^{-27}\,A}{14.15\times10^{-45}\,A}$ kg/m³ =1.18×10^{17}kg/m³
8. The p – p scattering is the only way to get direct evidence on proton-proton interaction force inside the nucleus.

9. nuclear forces are complicated in nature and do not obey any simple law.
10. β-decay is the process of emission of electrons from nuclear.
11. The Distance through which an α-particle travels in a substance before coming to rest is called the range (R) of the particle in that substance.
12. Continuous Spectrum: The β–particles have a continuous distribution of energy. The continuous spectrum energy ranging from 0 to a certain maximum value. The upper value is called the end point energy and is a characteristic of the emitter.
13. Discrete Spectrum: Some radioactive substances can emit beta particles which produce line spectra(D isctrete spectra) superimposed on the continuous faint background. These are called secondary spectra.

10.15 KEY WORDS:

Nucleons, mass, charge, density, angular momentum, radius, spin, magnetic dipole moment, binding energy, scattering, range.

10.16. SELF-ASSESSMENT QUESTIONS:

1. Explain binding energy and calculate the binding energy of deuteron.
2. Write a short note on size, mass,density, radius of nucleus.
3. Explain proton-proton scattering.
4. Explain neutron-proton scattering.
5. Explain nuclear forces.
6. Write a note on aipha particle range.
7. Write a note on Geiger- Nuttal law.
8. Discuss in detail Gqmow's thory of alpha decay.
9. Write a note on beta decay.

EXCERCISE:

1. A nucleus of mass 125 has radius 6 fermi.Find the radius of nucleus having mass number 64.
[Ans:4.8 fermi]

[Hint: formula $r = r_0 A^{1/3}$

$[r_2/r_1] = [A_2/A_1]^{1/3}$

$r_2 = r_1[A_2/A_1]^{1/3}$]

2.Calculate the binding energy of lithium (A=7,Z=3, Mass of lithium M= 7.016005, mp=1.007277, mn= 1.008665)
[Ans:37.7 MeV]

[Hint: formula Mass defect $\Delta m = [Z\ mp + N\ mn] - M$

$= [3x1.007277 + 4x1.008665]$

Binding energy $E = \Delta mc^2$]

3.In a thermonuclear reactions 1.000×10^{-3} kg hydrogen is converted into 0.993×10^{-3} kg helium i)calculate the energy released in joules ii) if the efficiency of the generator is 5%. Calculate the electrical energy in KWH. **[Ans:37.7 MeV]**

[**Hint:** formula Mass defect $\Delta m = 1.000 - 0.993\times10^{-3}\,\text{kg} = 0.007\times10^{-3}\,\text{kg}$

Energy released $E = \Delta mc^2 = 0.007\times10^{-3}\times3\times10^{10}\,\text{J}$

Electrical energy= $E\times5/100$]

10.17 REFERENCE BOOKS:

1. Unified physics vol-4	S.L. Gupta, Sanjeev Gupta.
2.Introductory of Atomic Spectra	H.F. White
3. Physics of atom	Wher and Richards
4. Prospective of Modern Physics	A.Beiser
5. Elements of Modern Physics	Patil
6. Atext book of common core physics	Vikas publications

UNIT-3

LESSON-11

NUCLEAR REACTIONS

OBJECTIVES :

After the completion of this lesson the student will be able to

1) **Understand the nuclear reactions and importance of nuclear reactions equations**
2) **Know about the channels**
3) **Understand the compound nucleus**
4) **Understand the direct reactions**

STRUCTURE :

11.1 INTRODUCTION:

The process in which the characteristic of incident nuclear particle undergoes a change in the bombardment of a nucleus is called a nuclear reaction. They are produced by exposing the target nuclear with fast moving nuclear particles like α - particles, proton, neutrons, γ – rays, etc. In case of nuclear reactions, (i) The atomic number of reactions must be equal to total atomic number of product particles. (ii) The total sum of atomic mass numbers on both sides of the equation must be equal.

The nuclear reactions or useful to discover and identify the new isotopes and provide the experimental verification of Einstein's equation $E = mc^2$.

11.2 NUCLEAR REACTIONS :

A nuclear reaction is the process of strong interaction of an atomic nucleus with an elementary particle resulting in the formation of a new nucleus and one or more new particles.

A nuclear reaction can be represented as $X + a \rightarrow Y + b$

where 'X' is the initial nucleus, a is the initial particle, Y in the final nucleus and b is the final particle.

During nuclear reaction the following physical quantities are consumed a) Charge b) Number of nucleus c) Total energy d) Linear momentum e) Angular momentum f) Parity g) Spin

Different types of nuclear reactions :

The following are some of the mechanisms.

(i) Elastic scattering : In this case the incident particle strikes the target nucleus and leaves with out loss of energy, but its direction may change.

Example : Scattering of α - particle from the thin gold foil.

$${}_2He^4 + {}_{79}Au^{197} \rightarrow {}_{79}AU^{197} + {}_2He^4$$

The target nucleus remains unaffected. Here there is no change in internal energy of the nucleus.

(ii) Inelastic scattering : In the case, the incident particle loses a part of its energy in exciting the target nucleus to a higher allowed energy level. The excited nucleus later decays to the ground state, radiating the excess energy in the form of γ - ray photon.

Example : $_1H^1 + {}_3Li^7 \rightarrow ({}_3Li^7)^* + {}_1H^1$ [$({}_3Li^7)^*$is in excited state]

$({}_3Li^7) \rightarrow {}_3Li^7 + \gamma$ - ray

(iii) Radioactive Capture: In this case the incident particle is captured by the target nucleus and new nucleus is formed. In general the new nucleus has a considerable excess energy and it decays with the emission of one or more γ - ray photons.

Example : $_1H^1 + {}_6C^{12} \rightarrow [{}_7N^{13}]^* \rightarrow {}_7N^{13} + \gamma$

(excited state compound nucleus)

Another example for radiative capture is

$_1H^1 + {}_{12}Mg^{26} \rightarrow ({}_{13}Al^{27})^* \rightarrow {}_{13}Al^{27} + \gamma$

(iv) Disintegration : Here the incident particle is absorbed by the target nucleus and the ejected particle is a different from one. The composition of the product nucleus is also different from the parent nucleus.

Example : The disintegration of beryllium by α - particle producing neutron.

$_2He^4 + {}_4Be^9 \rightarrow {}_6C^{12} + {}_0n^1$

(v) Photodisintegration : The γ – rays are absorbed by the target nucleus, as a result, the nucleus is excited to higher quantum state. This excited nucleus goes to ground state by emitting one or more particles.

Example : $_1H^2 + \gamma \rightarrow {}_1H^1 + {}_0n^1$

(vi) Spontaneous decay : The phenomenon of natural radioactivity during which α , β and γ - rays are emitted may also be considered as a nuclear reaction.

(vii) Spallation reaction: On capture of an incident particle, a heavy nucleus has sufficient energy for the ejection of several particles. Such a reaction is known as spallation reaction.

Example : The nuclear fission in which heavy nucleus splits mainly into two nuclei.

$_{92}U^{235} + {}_0n^1 \rightarrow {}_{40}Zr^{98} + {}_{52}Te^{136} + 2\,{}_0n^1$

(viii) Heavy ion reactions : In these reaction the target nucleus is bombarded by projectiles heavier than α - particles. Various types of products may be produced. The reactions usually take place at fairly high energies (several hundred MeV) of the projectile.

$_5B^{10} + {}_8O^{16} \rightarrow {}_{11}Na^{22} + {}_2He^4$

Another example for heavy in reaction is

$${}_7N^{14} + {}_{82}Pb^{207} \rightarrow {}_7N^{13} + {}_{82}Pb^{208}$$

11.3 CHANNELS :

A channel is a possible pair of product nucleus and outgoing particle, each in a definite quantum state.

In the reaction a + x →[ac] →y + b

a and x are called as incident channel and Y and b are final channel with reference to compound nucleus c.

When a given projectile bombards a given target more than one reaction may occur. The following are the proton induced reactions and neutron induced reactions.

(A) Proton induced reactions:

(i) (p, α) reactions such as

$${}_3L^{I7} + {}_1H^1 \rightarrow [{}_4Be^8] \rightarrow {}_2He^4 + {}_2He^4$$

(ii) (p, n) reactions such as

$${}_8O^{18} + {}_1H^1 \rightarrow [{}_9F^{19}] \rightarrow {}_9F^{18} + {}_0n^1$$

(iii) (p, d) reactions such as (here d stands for deuteron ${}_1H^2$

$${}_4Be^9 + {}_1H^1 \rightarrow [{}_5B^{10}] \rightarrow {}_4Be^8 + {}_1H^2$$

(iv) (p, γ) reactions such as

$${}_{13}Al^{27} + {}_1H^1 \rightarrow [{}_{14}Si^{28}] \rightarrow {}_{14}Si^{28} + \gamma$$

(B) Neutron induced reactions:

(i) (n, α) reaction such as

$${}_{12}Al^{27} + {}_0n_1 \rightarrow [{}_{13}Al^{28}] \rightarrow {}_{11}Na^{24} + {}_2He^4$$

(ii) (n, p) reaction such as

$${}_7N^{14} + {}_0N^1 \rightarrow [{}_7N^{15}] \rightarrow {}_5C^{14} + {}_1H^1$$

(iii) (n, γ) reaction such as

$$_{13}Al^{27} + {}_{0}n^{1} \rightarrow [{}_{13}Al^{28}] \rightarrow {}_{13}Al^{28} + \gamma$$

(iv) (n, 2n) reaction such as

$$_{13}Al^{27} + {}_{0}n^{1} \rightarrow [{}_{13}Al^{28}] \rightarrow {}_{13}Al^{26} + {}_{0}n^{1} + {}_{0}n^{1}$$

11.4 COMPOUND NUCLEUS :

In 1936 Bohr proposed the theory of compound nucleus. According to Bohr's theory the nuclear reaction takes place in two steps.

1. The incident particle is absorbed by the initial or target nucleus to form a compound nucleus.

   Incident particle + initial nucleus →Compound nucleus ....(1)

2. The compound nucleus disintegrates by ejecting a particle or a γ - ray leaving the final or product nucleus.

   Compound nucleus →Product nucleus + Outgoing particle ....(2)

The above two steps are taken as independent steps. The mode of disintegration of the compound nucleus depends only all its energy, angular momentum and parity. The mode of disintegration does not depend on the specific way in which the compound nucleus is formed. This is according to Bohr's assumption and is found valid.

The compound nucleus is a many body system of strongly interacting particle. It is formed by the amalgamation of an incident particle B with target nucleus A.

$$A + B \rightarrow C^{*}$$

The incident particle captured by a nucleus gives up its energy to few nucleons in the nucleus. Due to interaction of these nucleons with all the others, the energy is quickly distributed among all the nucleons of the compound nucleus. The new nucleus thos formed is in excited state.

A compound nucleus once formed can decay in a number of different ways each with its intrinsic probability.

Example : The bombardment of $_{11}Na^{23}$ with α - particle or by other methods. A compound nucleus $_{13}Al^{27}$ is formed. Then compound nucleus decays at least in following ways.

$$Al^{27} \rightarrow Na^{23} + \alpha;\ Al^{27} \rightarrow Mg^{27} + d$$

$Al^{27} \rightarrow Mg^{26} + p; Al^{27} \rightarrow Al^{26} + n$

$Al^{27} \rightarrow Al^{27} + \gamma$ - ray

The compound nucleus has a life time which is long (10^{14} to 10^{-15}s) compared to the time taken by the nucleon to traverse a nucleus (10^{-29} to10^{-23}s). This finite life time is because there can always be a statistical fluctuation in the energy distribution which concentrate enough energy on a nucleus allow to escape.

11.5 DIRECT REACTION :

A direct reaction is one which proceeds with out the formation of a compound nucleus. In this reaction the incident particle interacts with target nucleus for a very much shorter time ($\sim 10^{-21}$s) than the life time of a compound nucleus ($\sim 10^{-15}$s). At low energies compound formations mechanism and at high energies direct reaction mechanism will prevail. The term direct reaction is used for a variety of nuclear processes including inastic collisions or scattering, stripping and its inverse, the pick up reaction.

(i) In an inelastic scattering the incident nucleon, on entering the motion, it may strike another nucleon in the surface region, lose some energy and comes out with a reduced energy. The entire process occurs in times of the order of $\frac{R}{v} \sim 10^{-21}$s where R is the nuclear radius and v the velocity of the incident particle.

(ii) In stripping reaction the incoming compound particle consisting of more than one nucleon splits in to two fragments, one of which is absorbed by the target nucleus and the other continues more or less undisturbed.

(iii) In pickup reaction incident particle removes one or two nucleons from the target nucleus.

(p, α), (p, t), (p, He^3), (d, t) and (d, He^3) are the examples for pick up reaction.

11.6 SOLVED EXAMPLES:

1. Calculate the energy generated in KWH, when 0.1Kg of ${}_3Li^7$ is converted into ${}_2He^4$ by proton bombardment. [${}_3Li^7$ = 7.0183 amu, ${}_2He^4$ = 4.0040 amu, ${}_1H^1$ = 1.0081amu]

[Ans:6.47 × 10^6kwh]

Sol: Mass defect $\Delta m = ({}_3Li^7 + {}_1H^1) - 2({}_2He^4)$

$= (7.0183 + 1.0081) - 2(4.0040) = 0.0184$ amu

Energy released Q in the reaction $_3Li^7 + {}_1H^1 \rightarrow 2({}_2He^4) + Q$ is

Q= 0.0184 + 931 Mev $= 27.408 \times 10^{-13}$ joule. .... (1)

Mass of $_3Li^7$ = 7.183 amu = 1.176×10^{-28}kg .....———... (2)

Heat generated by $_3Li^7$ $= 1.176 \times 10^{-28} \times 24.408 \times 10^{-13} = 27.408 \times 10^{-13}$J

Heat generated by 0.1kg of $_3Li^7 = \left[\frac{27.408 \times 10^{-3}}{1.173 \times 10^{-26}}\right](0.1) = 6.47 \times 10^6$ kwh

2. **Find the amount of energy released when all the nuclear in 1Kg of deuterium fuse by the reaction. 6 $_1H^1 \rightarrow 2({}_2He^4) + 2p + 2n + 43$MeV.(Atomic mass of deuterium = 2.01478 amu)**
[Ans:21.413×10^{26} MeV]

Sol: Number of atoms in 1kg of $_1H^1 = \frac{6.02 \times 10^{23} \times 1000}{2.01478}$

One nucleas of $_1H^2$ produce energy $= \frac{43}{6}$ MeV

$\therefore$ energy induced by 1 kg of $_1H^2$ $= \frac{6.02 \times 10^{23} \times 1000}{2.01478} \times \frac{43}{6} = 21.413 \times 10^{26}$ MeV

11.7 SUMMARY :

1. A process in which the characteristic of incident nuclear particle undergoes a change in the bombardment of a nuclei is called a nuclear reaction.

2. In nuclear reactions (i) the atomic number of reactions must be equal to total atomic number of product particles (ii) the total sum of atomic mass encumber on both sides of be equation must be equal.

3. The unclear reactions are useful for experimental verification of eruption's equation $E = mc^2$

4. In elastic scattering the direction of incident particle changes but target nucleus remains unaffected.

5. In the inelastic scattering the change in direction and low of energy for incident particle and also the target nucleus excited.

6. A channel is a possible pair of product nucleus and outgoing particle, each in a definite nutum state.

7. A direct reaction is one which proceeds without formation of a compound nucleus.

11.8 KEY WORDS:

Nuclear reaction, scattering, disintegration, channels, compound nucleus, direct reaction.

11.9 SELF-ASSESSMENT QUESTIONS:

1. What is nuclear reaction
2. Explain the concept of nuclear reaction channel
3. Explain the concept of compound nucleus
4. Explain the concept of the direct reactions
5. Mention briefly the kinds of nuclear reactions with examples
6. Write an essay on Bohr theory of compound nucleus

11.10 REFERENCE BOOKS:

1. Unified physics vol4 Dr. S.C. Gupta & S.Gupta Jaiprakash nath and Co, meerit
2. A test book of common core physics Sri Vikas Publications, Guntur

UNIT-3

LESSON-12

NUCLEAR MODELS AND NUCLEAR FISSION AND FUSION

OBJECTIVES :

After the completion of this lesson the student will be able to

1. Understand about the Nuclear models i.e liquid drop model and shell model.

2. Understand about the Nuclear fission and fusion

3. Understand about the carbon – nitrogen cycle and carbon - carbon cycle

STRUCTURE :

12.1 INTRODUCTION :

To account for the aspects of nuclear properties and behaviour, various nuclear models have been proposed. Such models based on the macroscopic properties and electron shell of an atom. The corresponding models are called liquid drop model, shell model etc. The liquid drop model was proposed by Bohr. This model is based on certain assumptions but fails to explain the magic numbers. In shell model, the nucleus consists of series of proton's and neutrons placed in shells just like electrons in describe shells of atom.In shell model, the nucleus consists of series of proton's and neutrons placed in shells just like electrons in describe shells of atom.

The discovery of Nuclear fission stated from the attempts of Fermi in 1934, to produce transuranic elements. In 1939 Otto Hahn and Strassman discover that when Uranium-92 was bombarded with neutrons, it split into barium and krypton. Bohr and wheeler explained the process of nuclear fissionusing the liquid drop model.

In nuclear fusion process, the lighter nuclei are fused together to form a heavier and stable nucleus with release of large amount of energy. It is a thermonuclear reaction. Hydrogen bomb is based an this process. Bethe suggested that the production of stellar energy is by thermonuclear reactions in which protons are transformed into helium nuclei. According to Bethe the nuclear fusion takes place under proton-proton cycle and carbon – nitrogen cycle.

12.2 LIQUID DROP MODEL :

This model is proposed by Bohr. According to this model, the nucleus is similar to a small electrically charged liquid drop. The nucleons move within this encloses like molecules in liquid drop. The nucleons always remain a constant distant apart and share among them the total energy of the nucleus. The nucleons deep inside the nucleans are attracted from all sides by neighboning nucleus while those on the surface are attracted from one side only.

The spherical surface which encloses the nucleus may be regarded as analogous to surface tension which holds a water drop to the evaporation of particles from a liquid surface.

The following analogies between atomic nucleus and a small drop of liquid support the liquid drop model of the nucleus.

1. The small liquid drop is spherical because of surface tension effects and the atomic nucleus is assumed to be spherical.
2. The density of a spherical liquid drop is independent of its volume. This is also true for atomic nucleus.

3. The molecules in liquid drop interact over short ranges as compared to the diameter of the drop. Similarly the nuclear in a nucleus interact with their immediate neighbors.
4. The surface tension force acting at the surface of the drop are analogous to the potential barrier effects at the surface.
5. If a liquid drop is made to oscillate, it tends to separate into two parts of equal size. Similarly heavy nuclei break into lighter fragments after capturing neutrons (nuclear fission).
6. The molecules in the drop move over short distances with thermal velocities. If the temperature is increased due to the increase of thermal agitation, the evaporation of molecules takes place.

   Similarly the nucleus possess definite kinetic energy within the nucleus. If the energy is given to the nucleus by the bombardment of light particles a compound is formed, which emits nucleus almost immediately.

Merits :

1. It has been successfully applied in describing nuclear reaction and explaining fission.
2. The calculation of atomic masses and binding energy can be done with good accuracy.

   However the model fails to explain other properties in particular magic numbers.

12.3 THE SHELL MODEL:

The nucleus revolves round the center of mass of the nucleus, like the electrons round the nucleus. In addition to orbital motion they have spin. They from closed shells and sub shells similar to those of the electrons of an atom.

Each nucleus moves independently of one another in a potential (negative due to attractive force) which represents the all raged effect of its interaction with other nucleus. Each nuclear is surrounded by the same number of nearest neighbors, so that the potential constant. As we proceed towards the surface the number of neighbors is less and so the potential well the energies of the individual nucleus are determined. There exists a discrete set of allowed energy nucleus.

Separate energy levels exist for protons and neutrons. So protons and neutrons have separate shells and sub shells.

The lowest energy level is $IS_{1/2}$ The angular momenters for S is equal to zero. As j is equal to $(1 \pm \frac{1}{2})$, j an take two values $+\frac{1}{2}$ and $-\frac{1}{2}$. So two nuclears can be accomodated in this shell.

In $_2He^4$ the proton levels and nevtron levels are filled assigining stability to $_2He^4$.

The next higher level (second level) is 1P shell. The orbital angular moment is nor equal to zero. The spin – orbit coupling effect this level. In this level for p, $l = 1$ and $j = 1 \pm \frac{1}{2}$.

Sequential order of the energy levels of a nuclear in a square well is shown in the Fig12.2.1. The left side of the figure gives the energy levels without spin – orbit interaction; the right side fives the levels with spin orbit interaction. The levels indicate the energy of each shell when all the shells below it are felled and all shells above are empty. The numbers on the far right give the cumulative number of nuclears required to fill the shells.

$\therefore j$ can take the values of $\frac{3}{2}$ and $\frac{1}{2}$

m_j takes $(2j + 1)$ values for $j = \frac{3}{2}$ there are 4 values, so 4 nucleons exist in that level.

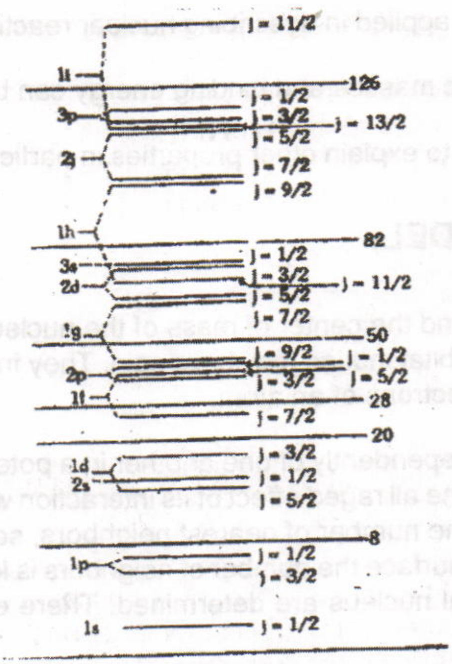


FIG12.2.1

Fig. 12.2.1 shows the number of energy levels and number of nucleons in each shell. For $j = \frac{1}{2}$ there are 2 values for m_j. So 2 nucleons exist in that level in total, 1P can accommodate 4 + 2 = 6 nucleons

For $_8O^{16}$, 1S level is filled with two nucleons and 1P level is filled with 6 nucleons. The proton shells are filled with 8 protons and the neutron levels are filled with 8 neutrons assigning stability to $_8O^{16}$. To fill all the two levels 8 nucleons either of proton or neutron levels are required.

The next higher level (3rd level) contains 1-d and 2-s sublevels 2-s level can accommodate two nucleons.

For 1-d level l = 2 and j has two levels 5/2 and 3/2. there com exist (2j + 1) nuclears with j = 5/2. This comes to 6 nucleus.

For j = 3/2 with four nucleolus can exist. So in total this level can accommodate 10 nuclears.

To fill all the three levels 20 nucleons either protons or neutrons are required.

Thus the forth level contains fine sublevels These are $1f_{7/2}$, $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$. Altogether (8 + 4 + 6 + 2 +10) 30 nuclears are accomodated. Upto foer levels it requires 50 nuclears to fill all four shells. The fifth level contains $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$, $1h_{11/2}$ states. The number of nuclears required for filling the shell is (8 + 6 + 4 + 2 + 12 = 32). To fill all the fine shells it requires 82 nucleons.

Consider Sn_{50}^{132}. The 50 protons fill the four proton levels and the remaining 82 neutrons fill all the fine neutron level assigning the stability to Sn_{50}^{132}

when Z or (A-Z) take the values 2,8,20,28,50,82,126 the nucleus is stable. These are called magic numbers.

Merits : The shell model has been successful to account for the magic numbers and also the observed angular moments, magnetic moments and electric quadrapole moments of nuclei and also for the distribution of nuclear isomers.

Demerits : It fails to explain and account for the large nuclear quadrapole moments and spheroidal shapes of many nuclei

12.4 NUCLEAR FISSION :

The process of breaking up of the nucleus of a heavy atom into two, more or less equal fragments with the release of a large amount of energy is known as nuclear fission.

For example when uranium ${}_{92}U^{235}$ is bombarded with a slow neutron ${}_{0}n^{1}$, Uranium nucleus captures the slow neutron and forms an unstable compound nucleus. The compound nucleus splits into nearly equal parts. Some neutrons are also released in the process.

The above nuclear fission can be written as follows

$$ {}_{92}U^{235} + {}_{0}n^{1} \rightarrow \left[{}_{92}U^{236}\right] \rightarrow {}_{56}Ba^{141} + {}_{36}Kr^{92} + 3\,{}_{0}n^{1} + \text{energy} $$

Bohr and wheeler explained nuclear fission phenomenon successfully on the basis of the liquid drop model of the nucleus. This type of reaction takes place in atom bombs.

12.5 NUCLEAR FUSION :

Nuclear fusion is a process in which two or more lighter nucleus combine together to form a single heavy nucleus.

For example when four hydrogen nuclei are fused together, a helium nucleus is formed.

$$ 4\,{}_{1}H^{1} \rightarrow {}_{2}He^{4} + 2\,{}_{1}e^{0} + 2\nu + 26.7\ \text{Me.V} $$

The fusion of two nuclei is more difficult to achieve as compared to fission of heavy nucleus. This is because of strong electrostatic repulsion between two positively charged nuclei while bringing them very close so that short range nuclear force is developed between them, to fire these nuclei. Hydrogen bomb is a device which makes use of the principle of nuclear fusion.

12.6 ENERGY PRODUCTION IN STARS (PROTON – PROTON AND CARBON – NITROGEN CYCLE) :

The temperature of stars are very high and they radiate enormous amount of energy. The sun is radiating energy at the rate of 3.8×10^{26} Joules of energy each second. Its age is 5×10^{9}years . Now the question is that what is the source of this stellar energy? The origin of this energy is neither chemical nor gravitational. The fusion of protons is supposed to be origin of energy of sun and other stars. According to Bethe, the fusion is taking place under the following two different cycles

(i) Proton – proton cycle (ii) Carbon – nitrogen cycle

(i) Proton – Proton cycle : In proton – proton cycle, the first step involves the fusion of two proton to form a deuteron nucleus releasing a positron and energy. The reaction is given by

$$_1H^1 + {}_1H^1 \rightarrow {}_1He^2 + {}_1e^0 + Q_1$$

The deuteron then combines with another proton and forms helium ($_2He^3$). The corresponding reaction is given below

$$_1H^2 + {}_1H^1 \rightarrow {}_2He^3 + \gamma$$

The two helium 2 nuclei fuse to produce helium (2He4) nuclei. The corresponding reaction is given below

$$_2H^3 + {}_2He^3 = {}_1He^4 + 2{}_1H^1 + Q_2$$

So that we have

$$4{}_1H^1 \rightarrow {}_2He^4 = 2{}_{-1}e^0 + Q$$

The proton - proton cy

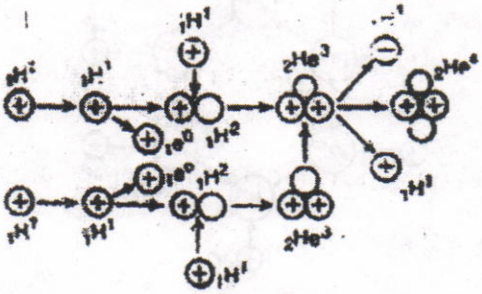


FIG 12.6.1

(ii) Carbon – nitrogen cycle : In this cycle the synthesis of hydrogen nuclei with carbon takes place. The carbon nuclei absorbs the protons in succession and ultimately discharge α - particle becoming carbon nuclei again.

The reactions are given below.

$$_6C^{12} + {}_1H^1 \rightarrow {}_7N^{13} + Q_1$$

Where Q_1 is the energy released

The radioactive nitrogen 13 decays as

$$_7N^{13} \rightarrow {}_6C^{13} + {}_{+1}e^0$$

Now stable $_6C^{13}$ nucleus reacts with another proton, thereby liberating more energy

$${}_6C^{13} + {}_1H^1 \rightarrow {}_7N^{14} + Q_2$$

Where Q_2 is additional energy released during nuclear reaction

The stable ${}_7N^{14}$ again combines with a proton to form oxygen (${}_8O^{15}$) with the release of more energy Q_3, thus

$${}_7N^{14} + {}_1H^1 \rightarrow {}_8O^{15} + Q_3$$

Now oxygen (${}_8O^{15}$) decay as

$${}_8O^{15} \rightarrow {}_7N^{15}\ {}_{+1}e^0$$

Nitrogen (${}_7N^{15}$)then again capture a proton to become carbon (${}_6C^{12}$) with the release of α - particle (${}_2He^4$)

$${}_7N^{15} + {}_1H^1 \rightarrow {}_5C^{12} + {}_2He^4$$

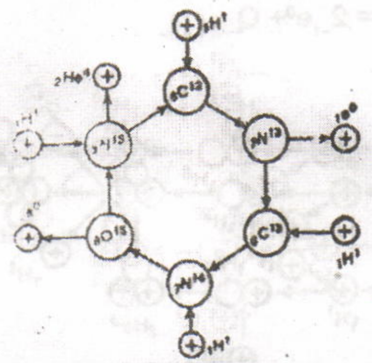


FIG 12.6.2

$$4\,{}_1H^1 \rightarrow {}_2He^4 = 2\,{}_{+1}e^0 + 27MeV$$

The entire carbon nitrogen cycle is shown in figure(12.6.2)

12.7 SOLVED EXAMPLES :

1. **If 7.2g of uranium is completely converted into energy how many KWH energy is obtained?** **[Ans:180 ×10⁶KWH]**

Sol: M = 7.2g = 7.2 × 10^{-3}kg

c = velocity of light = 3 × 10^8 m/s

Energy release $= E = mc^2$

$$= 7.2 \times 10^{-3} \times (3 \times 10^{8})^2$$

$$= \frac{7.2 \times 10^{-3} \times 9 \times 10^{16}}{36 \times 10^{5}} \text{KWH} = 180 \times 10^{6} \text{KWH}$$

2. In U^{235}_{92} fusion 200 MeV average energy is released. Calculate the number of fissions per second to produce one kilo watt of power? [Ans:31.25 × 10¹²]

Sol: The energy released per fission= 200 MeV = 200×10^6eV

$$= 200 \times 10^6 \times 1.6 \times 10^{-19} \text{J} = 3.2 \times 10^{-11} \text{J}$$

$$\therefore \text{Number of fissions per second} = \frac{\textit{Energyrequired}}{\textit{Energyreleased per fission}} = \frac{1 \times 10^3}{3.2 \times 10^{-11}} = 31.25 \times 10^{12}$$

3. Calculate the amount of energy released in Joules when 1gm of Uranium U^{235} under goes fission. (Avogadro's number = 6.023×10^{23}, average energy released per fission = 200 MeV) [Ans:8.2 × 10¹⁰ J]

Sol: The number of U^{235} of atom in 1gm of substaice $= \frac{6.023 \times 10^{23}}{235} \times 1 = 2.563 \times 10^{21}$ atoms

$\therefore$ Fission energy released= $2.563 \times 10^{21} \times 200$ MeV

$$= 2.563 \times 10^{21} \times 200 \times 10^6 \times 1.6 \times 10^{19} \text{J} = 8.2 \times 10^{10} \text{J}$$

4. The fusion ${}_1H^2 + {}_1H^2 \rightarrow {}_2He^4$ + energy is proposed to be used for production of power. The efficiency of process in 30%. Find how much kg of deuterium will be consumed in a day for an output of 50.000kw. (Mass of ${}_1H^2$ = 2.0178 amu and mass of ${}_2He^4$ = 4.00388 amu) [Ans:2.519 × 10⁻²kg]

Sol: The mass difference $\Delta m = (2.01478 \times 2) - 4.00388$

$$= 0.02568 \text{ amu} .$$

The energy released in each fission = $0.02568 \times 931 = 23.91$ MeV

The output energy $= \frac{30}{100} \times 23.91 = 7.173$ MeV

Output per each devterium atom $= \frac{7.173}{2} = 3.587$ MeV

No' of deuterium atoms required $= \frac{50{,}000}{3.587 \times 10^{6} \times 1.6 \times 10^{-19}} = 8.712 \times 10^{19}$

Equavalent mass of deuterium per second$= 8.712 \times 10^{19} \times \frac{2.01478}{6.02 \times 10^{23}} = 2.916 \times 10^{-7}$ kg s^{-1}

Consumption of deuterium per day$= 2.916 \times 10^{-7} \times 24 \times 60 \times 60 = 2.519 \times 10^{-2}$kg

5. **Certain stars obtain part of their energy by the fusion of three α - particles to from a $_{6}C^{12}$ nucleus. How much energy does each such reaction evolued? The mass of Helium atom is 4.00260 amu while the mass of electron is 0.00055 amu. the mass of $_{6}C^{12}$ is 12 amu.** **[Ans:7.26 MeV]**

Sol: Mass of $_{2}He^{4}$atom $= 4.00260$ amu

$\therefore$ Mass of Helium $= 4.0026 -$ mass of two electrons

$= 4.0026 - 2 \times 0.00055 = 4.00150$ amu

Simularly, the mass of $_{6}C^{12}$ nucleus

$= 12.0000 - 6 \times 0.00055 = 11.99670$ amu

When 3α - particle fuse a $_{6}C^{12}$ nucleus is formed. Hence the mass loss is given by

$3 \times 4.00150 - 11.99670 = 0.00780$ amu

Energy evolved $= 0.00780 \times 931 = 7.26$ MeV

12.8 SUMMARY:

1. To account for the aspects of nuclear properties and behaviour, various nuclear models have been proposed. Such models based on the macroscopic properties and electron shell of an atom. The corresponding models are called liquid drop model, shell model etc.

2. The liquid drop model was proposed by Bohr. This model is based on certain assumptions but fails to explain the magic numbers.

3. In shell model, the nucleus consists of series of proton's and neutrons placed in shells just like electrons.

4. The discovery of Nuclear fission started from the attempts of Fermi in 1934, to produce transuranic elements. In 1939 Otto Hahn and Strassman discover that when Uranium-92 was bombarded with neutrons, it split into barium and krypton.

5. The process of breaking up of the nucleus of a heavy atom into two, more or less equal fragments with the release of a large amount of energy is known as nuclear fission.

6. Nuclear fusion is a process in which two or more lighter nucleus combine together to form a single heavy nucleus.

7. The fusion of protons is supposed to be origin of energy of sun and other stars.

12.9 KEY WORDS:

Liquid drop Model, Shell Model, Nuclear fission, Nuclear fusion,Energy Production in stars Proton – proton cycle, Carbon – nitrogen cycle.

12.10.SELF-ASSESSMENT QUESTIONS:

1. Discuss the liquid drop model of the nucleus.

2. What are the various nuclear models. Give briefly the liquid drop model of the nucleus.

3. Explain how the shell model of nucleus accounts for the existance of magic numbers.

4. What is meant by nuclear fusion.Explain how energy released is more in fusion than in fission.

5. What is meant by nuclear fission.

6. Explain Proton – proton cycle, Carbon – nitrogen cycle in nuclear fusion.

7. Write a short note on energy production in stars.

EXERCISES:

1. Calculate the amount of energy released by fissioning one gram of uranium in Jouls. During fission only 0;1$ of mass is converted in to energy. [1 amu = 1.66 x 10^{-27}kg = 931 MeV, Mass of uranium = 235 amu]
Ans: 8.97 x 10^{-7} J

2. Calculate the amount of energy released by fusing two deuterium nuclei into helium nucleus.

(Mass of $_1H^2$ = 2.0178 amu and mass of $_2He^4$ = 4.00388 amu) **Ans: 24 MeV**

12.11 REFERENCE BOOKS:

1. Unified physics vol-4	Dr. S.C. Gupta & S.Gupta
2. A test book of common core physics	Sri Vikas Publications, Guntur
3. Introductory of Atomic Spectra	H.F. White
4. Physics of atom	Wher and Richards
5. Prospective of Modern Physics	A.Beiser
6. Elements of Modern Physics	Patil

UNIT-4

LESSON-13

CRYSTALLOGRAPHY

Objectives :

After studying this lesson the student is able to know about

i) Classification of solids as crystalline and amorphous and the distinction between them.

ii) Nature of crystalline materials, ordering, Translational vector.

iii) Lattice symmetry elements, unit and primitive cell, two and three dimensional Bravais lattices.

iv) Crystal systems.

v) Index system and Miller indices.

Structure :

13.1 Introduction :

Usually it is regarded that matter exists in three states - solid, liquid and gas. Liquids and gases togethe are referred to as fluids; property of flow being common for those two states. Rigidity in the form or shape is the criterion that distinguishes solids from fluids. In modern approach matter is classified into condensed matter and gaseous states taking "definite volume" as the criterion. Solids and liquids come under the class of condensed matter.

Matter in solid state can be divided into two classes.

i) Crystalline and (ii) non crystalline or amorphous.Crystalline matter, is further subdivided into single rystal and polycrystalline types.

3.2 Distinguishing Crystalline and Amorphous materials :

Crystalline and Amorphous materials are distinguishes as follows :

	Crystalline Solids	Amorphous Solids
1.	In these atoms or molecules or ions are arranged in a regular manner.	In these atoms or molecules or ions are arranged in a random manner.
2.	These are anisotropic (have different values for physical parameters like dielectric constant in different directions).	These are isotropic
3.	The order (i.e. arrangement) is of long range.	There is no long range order (practically no order, or said to have very short range order)
4.	These will have a sharp melting point (melting occurs at a definite temperature)	Melting occurs over a range of temperature i.e. starts at one temperature and completes at another temperature.
5.	The cooling [illegible] for these solids has a break.	Generally cooling curve for these solids is smoother and continuous.
6.	These solids have generally high densities.	Generally, these solids have low densities.
7.	These will have definite neat of fusions.	These will not have definite heat of fusion.
8.	These have clevage surfaces.	No clevage surfaces.
9.	These are considered as true solids.	These are considereed as pseudo solids.

13.3 Crystals - Ordering :

In Crystalline materials, atoms or molecules or ions are stacked in a regular array in three dimensions and such a regular arrangement is not there in amorphous materials. The repitition at regular intervals in three dimensions that occurs in crystals results in an environment at one location to be identical in all respects at another point inside the material periodically.

The structure of all crystals in which periodicity is there can be described in terms of "lattice".

Lattice : It is a mathematical (imaginary) concept and is defined as an infinite number of points with a property that the arrangement about any point is same or identical with that about any other point. If all the points are confined to a single plane it is called two dimensional lattice. If the points are distributed in three dimensional space, the corresponding lattice is called a space lattice.

An atom or group of atoms, identical in composition and orientation is called 'Basis' or 'motifi'. Attached to each lattice point, it gives the actual crystal structure. Thus

Latice + Basis = Crystal

13.4 Symmetry Considerations :

As crystals have some regular ordered arrangement and periodicity, they possess some types of symmetry. They can be described by certain operations. The "symmetries" are called symmetry elements and the operations for describing those are called symmetry operations.

13.4.1 Symmetry elements and operations :

Following are the examples of symmetry elements.

1. Translation 2. Rotation 3. Reflection

A symmetry operation is one that leaves the crystal and the environment invariant.

13.4.2 Translational Vector :

In order to represent lattice points in space, a coordinate system is required. All the lattice points can be generated by translating three non coplanar unit vectors in three directions. The three non coplanar directions constitute a coordinate system. The three coordinate axes constitute the three crystallographic axes.

Let a,b,c be the unit vectors in three dimensions along the crystallographic axes. By choosing any one lattice point as origin then the location of any other lattice point can be defined (w.r.to origin) by.

$T = n_1 a + n_2 b + n_3 c$ where n_1, n_2, n_3 are arbitrary integers.

T is called translational vector.

As Basis or motif is attahced to each lattice point in crystals, basis repeats itself in all directions by means of a translation operation T.

Rotation : Let us imagine a line (axis) passig through the centre of the cube. If the cube is rotated through $\pi/4$, and is left invariant, then the cube is said to have fourfold symmetry and the axis is called symmetry axis (Fig 13.1).

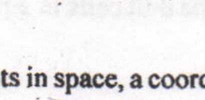


Fig 13.1

Reflection : Let us imagine a reflectory plane or plane mirror is the position PQRS. The part ASRDEPQH the cube is just as the image (SBCRPFGQ) projected by mirror placed at PQRS (Fig13.2(a)). Hence the cube is said to have reflection symmetry.The other two cases can be understood similarly.

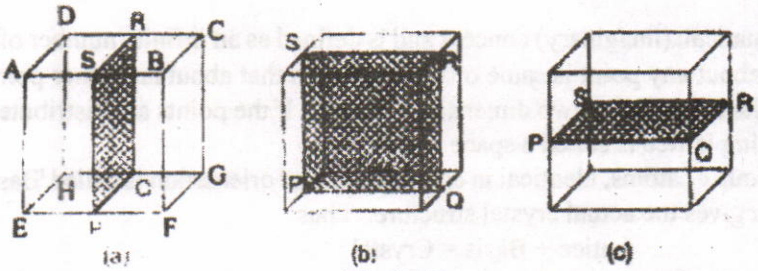
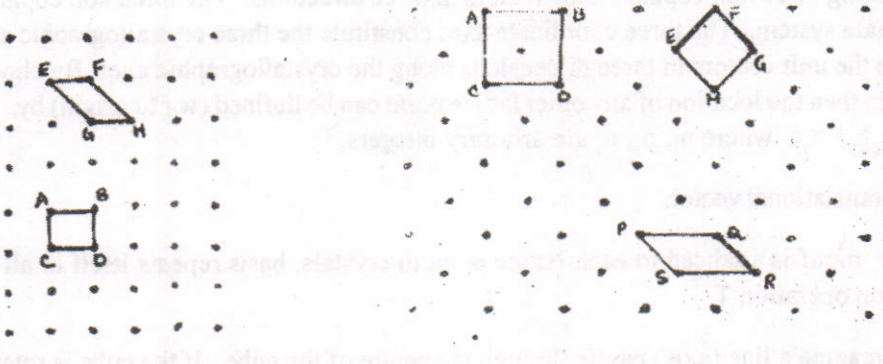


Fig 13.2

The reflection caused by PQRS keeps the cube invariant. Hence it has reflection symmetry and PQRS is called mirror plane or symmetry plane.

13.5 Unit Cell :

It is convinient to subdivide the cyrstal structure into small entities which by repitition in three dimensions describe the crystal as a whole. Such entitiy can be considered as a building block for the crystal and is called unit cell. We already considered that crystal structure can be described with the help of a lattice. Hence concept of unit cell can be understood also with respet to the lattice. The choice of "Unit Cell" is not unique. The Fig 13.3 (a) & (b) show the different ways of selecting the unit cells in a plane (two dimensional) lattice.



(a) (b)

Fig 13.3

A unit cell with only one lattice point attached to it is called primittive (unit) cell. Primittive cell is the smallest unit cell.

In Fig 13.3(a) ABCD & EFGH are the primittive cells.

In Fig 13.3(b) ABCD is non primittive unit cell (two lattice points are attached to it)

In Fig 13.3(b) EFGH and PQRS are primittive cells.

Note : In the cases of ABCD & EFGH of Fig 13.3 (a) and EFGH & PQRS of Fig Fig 13.3(b), the lattice points at the corner contribute only $\frac{1}{4}$ of it and the four points at four corners as a whole contribute $\left(4 \times \frac{1}{4} = 1\right)$ only one lattice point. In Fig 13.3(b) in case of ABCD the four lattice points at corners $\left(4 \times \frac{1}{4}\right)$ contribute one lattice point and further it has one lattice point inside. Thus two lattice points are attached to it and thus it is a non-primittive cell.

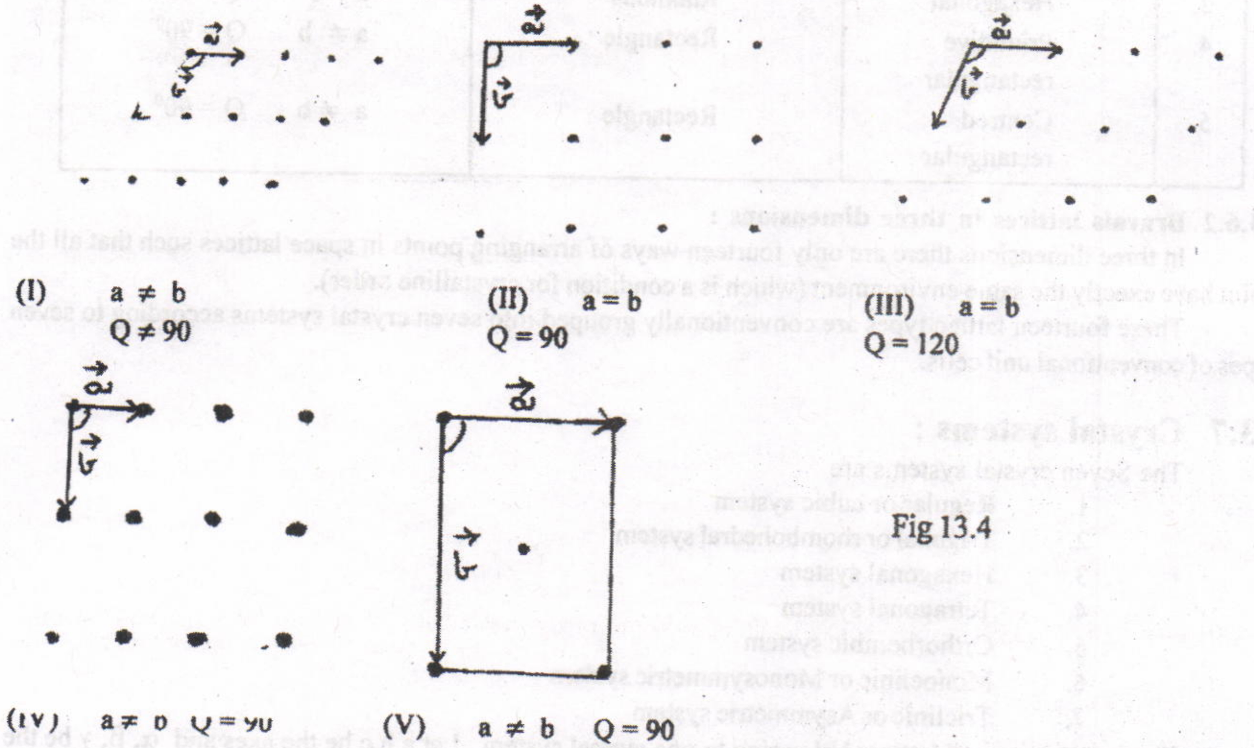
In (three dimensional) space lattice it is convinient to consider parallelopiped as a unit cell. The unit cell may be defined as the smallest volume which when repeated in all directions builds the crystal.

13.6 Bravais lattices :

As Bravais in 1948 introduced first the concept of lattice to describe the periodicity in crystals, these lattices are called Bravais lattices. In general infinite number of lattices are possible because there is no restriction on the lengths of unit vectors in the directions of crystallographic axes .

13.6.1 Bravais lattices in two dimensions :

Let a & b be the unit vectors in the directions of crystallographic axes and Q be the angle between those. The possible types in two dimensions are as follows :



(I) $a \neq b$ $Q \neq 90$

(II) $a = b$ $Q = 90$

(III) $a = b$ $Q = 120$

(IV) $a \neq b$ $Q = 90$

(V) $a \neq b$ $Q = 90$

Fig 13.4

(I) Oblique lattice : This lattice has rotational symmetry. The lattice is invarient only under a rotation of $\frac{2\Pi}{n}$ where n = 1 or 2. This is a general lattice.

The other four types are of special types.

(II) Here $a = b$ and $Q = 90$. It is called square lattice. Rotational symmetry under a rotation of $\left(\frac{2\Pi}{4}\right)$

(III) $a \neq b$ and $Q = 120$. Hexagonal lattice. It has rotational symmetry under a rotation of $\left(\frac{2\Pi}{4}\right)$

(IV) $a \neq b$ $Q = 90$ - Rectangular Lattice

(V) $a \neq b$ $Q = 90$ - Centered rectangular Lattice

Bravais lattices in two dimensions.

S.No.	Lattice Type	Conventional Unit Cell	Axes and angles	
1.	Oblique	Parallelogram	$a \neq b$	$Q \neq 90^0$
2.	Square	Square	$a = b$	$Q = 90^0$
3.	Hexagonal	Rhombus	$a = b$	$Q = 120^0$
4.	Primittive rectangular	Rectangle	$a \neq b$	$Q = 90^0$
5.	Centred rectangular	Rectangle	$a \neq b$	$Q = 90^0$

13.6.2 Bravais lattices in three dimensions :

In three dimensions there are only fourteen ways of arranging points in space lattices such that all the point have exactly the same environment (which is a condition for crystalline order).

These fourteen lattice types are conventionally grouped into seven crystal systems according to seven types of conventional unit cells.

13.7 Crystal systems :

The Seven crystal systems are

1. Regular or cubic system
2. Trigonal or rhombohedral system
3. Hexagonal system
4. Tetragonal system
5. Orthorhombic system
6. Monoclinic or Monosymmetric system
7. Triclinic or Asymmetric system

There may be no. of lattices belonging to one cyrstal system. Let a,b,c be the axes and α, β, γ be the angles between the directions of crystallographic axes in these lattices.

1) **Regular or cubic system :Fig 13.5**

In the cubic system there are three types of lattices depending upon the composition of unit cell. They are

a) Simple Cubic : In simple cubic, particles are only at the corners of cube.Fig 13.5(a)

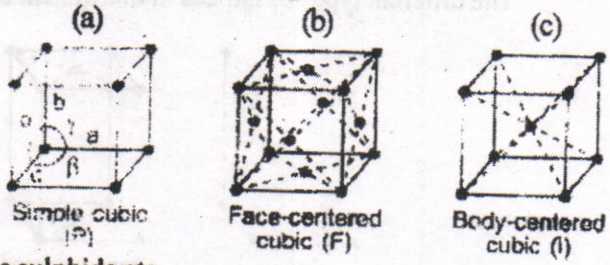
b) Body centered : In body centered, the particles are at the corners as well as at the centre of the cube.Fig 13.5(b)

c) Face Centered : In these, particles are at the corners as wll as at the centre of each of the faces of cube.Fig 13.5(c)

Ex: Examples of cubic crystal are diamond, zinc sulphide etc.

In these crystals, $a = b = c$ and $\alpha = \beta = \gamma = 90$

Fig 13.5



2. Trigonal or Rhombohedral system:Fig 13.6

In this system, a=b=c and $\alpha = \beta = \gamma \neq 90$

i.e. the crystals are made up of three equal axes.

Ex : Examples of this system are quartz and calcite.

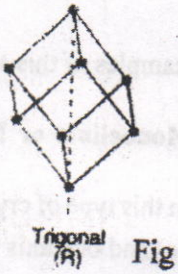


Fig 13.6

3. **Hexagonal system:Fig 13.7**

The Hexagonal system has eight faces. The two equilateral axes are equal (a=b) and intersect at an angle of $\gamma = 120$. The vertical axis has different length ($c \neq a$ or b) and is at right angles to the equilateral axes. $\alpha = \beta = 90$.

Ex: Zincite (Zno), Ice (H_2O) etc.

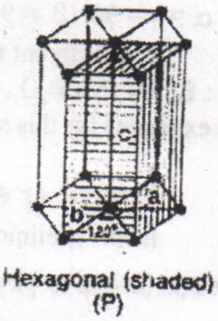


Fig 13.7

4. **Tetragonal system :Fig 13.8**

In this system, the three axes are right angles to each other i.e., $\alpha = \beta = \gamma = 90$ and the two lateral axes are equal i.e. $a = b \neq c$

The crystal is characterised by a four fold or tetragonal axis of symmetry.

The two sub types in these are as shown in Fig 13.8

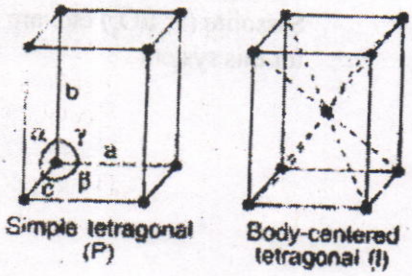


Fig 13.8

Ex : Examples for this system are ordinary white tin, Indium etc.

5. Orthorhombic system : Fig 13.9

In this system cyrstallographic axes are unequal i.e. $a \neq b \neq c$ and they are right angles to each other i.e. $\alpha = \beta = \gamma = 90$

The vertical axis is one of the two fold or diagonal symmetry only.

The different types of lattices in this system are as shown below.

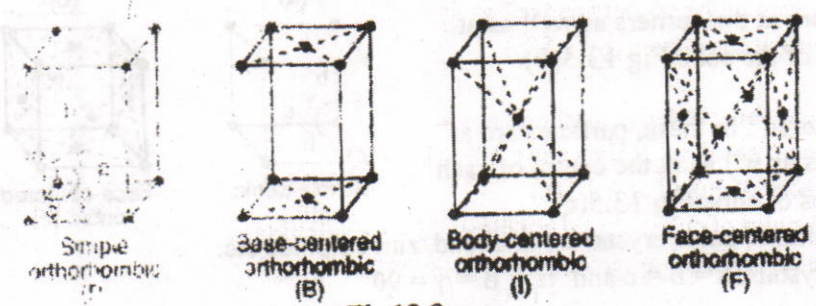


Fig 13.9

Ex: Examples of this system are celestine ($SnSo_4$), Olivine (Mg_2Sio_4), Carnallite ($Kel. Mgcl_2 . 5H_2O$) etc.

6. Monoclinic or Monosymmetric system :

In this type of crystals, crystallographic axes are uneuqal ($a \neq b \neq c$) and one axis is perpendicular to the other two axes i.e. $\alpha = \gamma = 90, \ \beta \neq 90$

The different types of lattices in this system are as shown here.

Ex : Borox ($Na_2B_4O_7 \cdot 10H_2O$), Cryolite (Na_3AlF_3) etc. are the examples for this system

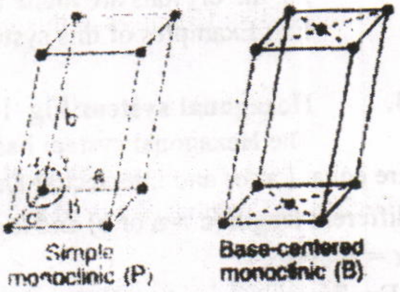


Fig 13.10

7. Triclinic or Asymmetric system :

In this triclinic system of crystals, crystallographic axes are unequal ($a \neq b \neq c$) also the three angles are ıneuqal ($\alpha \neq \beta \neq \gamma$), none of the angles is right angle.

Ex: Potassium dichromate ($K_2Cr_2O_7$)
Sassolite (H_3BO_3) etc. are the examples
for this system

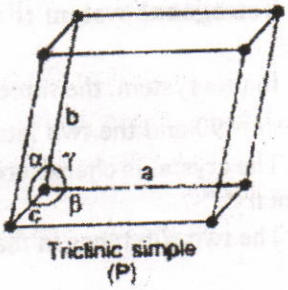


Fig 13.11

The notations used in the different types of lattices given above are referred to as

P	-	Primitive
C	-	Base centered
I	-	Body Centered
F	-	Face Centered

All the 14 types of Bravais lattices belonging to 7 crystal systems explained are tabulated as below.

System	No. of Lattices in system	Bravais Lattices	Lattice symbol	Nature of unit cell (axial length & Interaxial angles)
Cubic	3	1. Simple	P	a=b=
		2. Body centered	I	$\alpha = \beta = \gamma = 90$
		3. Face Centered	F	
Trigonal	1	1. Simple	P	a=b=c $\alpha = \beta = \gamma \neq 90$
Ortho rhombic	4	1. Simple	P	
		2. Base centered	C	$a \neq b \neq c$
		3. Body centered	I	$\alpha = \beta = \gamma = 90$
		4. Face centered	F	
Triclinic	1	1. Simple	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90$
Hexagonal	1	1. Simple	P	$a = b \neq c$ $\alpha = \beta = 90$ & $\gamma = 120$
Monoclinic	2	1. Simple	P	$a \neq b \neq c$
		2. Base centered	C	$\alpha = \gamma = 90$ & $\beta \neq 90$
Tetragonal	2	1. Simple	P	$a = b \neq c$
		2. Body centered	I	$\alpha = \beta = \gamma = 90$

13.8 Index system

Need : For understanding the structure and various physical properties, we have to know the positions of diffeent atoms in the unit cell as well as the orientations of various planes in the crystal. For this purpose, index system is used.

The orientations of a crystal plane is determined by the points in the plane, provided they are not collinear. If each point lay on a different crystal axis, the plane could be specified by giving the coordinates of the points (the intercepts on the axis).

points (the intercepts on the axis).

The equation of the plane can be written as

$$\frac{x}{p}+\frac{y}{q}+\frac{z}{r}=1$$ Where p,q,r are the intercepts on x, y, z axes.

13.8.1 Miller indices :

Miller used this equation to develop an index system. Thus the indices are called "Miller indices".

The steps in the determination of Miller indices of a set of parallel planes along axes can be illustrated as follows :

i) Determine the intercepts of the plane along the three crystallographic axes.
ii) Invert the intercepts; i.e., write the numbers as their reciprocals.
iii) If fractions result, multiply them by lowest common denominator.

The resulting integers are called Miller indices of a plane and are written in a parenthesis (Brackets). These are represented by (h, k, l)

The meaning of these indices is that a set of parallel planes (h,k,l) cuts the x-axis into h parts, the y-axis into k parts and the z-axis into 'l' parts.

Ex: If 2,3,6 are the intercepts along three axes.

Reciprocals of intercepts are $\frac{1}{2},\frac{1}{3},\frac{1}{6}$

Multiplying the reciprocals by L.C.M. of their denominators, 3,2,1

Hence the Miller indices will be 3,2,1.

Note : If a plane cuts an axis on the negative side of origin, then a bar is put over the corresponding Miller index.

Ex : (1,2,3)

Cubic planes having different Miller indices (see Fig 13.12)

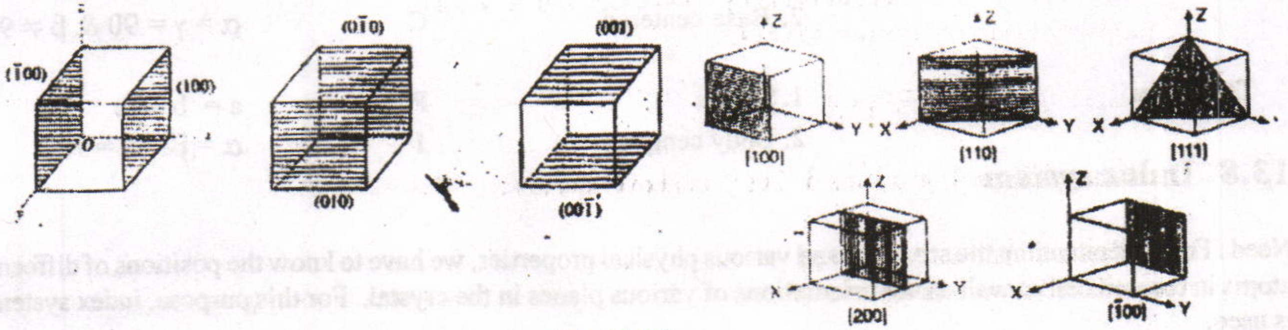


Fig 13.12

3.8.2. Interplanar distance of lattice planes :

Consider a simple unit cell of cubic in which the coordinate axes are orthogonal. Now we can use cartesian coordinates for calculating interplanar spacing.

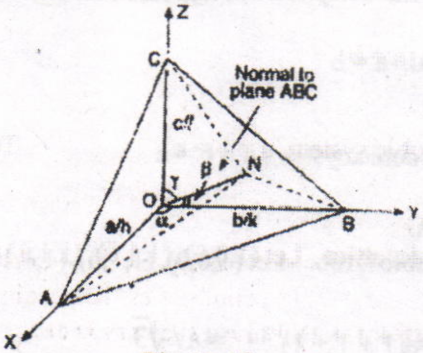


Fig 13.13

In the fig., origin 'o' is taken at any lattice point. ox, oy and oz are orthogonal axes. a,b,c are primitive vectors. Consider any set of crystal planes whose miller indices are (h,k,l). When the reference plane passes through the origin and the next plane cuts the intercepts a/h, b/k and c/l on x, y and z axes respectively. then 'd' gives the interplannar distance.

Draw a normal ON onto the plance ABC from origin. The interplanar distance is nothing but the distance 'd' between the normal from origin to the plane.

From figure $$\cos\alpha = \frac{ON}{OA}$$

$$\cos\beta = \frac{ON}{OB}$$

$$\cos\gamma = \frac{ON}{OC}$$

Where α , β, γ are the angles made by normal ON with x, y, z axes respectively.
According to law of direction cosines,

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

sub. the values of $\cos\alpha$, $\cos\beta$, $\cos\gamma$ in above equation.

$$\left(\frac{ON}{OA}\right)^2 + \left(\frac{ON}{OB}\right)^2 + \left(\frac{ON}{OC}\right)^2 = 1$$

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

Thus, $$d = \left[\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right]^{-1/2}$$

This relation is applicable to primitive lattices in orthorhombic, cubic and tetragonal because we assued orthogonal axes.

For tetragonal crystal, $a = b$

Then For cubic system, $a = b = c$

Then $$d = \left[\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}\right]^{-1/2}$$

Ratio of d's for different plane :

Consider a simple cubic lattice. Let (1,0,0), (1,1,0), (1,1,1) be the miller indices of any three planes in a cube.

Then, for (1,1,1) plane, $d = a(1 + 1 + 1)^{-1/2} = a/\sqrt{3}$

for (1,1,0) plane, $d = a(1 + 1+0)^{-1/2} = a/\sqrt{2}$

for (1,0,0) plane, $d = a(1 + 1 + 0)^{-1/2} = a$

∴ Taking the ratio of d's for different planes in case of cube

$$d_{100} : d_{110} : d_{111} = a : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}}$$

$$= 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}}$$

$$\Rightarrow \frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \sqrt{2} : \sqrt{3}$$

3.9 Summary :

1. **A lattice is a mathematical concept and it is an infinite array of points in three dimensions in which every point has an identical environment as any other point in array.**
2. **Anaton or group of atoms, identical in composition on orientation is called basis.**
3. **Lattice + Basis = Crystal structure**
4. **Crystals possess symmetry elements and the operations described those are called symmetry opera-**

5. Translation, Rotation, Reflection are some of the symmetry operations.
6. Translation vector $T = n_1a+n_2b+n_3c$ where a,b,c are the unit vectors along the crystallographic axes and n_1, n_2 and n_3 are arbitrary inte[illegible]
7. A unit cell is the building block by the repitition of which in 3- dimensions, a crystal is built up.
8. A unit cell is the only one latice point attached to it is called primittive cell.
9. Bravais first introduced 'latice' to describe the periodicity in crystals and those lattices thus called Bravais lattices.
10. Two dimentsional Bravais latices - 5
    Three dimensional latices - 14
11. In the dimentional case by considering the restrictions on lattice translations, a,b,c and α, β, γ angles we get only 7 classes of crystals.
12. crystal systems : Cubic, Tetragonal, Orthorhomic, Monoclinic, Triclinic Triogonal (or Rhomhedrel) and Hexagonal

13.10 Key words :

Crystal, lattice, Translational vector, Symmetry elements, unit cell, primittive cell, crystal systems, Index systems, Miller Indices.

13.11 Worked examples :

1. Find the Miller indices of a set of parallel planes which make intercepts in the ratio 3a : 4b on the X and Y axes and are parallel to Z-axis, a,b,c being primittive vectors of the lattice.

Ans: pa : qb : rc = 3a : 4b : αc

$p : q : r = 3 : 4 : \alpha$

$$\frac{1}{p}:\frac{1}{q}:\frac{1}{r}=\frac{1}{3}:\frac{1}{4}:\frac{1}{\alpha}=4:3:0$$

Thus the Miller indices of the plane are (4,3,0)

2. In a simple cubic crystal find the ratio of the intercepts of the three axes by a plane with Miller Indices (1,2,3)

Ans: For a simple cubic lattice a = b = c

$\therefore$ pa : qb : rc = p : q : r

$$h,k,l=\frac{1}{p}:\frac{1}{q}:\frac{r}{1}=\frac{1}{p}:\frac{1}{q}:\frac{1}{r}$$

$$1:2:3=\frac{1}{p}:\frac{1}{q}:\frac{1}{r}$$

$p : q : r = 1 : \frac{1}{2} : \frac{1}{3}$

$= 6 : 3 : 2$

Thus intercepts of (1,2,3) plane on the three axis of a simple cubic lattice are in the ratio $6 : 3 : 2$

3. **If unit cells have following characteristics**

(i) $a = 10.8Å$ $b = 9.47Å$ $c = 5.2Å$
$\alpha = 41^0$ $\beta = 83^0$ $\gamma = 93^0$

(ii) $a = b = 10.73$ Å, $c = 14.3Å$
$\alpha = \beta = 90^0$ and $\gamma = 120^0$

identify to which crystal system do these unit cells belong?

Ans: **(i) Since $a \neq b \neq c$ & $\alpha \neq \beta \neq \gamma \neq 90^0$. This shows that the three primitives are unequal and there is a compete lack of symmetry. This is a characteristic of Triclinic structure. Hence the unit cell belongs to a Triclinic system.**

(ii) In this case the given data reveals that $a = b \neq c$, $\alpha = \beta = 90^0$ and $\gamma = 120^0$ This is the characteristic of hexogonal structure. Hence the unit cell belongs to a hexagonal system.

4. **The primitives of a crystal are 1.2Å, 1.8Å & 2Å along whose Miller indices (2,3,1) cut intercept 1.2Å along x-axis. What will be the lengths of intercepts along y & z axes?**

Ans: Given that

$h : k : l = 2:3:1$

we have

$\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = h : k : l = 2 : 3 : 1$ $\therefore p : q : r = \frac{1}{2} : \frac{1}{3} : \frac{1}{1} = 3:2:6$

Now $pa : qb : rc$ $= 3 \times 1.2 : 2 \times 1.8 : 6 \times 2$
$= 3.6 : 3.6 : 12$

If lx, ly, lz be the lengths of intercepts on x, y and z axes respectively, then

$l_x : l_y : l_z = 3:6 : 3.6 : 12$

since $l_x = 1.2Å$

Hence $ly = \frac{3.6}{3.6} \times 1.2A = 1.2A$

$$lz=\frac{12}{3.6}x12.A=4A$$

Thus the length of intercepts along y & z axes are 1.2 Å and 4Å respectively.

13.12 Self-assessment questions :

1. Explain the concepts of lattice, basis and crystal structure?
2. Distinqyish between Crystalline and Amorphous materials
3. Explain various Bravais lattices in two and Three dimensions.
4. Explain translatonal vector, symmetry elements and symmetry operations?
5. Explain Miller indices and represent some planes with correspondin Miller indices?
6. Describe the Seven crystal systems with diagrams?
7. Describe the Crystal structures of 1) NaCl 2) CsCl 3) Diamond

13.13 Exercises :

1. A plane in an orthorhombic crystal (a:b:c = 2:3:4) makes intercepts of 4Å, 3Å, & 2Å on its coordinate axes. Find the Miller indices of the plane.

Ans: (1,2,4)

2. In a crystal whose primitives are 1.2Å, 1.8Å and 2Å, a plane (2,3,1) has an intercept of 1.2Å on the X axis. Find the intercepts on y and z axis.

Ans: (1.2 : 1.2 : 1)

3. Determine the Miller indices of a plane that makes intercepts of 2Å, 3Å, 4Å on the coordinate axes of an orthorhombic crystal with a : b : c = 4 : 3 : 2 .

Ans: (4,2,1)

4. An orthorhombic crystal has primittive translations a = 1.21Å, b = 1.84Å and c = 1.97 if a plane with Miller indices (2,3 -1) cuts an intercept of 1.21Å along the x-axis, find the length of intercepts on y & z axis.

Ans: $l = 1.21$, $l_2 = 3.68/3$ $l_3 = 3.94$

5. Find the Miller indices of a plane that makes intercepts on a,b,c axis equal to 3Å, 4Å & 3Å in a tetragonal crystal with $\frac{c}{a}=1.5$.

Ans: (4,3,6)

5. The orthohombic crystal has axial units in the ratio of 0.424 : 1 : 0.367. Find the Miller indices of a crystal face whose intercepts are in the ratio 0.212 : 1 : 0.183

Ans: (2,1,2)

13.14 Reference Books :

1.	Introduction to Solid State Physics.	Charles Kittel, John Wiley & Sons.
2.	Solid State Physics	S.O. Pillai, New Age International
3.	Solid State Physics	A.J. Dekkar, Mc.Millan India
4.	Solid State Physics	Dr. S.L. Gupta & Dr. V. Kumar,K. Nath & Co, Merut.

UNIT-4

LESSON-14

CRYSTAL STRUCTURE DETERMINATION X–RAY DIFFRACTION METHODS

OBJECTIVES:

After studying this lesson the student is able to know about

1. The principle of X–ray diffraction.
2. Braggs' law
3. Laue method for crystal structure determination.
4. Powder Method
5. Some simple structures of NaC*l*, CsC*l* & Diamond.

STRUCTURE:

14.1. INTRODUCTION:

The general symmetry of crystals can be studied by the measurements on the external surfaces and the knowledge of the bulk properties like conductivity and elastic constants. For knowing the complete details of the structure like the positions of the atoms inside and the distances between them, diffraction methods are used.

Structural determination of crystals is often done by the diffraction of photons (x–rays) and neutrons and rarely by the diffraction of electrons.

The diffraction effects from a family of planes in a crystal cannot be observed for any angle of incidence. Even when a monochronatic beam of X–rays is used a relation between d(interplanar spacing), λ the wavelength of X–rays and θ, the angle of incidence has to be satisfied. Bragg derived that relation.

14.2 BRAGG'S LAW :

Bragg's law was presented by W.H.Bragg and W.L. Bragg in 1913.

The conditions for diffraction in crystals is conveniently systematised by Bragg. He reduced the nomenclature of diffraction to specular reflection of the crystal planes. Equally spaced crystal planes may be indicated by lines in two dimensional plane(fig 14.1). These lines become planes in three dimensions.

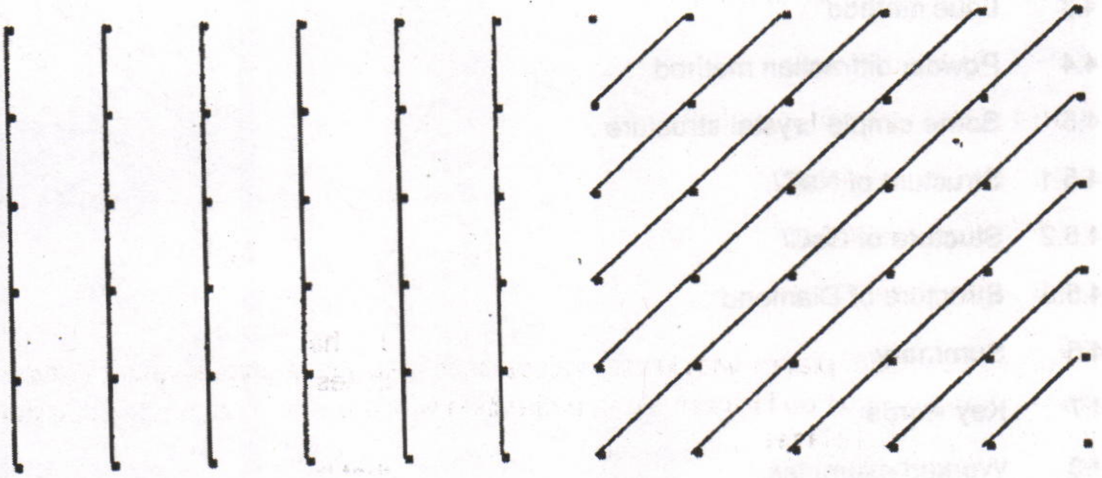


Fig. 14.1

Bragg's law in one dimension :

Bragg showed that any diffracted ray can be considered as the ray reflected by crystal plane just like by a mirror, parallel to planes. The diffracted beams are found only when reflected beams from parallel planes of atoms interfere constructively. The wavelength of photon does not change by reflection as it is considered to involve the Elastic Scattering.

The given wave can be reflected only when it satisfies the equation.

$$n\lambda = 2d \sin\theta$$

Where n = integer

λ = wavelength of the radiation

d = distance between adjacent planes and θ = grazing angle of the incident radiation.

Derivation of Bragg's equation :

Consider a series of parallel rows in which the atoms are arranged in a given plane of crystal. A parallel beam of x–rays is incident on the crystal plane making a glancing angle θ with the surface. Then each atom acts a .centre of disturbance. Since the X–rays are more penetrating, then we consider the rays reflected from several layers.

Let us consider two parallel rays LMN and PQR which are reflected by two atoms M and Q in adjacent layers as shown in the figure.

From the fig. 14.2, path difference is AQ + QB = n λ

From fig, AQ = BQ = d sin θ

$\therefore 2d \sin\theta \therefore = n\lambda$

This is known as Bragg's law.

Thus $\theta = \sin^{-1}\left(\frac{n\lambda}{2d}\right)$

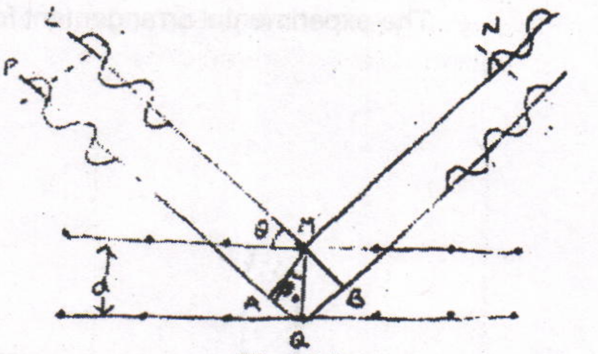


Fig 14.2

For a given set of planes with known values of 'n' and θ has unique value. Waves with given wavelength must be incident along a direction which lies in a cone, makes a definite angle with the crystal planes.

If a diffracted wave is observed, it may be concluded that the crystal possesses a set of planes with a normal which bisects the angle between incident and diffracted waves. Bragg reflection can occur only for wavelength $\lambda \geq 2d$ and $\sin\theta$ can not be greater than '1'.

For n = 1, $\lambda = \frac{2d\sin\theta}{n} < 2A^0 (\because \sin\theta \leq 1)$

i.e; X–rays with wave lengths less than 2A⁰ are most useful in studying crystals.

Energy of X–ray photon is given by,

$$E = h\vartheta = \frac{hc}{\lambda} \Rightarrow \frac{12.4}{E\ in\ k.e.v} = \lambda\ in\ \mathring{A}$$

$$\therefore E\ in\ e.v = \frac{12.4}{2} \times 1000 \quad \text{when } \lambda = 2\ A^0$$

$$= 6200$$

$$= 6.2\ kev$$

Energy is to be about 6.2 kev.

Thus, X–rays of energy in 10 to 50 kev range are used.

14.3 – LAUE METHOD :

This Laue method was the first method which produced X–ray photograph of crystals.

An X–rays beam of continuous range of wavelength is produced by an X–ray tube operated by about 65 kv which makes use of a tungston anticathode. This potential is insufficient to produce characterstic X–radiation and hence avoids the confusion. The available wavelengths are from 0.2 to 1A^0.

The experimental arrangement for Laue method is as shown in the figure.14.3

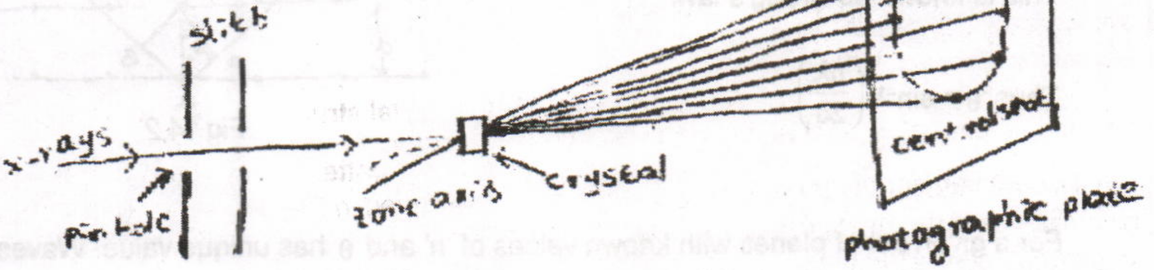


Fig. 14.3

In this method, first the crystal is held stationary in the beam of X–rays. First of all, X–rays are limited to a fine pencil by a slit system. Here, smaller the diameter of pin hole, sharper is the interference. This beam is made to fall on a small crystal. The diffracted rays are recorded on a photographic plate, kept near by about few cm's from the crystal. The crystal is kept in

a holder and can be rotated to change its orientation. For each orientation(set of planes) θ, the radiation of appropriate wavelength is got selected from the continuous range to satisfy the condition for diffraction, $n\lambda = 2d \sin\theta$.

If the incident ray makes an angle θ with the zone axis then the reflected ray will make the same angle with it and as the crystal is rotated, we get a set of points that lie on an ellipse. All the points that lie on an ellipse correspond to the same zone i.e, planes which are parallel to zone axis. If the incident ray make an angle with zone axis then the reflected ray makes the same angle with it and so they lie on a cone of semivertical angle 'θ' about the zone axis.

When a Laue photograph is taken with the rays parallel to an important axis of the crystal, the circular area at the centre of it is free of spots. As the inclination of the lattice plane of reflection is decreased, both θ and λ decrease inaccordance to $n\lambda = 2d \sin\theta$ until a point is reached where λ is less than the short wave-limit of the incident continuous X-rays. Then reflection is not possible. Only a rough estimate of the spacing between the lattice points can be made.

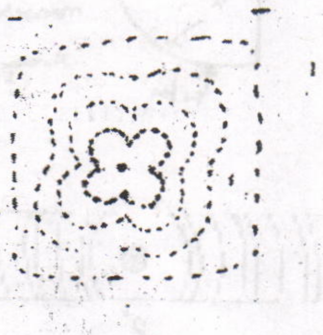


fig 14.4

Disadvantage: Obtaining the crystal structure from Laue photograph is complicated, as the intensities of spots of photograph do not depend on structure alone. Since the incident radiation of several wavelengths is reflected corresponding to different orders then,they may superpose on a single spot. Due to this, the determination of the crystal structure is difficult.

Advantage: Practically this method is never used but Laue pattern can be used to orient the crystals for solidstate experiments. The Laue pattern obtained in this case shows the fourfold symmetry.fig. 14.4

14.4 POWDER METHOD:

This is the only method used for a large class of substances which can not be obtained easily in the form of single crystals of required size. This method was devised by Debye scherrer and Hill.

In this method, fine powder of crystals having random or chaotic orientations is used instead of single crystal, and a monochromatic X–ray beam is used. The diffraction depends on the fact that in a fine powder, the grains are arranged in a chaotic manner. Some of them will be in a position to reflect the radiation from an important set of planes. The diffracted rays makes an angle θ with the beam satisfying the Bragg equation.

Since all orientations of the fragment normal to the plane are equally likely, the reflected rays will form a cone, concentric with the original beam whose semi-vertical angle is 2θ. For each set of planes, a cone of diffracted rays forms. The cones intercept the film in a series of concentric circular arcs. Using the radii of these circular arcs angle θ and the space of the planes can be deduced.

The formation of powder photograph is as shown in figure 14.5.

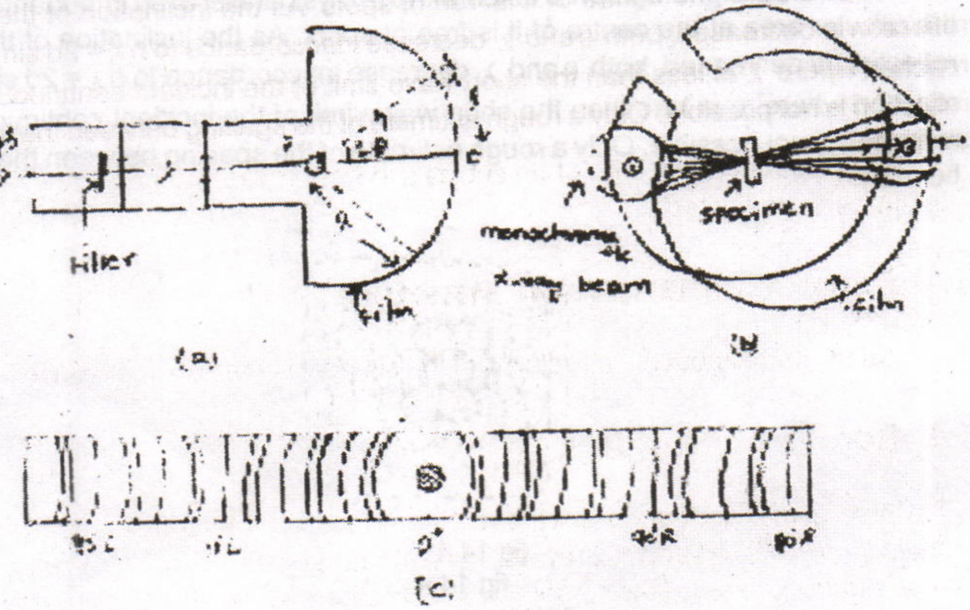


Fig. 14.5

The radiation is made monochoromatic with the help of a filler as shown in fig 14.5(a). Here p is the powder and 'o' is the point where the direct beam have to struck the film. Point 'A' on the film correspond at which a spectrum with glancing angle θ is formed. The max diffraction lie on cones. If a photographic plate is kept normal to the direct beam, concentric circles are registered upon it as shown in fig 14.5(b). They appear as arcs of the circles as in the film is in the form of cylindrical shape as shown in fig 14.5(c).

From Fig.14.5(c), it is observed that when rays are diffracted through small angles, they make arcs around the centrol spot. When diffraction angle is 90°, cones become flat and arc becomes straight line. When a angle is 180°, traces are nearly circular.

Now from fig 14.5(a), OA=l measured on the film and R is the radius of camera then $\theta = l/2R$.

Advantage: This method is very useful in finding the structures of simple crystals like cubic system. In these crystals, the spacing of all planes parallel to faces of the same form (h K *l*) are equal and produce spectra at the same angle. In general where h, k, *l* are different, there are 4s faces in the form and 24 sets of planes having same spacing. These all produce one line on film.

An interesting feature which is shown best by.the powder photograph is that the 'resolving power' becomes very high when angle is 180°. If.d varies in the eq., $n\lambda = 2d \sin\theta$, we have

$$\Delta d . \sin\theta + d . \cos\theta . \Delta\theta = 0$$

$$\Rightarrow \frac{\Delta\theta}{\Delta d} = \frac{-\text{Tan}\theta}{d} . \text{ (If } \theta = 90^0, \frac{\Delta\theta}{\Delta d} \text{ becomes very great].}$$

Disadvantage : crystals other than cubicals in which axes are not at right angles, this method becomes complicated.

14.5: Some simple crystal structures:

Let us study about the structures of the simple crystals such as NaC*l*, CsC*l* and diamond.

14.5.1 Sodium chloride:

In sodium chloride, both Na and C*l* are ions of opposite charge. Due to electrostatic forces between these two, they attract each other. But because of repulsion due to outer most electrons, they cann't approach each other, when attraction and repulsion balance, equilibrium is obtained.

i) Bravais lattic is a face centered cube.

ii) In each unit cell, there are four Formula units ok NaC*l*.

iii) Basis consists of Na atom and C*l* atom

iv) Coordination number = 6 since each ion is surrounded 6 nearst neighbours of the opposite kind.

v) Positions of Na and C*l* in a unit cell are (Fig. 14.6)

Na – (1/2, 1/2, 1/2), (0, 0, 1/2), (0, 1/2, 0), (1/2, 0, 0)

C*l* – (0, 0, 0), (1/2, 1/2, 0), (1/2, 0, 1/2) (0, 1/2, 1/2)

vi) Separation beteen Na and C*l*, d = a/2

$$a = \left(\frac{nM}{N\rho}\right)^{1/3} = \left(\frac{nM}{N\rho}\right)^{1/3}$$

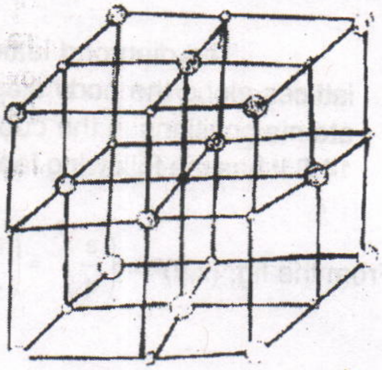


Fig. 14.6

$$\therefore d = \frac{1}{2}\left(\frac{Mn}{N\rho}\right)^{1/3}$$

Others having similar structure are

KCl, KBr, MgO, AgBr etc.

14.5.2: Cesium chloride :

i) The space lattice is simple cubic

ii) The primitive cell has one formula unit.

iii) Each ion is at the centre of a cube of ions of opposite kind. So, coordination number is eight.

iv) Basis contains two atoms of opposite charges Cs and Cl.

v) The positions of Cs and Cl are

Cs – (0, 0, 0)

Cl – (1/2, 1/2, 1/2)

vi) This is not body centered and it is a simple cube.

vii) Lattice parameter = 4.11 A°

viii) Unit cell has 1 formula unit

ix) Unit cell is primitive cell.

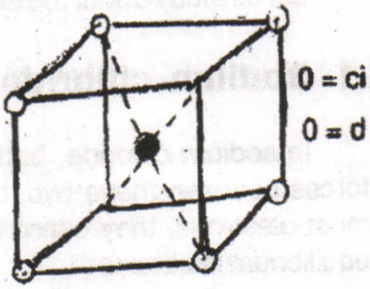


Fig. 14.7

Cesium chloride structure can be determined from all the above points (Fig. 14.7).

Ex : RbCl, LiHg.

14.5.3: DIAMOND CUBIC STRUCTURE:

The diamond lattice can be considered to be formed by interpenetrating two fcc lattices along the body diagonal by 1/4th of cube edge. The basic diamond lattice and the atomic positions in the cubic cell of diamond projected on a cube face are as shown in fig 14.8.It has the following features.

i) From the fig, $(x,y)^2 = \left(\frac{a}{4}\right)^2 = \left(\frac{a}{4}\right)^2 = \frac{a^2}{8}$

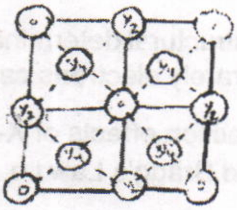


Fig. 14.8

$$(xz)^2 = (xy)^2 + (yz)^2 = \frac{a^2}{8} + \frac{a^2}{16} = \frac{3a^2}{16}$$

But xz = 2r.

$$\therefore (2r)^2 = \frac{3a^2}{16}$$

$$\therefore \text{Nearest neighbour distance, } 2r = \frac{\sqrt{3}a}{4}$$

ii) Lattice constant, $a = \frac{8r}{\sqrt{3}}$

iii) Basis consists two atoms of same type

iv) Coordination number = 4

v) No. of atoms in unit cell = 8

vi) One sublattice has its origin at the point (0, 0,0) and other at a point quarter of the body diagonal (a/4, a/4, a/4).

vii) The fractions denote height about the base in units of a edge.

The point at 0 and 1/2 are on thefcc lattice, that 1/4 and 3/4 are one a similar lattice displaced among the body diagonals by 1/4 of the cube edge.

viii) Packing factor = $\frac{v}{V}$

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

$$= \frac{32}{3}\times\pi r^3\times\left(\frac{\sqrt{3}}{8r}\right)^3 = \frac{32}{3}\times\pi r^3\times\left(\frac{\sqrt{3}}{8r}\right)^3 = \frac{\pi\sqrt{3}}{16} = 0.34 \text{ or } 34\%$$

Thus it is a loosly packed structure.

Ex: Carbon, silicon and germanium crystallize in this structure.

Thus using all the above points, Diamond structure can be illustrated

14.6 SUMMARY :

1. For structural determination of crystals, methods involving the diffraction of X–rays, neutrons and rarely electrons can be used.
2. Diffraction effects of X–rays (monochromatic) can be observed only by satisfying a relation called Bragg's Law i.e., $2d \sin\theta = n\lambda$.
3. In Laue method X–rays of continuous wavelengths (non-monochromatic) is used and the material under study is taken in the form of single crystal.
4. In powder method, the sample under study is a powder (consisting of several small crystals randomly oriented) and a monochromatic beam of X–rays is used.
5. Powder method has an advantage in the sense that it can be used for a large class of materials which cannot be obtained in the form of single crystals of required size.

14.7 Key Words:

Braggis Law, powder method, Laue method.

14.8 Worked Examples:

1. **Bragg reflection of second order occured, when X–rays of wavelength 0.12 nm was incident on a set of planes of a crystal at a grazing angle $\theta = 28^0$. Find the interplanar spacing of those reflecting planes**

Solution.

$2d \sin\theta = n\lambda$ (Bragg's Law)

$d = \dfrac{n\lambda}{2\sin\theta}$ given $n = 2$, $\lambda = 0.12 \times 10^{-9}$m and $\theta = 28^0$

$d = \dfrac{2 \times 0.12 \times 10^{-9}}{2 \times \sin 28^0}$ (because $\sin 28^0 = 0.4695$)

$= 2.56$ nm

2. **The interplanar spacing of principal planes of NaC*l* crystal is 2.82 A°. It is found that the first order Bragg reflection occurs at an angle of 10°. Find the wavelength of the used X–rays.**

Accordfing to Bragg's Law $2d \sin\theta = n\lambda$

$\therefore \lambda = \dfrac{2d\sin\theta}{1}$ as $n = 1$

Given $n = 1$, $d = 2.82 \times 10^{-10}$m and $\theta = 10^0$

$$\lambda = \frac{2 \times 2.82 \times 10^{-10} \sin 10^0}{1}$$ since ($\sin 10^0 = 0.1736$)

$\lambda = 0.9793A^0$

3. A beam of X–rays of wavelength 0.71 A⁰ undergoes Bragg's reflection at (110) planes of rock salt with lattice constant 0.28 nm. Find the glancing angle for second order diffraction

$2d \sin\theta = n\lambda$ (Bragg's law)

given $n = 2$, $\lambda = 0.71\times10^{-10}$ m, $a = 0.28\times10^{-9}$ m

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.28 \times 10^{-9}}{\sqrt{2}} = 0.198 \times 10^{-9}$$

$$\sin\theta = \frac{n\lambda}{2d} = \frac{2 \times 0.71 \times 10^{-10}}{2 \times 0.198 \times 10^{-9}} = \frac{0.071}{0.198} = 0.3586$$

therefore $\sin\theta = 0.3586$

$\theta = 21^0$.

4. Calculate the longest wavelength that can be analysed by a rock salt crystal of spacing d = 2.82 A⁰ in the first order.

$2d \sin\theta = n\lambda$ (Braggs law equation)

given that $n = 1$ and $d = 2.82\times10^{-10}$m

when wavelength is to be longest $\sin\theta = 1$

$$\therefore \lambda = \frac{2d\sin\theta}{n} = \frac{2 \times 2.82 \times 10^{-10} \times 1}{1} = 5.64\times10^{-10} \text{ m}$$

λ max = $5.64A^0$

5.A beam of X–rays is incident on a NaCl crystal with a lattice spacing of 2.82 A⁰. Calculate the wavelength of that X–ray ray beam if the first order Bragg reflection takes place at a glancing angle of 8⁰ 35'. Also calculate the possible maximum order of diffraction

$2d \sin\theta = n\lambda$ (Braggs law equation)

given $\theta = 8^0\ 35'$, $n = 1$ and $d = 2.82 \times 10^{-10}$m

$\therefore \sin\theta = 0.1490$

$$\lambda = \frac{2d\sin\theta}{n} = \frac{2 \times 2.82 \times 10^{-10} \times 0.1490}{1}$$

According to Braggs law $2d\sin\theta = n\lambda$

case 1: $\theta_1 = 60^0$ $\theta_1 = 30^0$ and $n_1 = 1$

case 2: $\theta_2 = 60^0$ and $n_2 = 3$ and given $d_1 = d_2$ $\lambda_2 = 0.97A^0$

$$d_1 = \frac{n_1\lambda_1}{2\sin\theta_1} = \frac{n_2\lambda_2}{2\sin\theta_2}$$

$$\therefore \frac{1\times\lambda_1}{2\times\sin 30^0} = \frac{3\times0.97\times10^{-10}\,m}{2\times\sin 60^0}$$

$$\therefore \lambda_1 = \frac{3\times0.97\times10^{-10}\times2\times\sin 30^0}{2\times\sin 60^0}$$

$$\lambda_1 = 1.68A^0$$

7. In X–ray analysis of a crystal, using X–rays of wavelength 0.58A° Bragg's reflections are obtained with glancing angles of i) 6.45° ii) 9.15° and iii) 13°. Find the interplanar spacing f.

$2d\sin\theta = n\lambda$ (Bragg's law)

$$\therefore \frac{d}{n} = \frac{\lambda}{2\sin\theta}$$

1. When q = 6.45° corresponding $\frac{d}{n} = 2.568$ $\left[\because \frac{d}{n} = \frac{1.58}{2\sin 6.45^\circ}\right]$

2. When q = 9.15° corresponding $\frac{d}{n} = 1.817$

3. When q = 13° corresponding $\frac{d}{n} = 1.288$

Taking equations 1 and 3, we can find that $\frac{d}{n}$ of equation (2) is almost (1). Hence 6.45 and 13° are gancing angles corresponding to first ands second order brags reflections on the same set of planes and thus their interplanar spacing can be obtained by putting n = 1 is equation (1) or n = 2 in e1quation (3) i.e

d = 2.658A°.

The second equation corresponds to another set of planes and the corresponding another set of planes and the corresponding inter planar spacing is obtained as

$(d/1) = 1.817$ or $d = 1.817^o$

8. Monochromatic X-rays of wavelength 1.5A° are incident on the face of a crystal with a set of planes of inter planar spacing o 1.6A°. Find the various orders of Bragg's reflections that take place.

2d sin q = n l (Brâgg's law)

taking equations 1 and 3, we can find that $\frac{d}{n}$ of equation (2) is almost twice that (1). Hence 6.45 and 13^0 are galncing angles corresponding to first and second order Bragg reflections on the same set of planes and thus their interplanar spacing can be obtained by putting n = 1 in equation (1) or n = 2 in equation (3) i.e. d = 2.568Å

The second equation corresponds to another set of planes and the corresponding interplanar spacing is obtained as

$$\frac{d}{1} = 1.817 \text{ or } d = 1.817^O$$

Monochromatic x-rays of wavelength 1.5Å are incident on the face of a crystal with a set of planes of interplanar spacing of 1.6Å. Find the various orders of Bragg's reflections that take place.

$2d \sin\theta = n\lambda$ (Bragg's law)

$\sin\theta = \frac{n\lambda}{2d}$ where n = 1 $\sin\theta_1 = \frac{\lambda}{2d}$

similarly n = 2 $\sin\theta_2 = 2\left(\frac{\lambda}{2d}\right)$ and $\sin\theta_3 = 3\left(\frac{\lambda}{2d}\right)$

$\sin\theta_1 : \sin\theta_2 : \sin\theta_3$ is same as 1:2:3 and so on

$\sin\theta_1 = \frac{\lambda}{2d} = \frac{1.5}{2x1.6} = 0.468 \therefore \theta_1 = 28^o$

$\sin\theta_2 = 2 \times 468 = 0.938$ and $\theta_2 = 69^0 42^1$

$\sin\theta_3 = 3 \times 0.468$ is greater than 1 and thus $\theta > 90^0$

Thus we now that third order is not possible maximum possible order is 2.

14.9. Self assessment Questions :

1) Derive Bragg's law for X-ray diffraction in crystals.

2) Describe the powder method for analysis of crystal structure. Mention the advantages of this method.

3) Describe Lave's method for x-ray diffraction in crystals.

4) Explain the structure of NaCl

5) Explain the structure of CsCl

6) Explain the structure of Diamond.

14.10 Exercises :

1. X-rays of wavelength 0.36Å are diffracted in the first order at an angle of 4.8^0 in Bragg spectrometer. Find the interplanar spacing of atomic layers in that crystal [Ans. 2.15Å]

2. Find the glancing angles at which first and second order diffraction maxima occur when x-rays of x = 1.92Å are incident on a calcite crystal surface with inter planar spacing d = 3.029Å [Ans : $\theta_1 = 18^0 30^1$, $\theta_2 = 39^0 20^1$]

3. The spacing between successive (100) planes in Nacl is 2.820Å. X rays incident on the crystal surface cause Bragg reflection maximum at a glancing angle of $8^0 35^1$. Calculate i) the wavelength of the x-rays and ii) the angle at which second order Bragg reflection takes place

   [Ans : $\lambda = 0.842$Å, $\theta = 17^0 22^1$]

4. When a nickel target is used in an x-ray tube, two short wavelengths are emitted and first order Bragg reflection occurs with those wavelengths at angles 15.1^0 and 17.1^0 respectively. Find their wavelengths assuming interplanar spacing to e 2.81Å

   [Ans: $\lambda_1 = 1.468$Å $\lambda_2 = 1.652$Å]

5. At what Bragg angles x-rays with λ = 1Å be incident on a family of parallel planes with d = 2.5Å so as to result diffraction intensity maxima.

   [Ans : $\theta_1 = 11.52^0$, $\theta_2 = 23.60^0$, $\theta_3 = 36.90^0$, $\theta_4 = 53.1^0$, $\theta_5 = 90^0$ corresponding to n = 1,2,3,4,5. Further higher ordes like n = 6 and more are not possible]

6. Calculate the wavelength of an x-ray beam incident at 12^0 for the first order reflection from a calcite crystal, if the grating constant of the crystal is 3.035Å. Find the maximum order possible with that x-ray beam.

   [Ans : $\lambda = 5.64$Å. Only first order is possible]

   [Hint : $n_{max} = \dfrac{2xd}{\lambda}$]

14.11 Reference books:

1.	**Introduction to Solid State Physics**	**Charles Kittel, John Wiley & Sons.**
2.	**Solid State Physics**	**S.O. Pillai, New Age International**
3.	**Solid State Physics**	**A.J. Dekkar, Mc.Millan India**
4.	**Solid State Physics**	**Dr. S.L. Gupta & Dr. V. Kumar, K. Nath & Co, Merut.**

Unit-4

Lesson-15

INTER ATOMIC FORCES

Objectives :

After studying this lesson the student is able to know about

1. Nature of atomic forces and bonding in crystalline solids.
2. Different types of bonding
3. Lattice energy cohesive energy.
4. Born's theory and calculation of repulsive exponent.
5. Born-Haber cycle.

Structure :

15.1 Introduction
15.2 Classification at solids basing on the bonding.
15.2.1 Ionic bonding
15.2.2 Covalent bonding
15.2.3 Metallic bonding
15.2.4 Molecular bonding
15.2.5 Hydrogen bonding
15.3 Potential energy of a system of two atoms
15.3.1 Cohesive energy
15.4 Born's theory
15.4.1 Madelung constant
15.4.2 Lattice energy - Nacl
15.5 Calculation of repulsive exponent
15.6 Born-Haber cycle

15.1 Introduction:

It is known that material in solid state is rigid. It indicates that there m ust be attactive forces between the constitutent units of the solid body and further there exist repulsion forces also inside the body to ensure definite size. We recall that solids can be classified as crystalline and amorphous. Crystalline materials can be classified in different ways. The basis for classification may be lattice structure which is dealt with in the previous chapter. Classification may be based on thermal, electrical and magnetic properties. The most convenient basis for classification can be the character in inter atomic bonding in the crystalline materials.

15.2 Classification of Solids :

The forces which bind the atoms in a molecule and molecules in a solid play an important role in the study of solid state physics.It is observed that these forces are electrostatic in nature. These forces depend on the distribution of valence electrons in different atoms. There are various types of distributions in different crystals. Based on the positions of valence electrons, different types of bonding take place.

Based on the bonding between atoms, solids are divided into different groups. They are

1. Ionic crystals
2. Covalent crystals
3. Metallic crystals
4. Molecular cyrstals
5. Hydrogen-bonded crystals.

15.2.1 Ionic Crystals :

Crystals in which ionic bonding is used are known as ionic crystals.In this type of solids, one or more electrons of one atom are transfered to another atom. This results in the formation of positive ion and negative ion.

The ions which are able to give electrons are called electro positive ions. Na, K, Ca and some other metals are electropositive ions. The ions which acquire electrons are called electronegative ions. F, Cl, O and non-mentls asre electronegative ions.

Sodium chloride is the best example for the one with ionic bonding. The valence of Na is +1 i.e. it has one electron in its outer most orbit which can easily lose and Na becomes a positive ion. The valence of Cl is -1, i.e. for stable electronic configuration it requires one electron.

Due to the coulombian attraction between oppositely charged ions, ionic bond is developed between Na and Cl by transfering one electron from Na to Cl.

The coulombian force of attraction between two different atoms provides the cohessive energy which binds them together. It is called binding energy. The magnitude of the cohesive or binding energy per molecule in ionic solids is generally about 5 to 10 ev. In case of NaCl it is 7.8 ev.

The arrangement of all the ions (+ve & -ve) will be such that the attraction between ions of different nature is more than the repulsion between the similar type of ions.

Characteristics of ionic cyrstals :

Generally ionic bonded crystals will have the following properties.

i) The ionic bond is very strong.

ii) The ionic crystals have high melting and boiling points.

iii) These are poor electical conductors at normal temperature because the valence electrons are bonded tightly to the nucleus. At high temperature, ions themselves begin to move giving property of conductivity.

iv) These are transparent to all frequencies upto fundamental absorption frequency. After this, they are opaque.

v) These are soluble in ionizing solvents such as water. Solution is dissociated into free ions.

vi) The electronic structure of ions is same as nearest inert gas atoms except that these are electrically charged.

vii) These [illegible] usually crystalized in relatively closed packed structure. Actual structure depends on the ratio of radii of two ions.

viii) Charge distribution in ions is spherically symmetric.

ix) This bond is non-directional but it has direction in some special cases.

x) Most of the insulators are ionic cyrstals. All Alkyl halides, Alkyl oxides are ionic bonded.

15.2.2 Covalent Crystals :

Crystals in which covalent bond takes place are called covalent crystals. In this bonding the valence electrons of the two neighbouring atoms are shared but not transfered. In case of diamond each carbon atom shares into four valence electrons with its four nearest neighbours. Chlorine atom has 7 electrons in its outermost orbit. The spins of six electrons are paired and that of seventh electron is unpaired. This unpaired electrons of two chlorine atoms are paired up and so, the spins are antiparallel. The covalent bonding between chlorine atoms is as shown below.

Characteristics of covalent crystals :

The covalent crystals have the following properties.

i) Covalent crystals are usually hard, brittle materials with high binding energy. So, these are having high melting and boiling points.

ii) These are strongly directional in nature and has property of saturation.

iii) The conductivity of covalent crystals varies over a wide range.

Ex : - Tin - good conductor, Ge - Semi conductor, Diamond - Insulator

iv) These are transparent to long wave-length radiation but opaque to shorter wavelengths.

v) It has dipole moment. When bonds are distributed symmetrically, even though a molecule contains dipoles, it may have net zero dipole moment. In this case individual dipoles cancel each other. Such a molecule is called non-polar molecule.

Ex : Carbon dioxide and carbon tetra chloride are non-polar molecules.

vi) The bond length and bond energy varies according to the no. of shared electrons.

15.2.3 Metallic Crystals :

These crystals are bonded by electrostatic attraction between lattice of ion cores and the free electron gas. In these valence electrons move freely throughout the whole metal, not bound to any nucleus and considered as electron gas.

The bonding is due to the attraction between the electron gas and the positive nuclei. In metallic crystals, the valence electrons have high degree of mobility and the cohessive energy is provided by the coulomb interaction between the positive ions and the negative smeared out charge of conduction electrons.

The classical theory fails to explain the metallic character of solids on the basis of number of valence electrons. According to this, as the valence electrons number increases, the metallic nature of element decreases. Metallic bond can be expalained on the basis of quantum mechanics. According to this, a metallic bond is regarded as an unsaturated covalent bond.

Consider Na atoms (z = 11). Each Na atom has one unpaired 3s electron. When the spins of these unpaired electrons are of opposite kind, a bond is formed due to attraction between them. Let a third sodium atom which has also one unpaired 3s electron approache the bonded pair. Since both the 3s quantum states are occupied, this atom experience repulsion according to Pauli's exclusion principle. But the energies of unoccupied 3p-states is nearly same as the energy of 3s-electron; third electron can enter into 3p-state. Now it can also form an electron-pair bond with either of the valence electrons of previous pair.

In this way very large number of atoms can be surrounded by a single sodium atom. The central atom has one unpaired electron which can form by turns electron-pair bonds with unpaired electrons of neighbouring atoms. Thus it forms less than a whole electron pair bond with each neighbouring atom. Solid sodium has this type of bonding. It has b.c.c. structure and on an average, each sodium atom forms one-eighth of an electron-pair bond with its neighbours. Such type of bonds are called as unsaturated covalent bonds.

Characteristics of Metallic crystals :

Metallic crystals have the following characteristics.

i) They have high electrical and thermal conductivity.

ii) Metals are opaque to all electromagnetic radiation, transparent to the middle ultraviolet. Metals have high optical reflection and absorption coefficient.

iii) These are having low melting and boiling points.

iv) The similarity between the metallic and covalent bond is the sharing of electrons. Difference is in metallic bond, the electrons belong to metal as a whole not to any particular atom which happens in case of covalent bond.

v) The binding energies are low for sodium 1.13ev and for Alluminium 3.23 ev.

vi) These have high ductility and malleibility

vii) Examples are Cu, Si, Ag and Al.

15.2.4 Molecular Crystals :

These crystals are bonded by weak van der waal's forces. In case of innert gases, such as argon, the atoms or molecules have a tendency to give up or share electrons with other atoms. In liquid and solid state, the forces of attraction are called dispersion forces.

The combination of moving negative electrons and the nucleus of an atom may be considered as a fluctuating dipole. The interaction between these dipoles with those of induced ones give rise to a relatively weak binding force called van der waal's force.

The binding is solely due to dipolar forces. It has no permanent dipolemoment. Molecular bond has instaneous fluctuating dipole moment. This instantaneous dipolement induces a moment in the neighbour atom. This interaction between its dipolemoment and induced dipole moment causes a little attraction between them. Due to this reason van der waal's forces arise.

Characteristics of molecular bond :

i) Molecular crystals have small binding energy.

ii) They have low melting and boiling points.

iii) They are poor electrical conductors.

iv) They are usually transparent to electromagnetic radiations down to the very short ultraviolet.

Ex : He, Ne, Ar, Kr, Xe, O2, H2 etc., are molecular bonded atoms.

15.2.5 Hydrogen-bonded crystals :

These crystals are bonded by hydrogen bonds:

Ex : Ice, some flourides etc.

A hydrogen atom can be attracted simultaneously by two different atoms and thus serves as a bridge between the two species. It is considered as a basis of a bond bewteen the two atoms. This is hydrogen bond.

Hydrogen bond is largely ionic in character. Since hydrogen has one electron, it can loose it to either of its adjoining ions resulting a probability of finding the electron on either ion.

The positive hydrogen ion tends to draw the two anions more closely together than their normal separation in the crystal. Thus hydrogen bond connects only two atoms.

This bond is much weaker than a covalent bond. The hydrogen bond may be imagined to be formed by a process of this type.

X-H+Y X-H ... Y

Where X and Y can be the same or differnet atoms. Thus the hydrogen atom is bonded to X and Y simultaneously.

15.3 Inter atomic forces and P.E. of a system of two atoms :

Here we discuss about the forces that hold together the atoms or molecules or ions in the solid. In this consideration, a casual thinking itself leads to the following general conclusions.

i) There must be attractive forces between the atoms or molecules in a solid to keep them together.

ii) There must be repulsive forces acting between the atoms since large external pressures are needed to compress a solid to any appreciable extent.

Without these two forces the atoms can not stay together to form a solid.

To understand the importance of these two forces, let us consider a simplest system consisting of two atoms separated by a distance 'r' and which forms a stable chemical compound. If the two atoms A and B are separated by an inifinite distance, then the potential energy of the system is zero. When they are brought closer to a finite separation, there will be a potential energy for system. It's sign depends ont he magnitudes of the attractive and repulsive forces.

The potential energy of attraction is negagive and is inversly proportional to some power of r (say m)

i.e. U attractive $= -\dfrac{A}{r^m} \longrightarrow$ ①

Where A is attraction constant.

The potential energy of repulsion is positive and it is inversly proportional to some power of r (say n)

$$\text{i.e., U repulsive} = -\frac{B}{r^n} \longrightarrow \textcircled{2}$$

Where B is repulsion constant.

This situation is described by the potential energy diagram as shown in the figure 15.1.

The total P.E. is given by,

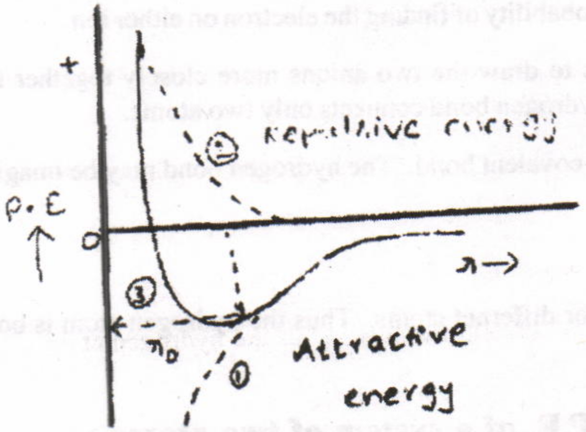


Fig 15.1

$$U_{total} = U_{att} + U_{rep}$$

$$= -\frac{A}{r^m} + \frac{B}{r^n} \longrightarrow \textcircled{3}$$

The constants A, B, m and n are characters of a molecule

The force between the atoms can be written as,

$$F = \frac{-du}{dr} = \frac{-d}{dr}\left[-\frac{A}{r^m} + \frac{B}{r^n}\right]$$

$$= -\left[\frac{Am}{r^{m+1}} - \frac{Bn}{r^{n+1}}\right]$$

$$\Rightarrow F = -\frac{Am}{r^{m+1}} + \frac{Bn}{r^{n+1}} \longrightarrow \textcircled{4}$$

From the above fig., we can say that the curve (3) has a minimum P.E. at $r = r_o$ which is the equilibrium position

i.e., when the system is in equilibrium

$$\left(\frac{du}{dr}\right)_{r=r_0} = 0$$

$$\Rightarrow -\frac{Am}{r_o^{m+1}} + \frac{Bn}{r_o^{n+1}} = 0$$

$$\Rightarrow \frac{Am}{r_o^{m+1}} = \frac{Bn}{r_o^{n+1}}$$

$$\Rightarrow \frac{Am}{Bn} = r_o^{m-n}$$

$$\Rightarrow \frac{A}{B}.\frac{m}{n} = r_o^{m-n} \longrightarrow ⑤$$

Now total P.E. at r_o, is given by

$$U_{r_0} = -\frac{A}{r_0^m} + \frac{B}{r_0^n}$$

$$= -\frac{A}{r_0^m}\left[1 - \frac{B}{r_0^n}.\frac{r_0^m}{A}\right]$$

$$= -\frac{A}{r_0^m}\left[1 - \frac{B}{A}.r_0^{m-n}\right]$$

From eq. ⑤, $r_o^{m-n} = \frac{A}{B}\frac{m}{n}$

$$\therefore\ U_{r_0} = \frac{-A}{r_0^m}\left[1 - \frac{B}{A}.\frac{A}{B}.\frac{m}{n}\right]$$

$$\Rightarrow U_{r_0} = \frac{-A}{r_0^m}\left[1 - \frac{m}{n}\right] \longrightarrow ⑥$$

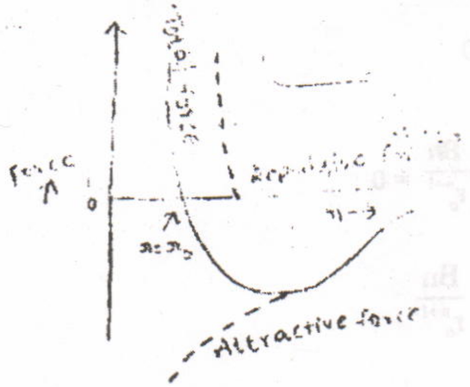


Fig. 15.2

This is the generalised expression for total P.E. of system which is minimum at $r = r_o$

If we plot a graph for variation of force with distance, it is as shown in the figure 15.2.

When the distance of separation is large, the significant force is the negative attractive force. This comes from electrostatic forces.

As the interatomic separation decreases, the magnitude of repulsive forces increases. This is evident in the non-compressible property of solids.

At $r = r_o$, due to equilibrium, $F = 0$ and has minimum P.E. U_o.

The magnitude of minimum P.E. is called the bond energy. This is possible only if $n >> m$

15.3.1 Cohessive energy :

The energy needed to break the crystal into individual atoms is called cohessive energy.

15.4 Born's Theory :

The calculation of binding energy of a crystal is the fundamental problem in the theory of solids. Ionic crystals are the simplest type of crystals.

Assumptions : In 1910 Born and Madelung gave a theory for cohesive energy or lattice energy or binding energy.

The theory is based on the following assumptions.

1. Crystals are built up of positive and negative ions.

II. The charge on the ions is spherically symmetric. The force between two ions is dependent on the distance between the ions and is independent of direction.

If there is only attractive force between the two ions, they have finally coalesced. But due to the electron clouds of two ions, a repulsive force acts between them. The repulsive force increases as the distance decreases. At a certain distance of separation the two forces balance each other and then the P.E. is minimum so that the solid is stable.

15.4.1 Madelung constant

The coulomb energy of attraction betwen two ions separated by a distance 'r' is given by

$$U_c = -\frac{Ae^2}{r}$$

Where 'e' is the charge on each ion, same for all ions and A is called as Madelung constar [illegible] t's value depends on the crystal structure.

The two ions can not continuously approach each other under coulomb attraction. But when they are at a small distance of separation, they begin to repet each other the repulsive force increases very rapidly with decrease in distance Born's experession for repulsive energy is given by,

$$U_R = \frac{B}{r^n}$$

Where B is a repulsive constant and 'n' is a number.

The total energy is given by,

$$U_T = U_c + U_r$$

$$\Rightarrow U = -\frac{Ae^2}{r} + \frac{B}{r^n} \longrightarrow ①$$

At euqilibrium, P.E.is minimum at $r = r_o$

$$\text{Thus, } \left(\frac{du}{dr}\right)_{r=r_0} = 0 \qquad \Rightarrow \left[\frac{d}{dr}\left(\frac{B}{r^n} - \frac{Ae^2}{r}\right)\right]_{r=r_0} = 0$$

$$\Rightarrow \frac{-nB}{r_o^{n+1}} + \frac{Ae^2}{r_o^{\ 2}} = 0 \Rightarrow \quad \frac{nB}{r_o^{n+1}} + \frac{Ae^2}{r_o^{\ 2}} \qquad \Rightarrow B = \frac{Ae^2}{n}.\, r_o^{n-1}$$

ubstituting the value of B in eq. (1),

$$U = -\frac{Ae^2}{r} + \frac{Ae^2}{n}, r_0^{n-1}.\frac{1}{r^n}$$

$$U = \frac{-Ae^2}{r}\left[1 - \frac{1}{n}\left(\frac{r_o}{r}\right)^{n-1}\right]$$

At equilibrium, $r = r_o$

$$\therefore U_0 = -\frac{Ae^2}{r_o}\left[1 - \frac{1}{n}\right] \qquad \longrightarrow ②$$

$$\Rightarrow U_0 = \frac{-Ae^2}{4\pi\epsilon_0 r_0}\left[\frac{n-1}{n}\right] \quad \text{in jouls in SI system}$$

$$= \frac{-Ae}{4\pi\epsilon_0 r_0}\left[\frac{n-1}{n}\right] ev$$

This equilibrium energy U_o is called the lattice energy.

15.4.2 Lattice energy :

This is defined as the energy released in the process when the constituent ions are placed in their repective positions in the crystal lattice (for NaCl this is equal to the energy needed to break are NaCl crystal into Na^+ and Cl^- ions)

This is the amont of energy which is spent to separate the solid ionic crystal into the constituent ions.

It is experimentally measured from the Born-Haber cycle data.

Lattice energy of NaCl :

For NaCl, we know , r is the distance between neighbour atoms, 2r is the side of the cube.(Fig. 15.3)

A sodium atom is surrounded by 6Cl atoms at closest distance 'r', 12 Na atoms at $\sqrt{2}$ r, 8 Cl^- ios at $\sqrt{3}$ r as shown figure 15.3 and another 6 Na+ ions at a distance 2r and so on.

The attractive potential energy :

1. between Na^+ and $6Cl^-$ ions at a distance $r = \frac{-6e^2}{r}$

2. between Na^+ and $8Cl^-$ ions at a distance $\sqrt{3}\,r = \frac{-8e^2}{\sqrt{3}r}$

The repulsive potential energy

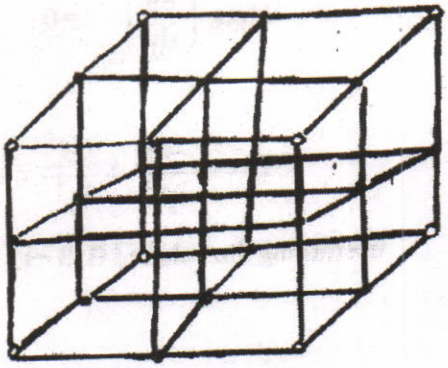


Fig. 15.3

3. between Na^+ and $12Na^+$ ions at a distance $\sqrt{2}\,r = \frac{12e^2}{\sqrt{2}r}$

4. between Na^+ and $6Na^+$ ions at a distance $2r = \frac{6e^2}{2r}$

The coulomb energy of this ion in the field of all other ions is,

$$U_c = -\frac{6e^2}{r} - \frac{8e^2}{\sqrt{3}r} + \frac{12e^2}{\sqrt{2}r} + \frac{6e^2}{2r}$$

$$\Rightarrow U_c = -\frac{e^2}{r}\left[\frac{6}{\sqrt{1}} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} + \dots\dots\right]$$

So, the coefficient of $\frac{e^2}{r}$ is a pure number

$$\therefore U_c = -A\frac{e^2}{r} \quad \text{where } A = \frac{6}{\sqrt{1}} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} + \dots$$

$$= 1.74756$$

Hence Madelung constant for Nacl = 1.74756. $\longrightarrow$ ③

In sodium crystal, the equilibrium distance between the ions is, $r_0 = 2.81\ \mathring{A}$ and Madelung constant $A = 1.748$. Now we have to find out the value of "n".

15.5 Calculation of repulsive exponent 'n' :

Born obtained the value of 'n' from the compressibility measurement of crystal.

The compressibility k of a solid is given by

$$k = -\frac{1}{v}\left(\frac{dv}{dp}\right) \longrightarrow ④$$

According to I law of thermadynamics,

$$dQ = du + dw$$

$$\Rightarrow du = dQ - pdv \ (\because dw = pdv)$$

We know that $dQ = C_v\,dT$.

At absolute zero temp, C_v is negligible

$\therefore du = -pdv$

$$\Rightarrow \frac{d^2u}{dv^2} = \frac{-dp}{dv} \longrightarrow ⑤ \quad \left[\because \frac{du}{dv} = -p\right]$$

Using eqs ④ and ⑤.

Compressibility at absolute zero is given by,

$$k_0 = \frac{1}{v_0}\left(\frac{dv}{dp}\right)$$

$$\Rightarrow \frac{1}{k_0} = v_0\left(\frac{dp}{dv}\right) = v_0 . \frac{d^2u}{dv^2}$$

$$\Rightarrow \frac{1}{k_0} = v_0 . \frac{d^2u}{dv^2} \longrightarrow ⑥$$

We have $\frac{du}{dv} = \frac{du}{dr} . \frac{dr}{dv}$

$$\Rightarrow \frac{d^2u}{dv^2} = \frac{du}{dr} . \frac{d^2r}{dv^2} + \frac{d^2u}{dr^2}\left(\frac{dr}{dv}\right)^2 \longrightarrow ⑦$$

At equilibrium, $r = r_0$ and $\frac{du}{dr} = 0$

$$\therefore \left(\frac{d^2u}{dv^2}\right)_{r=r_0} = \left(\frac{d^2u}{dr^2}\right)_{r=r_0}\left(\frac{dr}{dv}\right)^2_{r=r_0} \quad \text{..........} \quad 6a$$

For Nacl crystal, $V = 2Nr^3$ where N is total no. of molecules a 'r' is the inter ionic distance

$$\therefore \frac{dv}{dr} = 6Nr^2 \Rightarrow \left(\frac{dr}{dv}\right)^2 = \frac{1}{36N^2r^4}$$

At equilibrium, separation $r = r_0$

$$\therefore \left(\frac{dr}{dv}\right)^2_{r=r_0} = \frac{1}{36N^2r_0^4} \quad \text{....7a}$$

Sub. 7a in 6a

$$\left(\frac{d^2u}{dv^2}\right)_{r=r_0} = \left(\frac{d^2u}{dr^2}\right)_{r=r_0}\left(\frac{1}{36N^2r_0^4}\right)$$

$$\Rightarrow \frac{d^2u}{dv^2} = \frac{d^2u}{dr^2}.\frac{1}{36N^2r_0^4}$$

Sub. this in eq. ⑥,

$$\frac{1}{k_0} = v_0\left(\frac{d^2u}{dv^2}\right) \Rightarrow \frac{1}{k} = v_0.\left(\frac{d^2u}{dr^2}\right)\frac{1}{36N^2r_0^4} \longrightarrow \text{⑧}$$

we know that potential energy 'u' for N molecules is,

$$U = \frac{-NAe^2}{r}\left[1 - \frac{1}{n}\left(\frac{r_0}{r}\right)^{n-1}\right].$$

$$= \frac{-NAe^2}{r} + \frac{NAe^2}{n}.\frac{r_0^{n-1}}{r^n}$$

$$\Rightarrow \frac{du}{dr} = \frac{NAe^2}{r^2} + NAe^2.\frac{r_0^{n-1}}{r^{n+1}}$$

Again diff. w.r.t. 'r',

$$\Rightarrow \frac{d^2u}{dr^2} = \frac{-2NAe^2}{r^3} + NAe^2r^{n-1}\frac{(n+1)}{r^{n+2}}$$

At equilibrium, $r = r_0$

$$\therefore \left(\frac{d^2u}{dr^2}\right)_{r=r_0} = \frac{-2NAe^2}{r_0^3} + \frac{(n+1)NAe^2r_0^{n-1}}{r_0^{n+2}} = \frac{-2NAe^2}{r_0^3} + \frac{(n+1)NAe^2}{r_0^3}$$

$$\therefore \left(\frac{d^2u}{dr^2}\right)_{r=r_0} = \frac{NAe^2(n-1)}{r_0^3} \longrightarrow \text{⑨}$$

∴ sub this in eq. ⑧,

$$\frac{1}{K_0} = v_0 . \frac{NAe^2(n-1)}{r_0^3} \frac{1}{36N^2r_0^4}$$

But for Nacl, Vo = 2 Nro3, where N is the total no.of molecules and ro is the nearest distance between two ions.

$$\therefore \frac{1}{K_0} = 2Nr_0^3 . \frac{NAe^2(n-1)}{r_0^3} \frac{1}{36N^2r_0^4}.$$

$$\Rightarrow \frac{1}{K_0} = \frac{Ae^2(n-1)}{18r_0^4}$$

$$\Rightarrow n-1 = \frac{18r_0^4}{AK_0e^2}$$

$$\Rightarrow \quad n = 1 + \frac{18r_0^4}{AK_0e^2} \quad \longrightarrow ❶$$

We have the values of r_0 and A for NaCl crystal as 2.81 Å and 1.478 (refer 15.4.2). So by substituting these values in the following equation alongwith n.

$$u_0 = \frac{-Ae^2}{r_0}\left(1 - \frac{1}{n}\right)$$

We can get the value for lattice energy u_0

This is the Born's theory for calculating the lattice energy for simple crystals like NaCl, Cs Cl --- etc.

15.6 Born - Haber cycle

Lattice energy may be defined as the amount of work to be done to disperse a crystal into a widely separate ions.

It leads to the following conclusions

1. It can not be compared with any directly and readily measurable quantity.
2. It is not same as the heat of formation which is equal to the energy necessary to disperse the crystal into molecular gas.
3. It is not the chemical heat of formation which is the energy released when crystal is formed from metal atoms and diatomic halogen molecules.

Though in some cases lattice energies are determined directly, in majority cases an indirect estimative is done in terms of cyclic process involving certian steps called Born- Haber cycle. For NaCl it is shown in fig 15.4. The formtion of NaCl may be regarded as a process involving some steps and in each step, energy is either released or absorbed.

Energy absorbed is taken as positive and that released is considered negative

The cycle may be understood as follows :

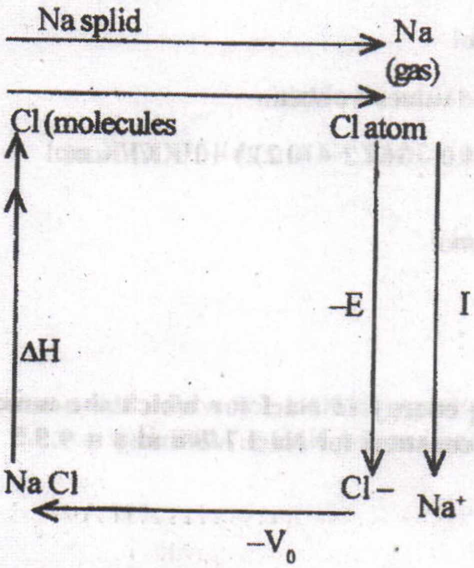


Fig 15.4

1. In the first stage solidium and chlorine molecules are dissociated into constituent atoms. Solid sodium is vaporised by supplying an energy equivatent to its sblimation energy (S), while chlorine morecule is dissociated by the supply of energy equal to the dissociation energy (D), where D/2 is the energy per chlorine atom.
2. Then in the second stage gaseous sodium and chlorine atoms are ionised. This process requires ionisation energy I to remove the outer most electron from Na atom. When this election is added to Cl atom, energy equivalent to the (E) electron affinity is released.
3. In the third stage, the two ions, Na^+ and Cl^-, in getting arranged in the lattice, energy is released (U_0).
4. In the fourth stage, the lattice gets broken into solid Na and Cl molecules and thus reaches the starting point absorbing and energy known as heat of dissociation ΔH.

According to the law of thermodynamics, we write.

$S + (D/2) + I - E - U_0 + \Delta H = 0$, beacuse in cyclic process total energy is equal to zero.

$\therefore U_0 = S + (D/2) \mid I - E + \Delta H$

In this equaltion all the quantities on the right hand side can be experimentally determened and hence lattice energy can be found.

Ex : For Nacl, details are as follows

$S = 108.8 \times 10^3$ KJ/Kmol

$D = 2.42.8 \times 10^3$ KJ/Kmol

$I = 494.0 \times 10^3$ KJ/Kmol

$E = 364.2 \times 10^3$ KJ/Kmol

$\Delta H = 410.2 \times 10^3$ KJ/Kmol

Substituting the above mentioned values we obtain

$$U_0 = (108.8 + 121.4 + 494.0 - 364.2 + 410.2) \times 10^3 \text{ KJ/K mol}$$

$$u\ U_0 = 770.2 \times 10^3 \text{KJ/K mol}$$

15.7 Worked examples :

1. **Calculated the finding energy fo Nacl for which the nearest neighbour distance is 0.324 nanometres madelung constant for Nacl 1.748 and n = 9.5**

Solution :

$$U_0 = \frac{Ae^2}{4p \in_0 r_0}\left[\frac{n-1}{n}\right] \text{ Joules}$$

$e = 1.6 \times 10^{-19}$ coulomb $\in_0 = 8.85 \times 10^{-12}$ fermi m^{-1}

$r_0 = 0.324 \times 10^{-9} m$ $n = 9.5$ $A = 1.748$

$$U_0 = \frac{1.748(1.6 \times 10^{-19})^2}{8.85 \times 10^{-12} \times 4\pi \times 0.324 \times 10^{-9}} \times \frac{8.5}{9.5}$$

$$= \frac{-1.748(1.6 \times 10^{-19})^2}{4\pi.8.85 \times 10^{-12} \times 0.324 \times 10^{-9}} \times \frac{8.5}{9.5} = 6.9 \text{ ev}$$

2. **Madelung constant of Kcl = 1.75. Its nearest neighbour separation is 0.314 nanometres. Calculate the cohesive energy. n = 5.77, I = 4.1 ev and E. 3.6 ev**

Solution :

Potential energy per pair of ions is given by $U_0 = \frac{Ae^2}{4p \in_0 r_0}\left[\frac{n-1}{n}\right]$

$e = 1.6 \times 10^{-19}$ coulomb $n = 5.77$

$\in_0 = 8.85 \times 10^{-12}\ Fm^{-1}$, $r_0 = 3.14 \times 10^{-9} m^{\prime}$ $A = 1.75$

$$U_0 = \frac{1.75 \times \left(1.6 \times 10^{-19}\right)^2}{4\pi\left(8.85 \times 10^{-12}\right) \times 0.314 \times 10^{-9}} \times \left(\frac{4.77}{5.77}\right)$$

$$= -1.06 \times 10^{-18} J = -6.63 ev$$

Potential energy per ion $= \frac{-6.63}{2} = -3.315$ (1)

The energy required to form an ion(K^+, Cl^-) from a pair of K and Cl atoms is equal to the ionisation energy of K atoms minus electron affvity of C*l* atom

Each atom therefore contribute $\frac{4.1 - 3.6}{2} = 0.25ev$ (2)

Thus colerive energy per atom = (1) + (2)

$= - 3.315 + 0.25 + -3.065$ ev

15.8 Summary :

1. Basing on the character of inter atomic binding follows in crystals these are classified as 1) molecular crystals, 2) covalent crystals 3) zonic crystals, 4) metallic crystals and 5) hydrogen bonded crystals.
2. Basing on the strength bonds are classified as primary bonds and secondary bonds.

Ex : for primarly bonds : covalurt, metallic and ionicbonds

Ex. for secondary bonds : Hydrogen bond

3. Born's theory gives the expression for equilibrirum value of the energy (called latice energy)

$$U_0 = \frac{Ae^2}{r_0}\left(1 - \frac{1}{n}\right)$$

Where A is called Madelung constant and 'n' is the repulsive exponent

4. Lattice energy of an ionic crystal is defined as the energy released in the process when the constituent ions are placed in the respective positions in the crystal lattice.
5. Cohesive energy is the energy needed to break the crystal into individual (nutural) atoms.
6. Repulsive exponent 'n' is given by $n = 1 + \frac{18 r_0^4}{AK_0 e^2}$

15.11 Excercises :

1. Madelung constant forCs *Cl* is 1.763. The nearest nighbour separation is 3.36 Å. Repulsive exponent n = 10.5. the ioisation of Cs in 3.89 ev and electron exffivity of Cl is - 3.61 ev. Find the conesive energy per atom. (Ans : -3.085 ev)

2. The potentioal energy of a system of two atoms is given by the expression

$$U = \frac{-A}{r^2} + \frac{B}{r_{10}}$$

A stable molecule is formed with a release of 8.0 ev of of energy when the intevatonic distance is 2.8 Å. Calculate the constants A and B. Determine the force needed to dissociate this molecule and the intuatomic distance at which dissociation takes place.

[Hint : $F = \frac{-dv}{dr} = \frac{-2A}{r^3} + \frac{10B}{r^{11}}$

$F = 0$ at equilibrium positeem $r = r_0$

Thus $A = \frac{5B}{r_0^8}$

As $r_0 = 2.8$ Å. We can show $A = 1.32 \times 10^{77}B$.

$$U_0 = \frac{-A}{r_0^2} + \frac{B}{r_0^{10}} = \frac{A}{r_0^2}\left[1 - \frac{B}{Ar_0^8}\right]$$

We know $A = \frac{5B}{r_0^8}$

Using this relation

$$U_0 = \frac{-4}{5}\ \frac{A}{r_0^2}$$

U_0 is given as 8.ev

$\therefore A = 1.256 \times 10^{-37} Jm^2$

$\therefore B = 9.52 \times 10^{-115} Jm^2$

For required to dissociate the molecule at a critical distance r_c becomes minimum.

$$\therefore \left|\frac{dF}{dr}\right|_{r=r_c} = 0$$

This gives $r_c = 3.30 \times 10^{-10}$m

Substituting this in the equation for F

We get $F = -5.08 \times 10^{-9}$N]

15. Reference books

1.	Introduction to Solid State Physics.	Charles Kittel, John Wiley & Sons.
2.	Solid State Physics	S.O. Pillai, New Age International
3.	Solid State Physics	A.J. Dekkar, Mc.Millan India
4.	Solid State Physics	Dr. S.L. Gupta & Dr. V. Kumar,K. Nath & Co, Merut.

UNIT-4

LESSON-16

MAGNETISM AND SUPERCONDUCTIVITY

Objectives :

After studying this lesson the student is able to know about

1. The magnetic property of materials
2. The classification of the magnetic materials into dia, para and ferro magnetic materials.
3. comparitive study of these three types of magnetic materials.
4. Weiss theory of Ferromagnetism.
5. Ferromagnetic domains.
6. Anti-ferromagnetism and Ferrimagnetism
7. Rudiments of Superconductivity.
8. Properties and Application of Suerconductivity materials.

Structure :

16.1 Introduction :

Magnetism was one of earliest recognised Scientific Phenomenon. This phenomenon, through in early days seemed to be independent of electrical Phenomenon, later the inseparable link between the two phenomena was realised.Now it is established that the magnetic properties of matter are due to the orbital and spin motion of electrons of atoms with which the matter is composed.

Dia, Para and Ferromagnetism :

With reference to the magnetic property, substances can be classified into three types 1. Diamagnetic, 2. Paramagnetic and 3. Ferromagnetic. On the basis of electron theory of magnetism the nature of above three groups can be explained.

16.2 Diamagnetism :

In diamagnetic substances there are no unpaired electrons. The two electrons in a pair possess equal but opposite magnetic memonets and hence they cancel each other resulting in zero magnetic moment. Thus the magnetic moment of a pair of electrons due to orbital motion is zero. Hence the effective magnetic moment in a diamagnetic substance is zero (Fig. 16.2.1)

When the substance is subjected to an external magnetic field of induction $\vec{B}$, then the on electron

$\vec{F} = e(\vec{V} \times \vec{B})$ where $\vec{V}$ is the velocity of the electron. As the velocities of two electrons of in pair are in opposite directions, then forces due to external magnetic field on those two electrons are in opposite directions causing changes in their magnetic moments and thus induced some resultant magnetic moment. let the magnatic field $\vec{B}$ be into the plane of the paper.

When no field Electron -A Electron-B

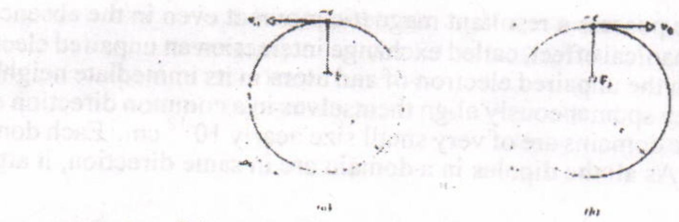


Fig.16.1

when field is present The field is into the paper

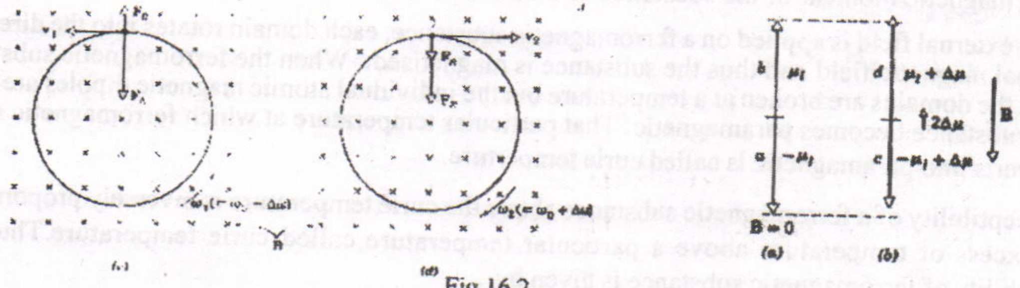


Fig.16.2

In the case of electron a which is moving in anticlock wise direction, the force due to magnatic field on it is away from the center. The force on electron B, (moving in clockwise direction) due to magnatic field is towards the center. Thus the angular velocities of A and B and thus their magnatic moments change. The resultant change in the magnetic moment is $2\Delta\mu$ (Fig.16.2).

16.3 Paramagnetism :

In case of paramagnetic substances the atom inherently possesses some resultant magnetic moment even in the absence of external field. This is due to the nature of the orbital and spin motions of the electrons in that atom. These atomic magnetic dipoles are weak and randomly oriented due to thermal agitations. The thermal agitations increase with increase of temperature.

When an external magnetic field is applied the magnetic dipoles in the substance tend to rotate and into the direction of the external field. Due to thermal agitation complete alignment is not possible. As the external field is made stronger more dipoles align with the direction of external magnetic field.

At a certain temperature, if the field is sifficiently stronger complete alignment of dipoles may become possible and then saturation value is reached for intensity of magnetisation. Intensity of magnetisation is inversly proportional absolute temperature and directly proportional to magnetising field.

$I \alpha H$ and $I \propto \frac{1}{T}$ or $I = C\frac{H}{T}$ where C is called curie constant. $\frac{I}{H}$ is called susceptibility χ, we can write $\chi = \frac{C}{T}$.

Hence susceptibility of paramagnetic substance is inversely proprotional to absolute temperature. This is called curie's law.

16.4 Ferromagnetism :

The atom of a ferromagnetic substance possess a resultant magnetic moment even in the absence of an external field. Due to quantum mechanical effect, called exchange interaction an unpaired electron in one atom interacts very strongly with the unpaired electron of and atom in its immediate neighborhood. As a result of this interaction they spontaneously align themselves in a common direction over a small volume called "domain". These domains are of very small size nearly 10^{-18} cm. Each domain contains very large magnetic dipoles. As all the dipoles in a domain are in same direction, it attains saturation.

Though all the dipoles in a domain allign in a direction, the domains are randomly oriented such that the resultant magnetic moment of the substance as a whole is zero.

When an external field is applied on a ferromagnetic substance, each domain rotates into the direction of external magnetic field and thus the substance is magnetised. When the ferromagnetic substance is heated the domains are broken at a temperature but the individual atomic magnetic dipoles are there and the substance becomes paramagnetic. That particular temperature at which ferromagnetic material converts into paramagnetic is called curie temperture.

The susceptibility of a ferromagnetic substance above the curie temperature is inversely proportional to the excess of temperature above a particular temperature called curie temperature.Thus the susceptability of ferromagnetic substance is given by

$$\chi = \frac{C}{T - \theta}$$

When C is curie constant, T is temperature of the substance and θ is curie temperature.

S.No	Parameter	Para Magnetic	Dia Magnetic	Ferromagnetic
1	Effect of the magnetic field a) Alignment	In uniform field they rotate fill their longest axis is parallel to the field	In uniform field they get their self, perpendicular to the director of the applied field	
	b) Movement	In non uniform field they tend to move from low fields to high fields (towards the stronger parts of the field)	In non uniform field they move from stronger to weaker parts of the field	
2.	Magnetisation	a) It is in the same sense of the applied field	It is opposite to the sense of the applied field	They get high degree of magnetization in the sense of the field
		b) Intensity of magnetising is proportional to the magnetic field	Intensity is proportional to the applied field	Increases very rapidly with the field and attains constant for large H
3.	Permeability	Is > 1, positive	Is < 1 but never negative + Ve	Very high permeability of the order of hundreds, thousand varies with temp.
4	Susceptibility	a) It is positive, and > 1	Small, negative	Positive, very large
		b) Varies inversely as the absolute temperature	Independent of temperature (Bismuth an exception)	Decreases steadily with the rise of temp. Above a certain temp (curie point Ferro magnetic become para.
		c) Susceptibility does not vary with the magnetising field at a given temperature	It does not very with field	Increases with large fields and decreases for larger values of field
5.	Examples	Aluminum, platinum, chromium, calcium oxygen, manganese, Ferric & cupric chloride, magnesium	Bismuth, copper, mercury, Antimony, gold water, Alcohol, tin, Zinc, phosphoras, Hydrogen, air.	Iron, cobalt, Nickel, Steel

16.5 Weiss theory of Ferromagnetism :

Weiss modified his theory of internal molecular field (for paranagnetism) by proposing the concept of 'domains'. This theory of ferromagretism helps us to understand not only the actual relation between para and ferromagretics but also ferromagnetics in particular.

He predicted that any ferromagretic material, at any temperature below curie point is sturated magnetically to a value apropriate to that temperature even when the applied field is zero. Although the substance is everywhere magnetically self saturated, it is diveded into small regions called domins. The magnetisation vectors of those domians are oriented in different dirctions such that the resultant intensity of magnetisation is zero. The sizes of the domains are from 10^{-6} c.c. to 10^{-2} c.c. and the number of molecules per domain is from 10^{12} to 10^{21} molecules in the domain. Due to the mutual friction, the molecules align themselves parallel to one another and attain saturation for the domain. When an external field is applied some of the domains roate and align with the direction of the field and as a whole, the material exhibits magnetic property. But even in the absence of the field, the individual domains, due to the internal molecular field are magnetically saturated. This is called as spontaneous magnetisation.

The field due to the domains, as in the paramagnatic case is taken as βI. The spontaneous magnetisation of domins accurs when β is positive.

The condition for a stable spontaneous magnetisation of the domains can be obtained as follows :

Consider one gram mole of the substance. Let its molecular weight be M, density ρ, magnetic moment σ, its saturation value σ_0. These ferromagnetic domains obey the paramagnetic conditions. So, we can write $\frac{\sigma}{\sigma_0} = (\coth a - \frac{1}{a})$, where $a = \frac{\mu H_e}{KT}$, $H_e = H+\beta I$

When the applied field is zero, $H = 0$, $\therefore H_e = \beta I$ and $a = \frac{\mu \beta I}{KT}$

We have $I = \frac{\sigma\rho}{M}$ and $\mu = \frac{\sigma_0}{N_M}$

$$\therefore \quad a = \frac{\sigma_0 \beta \sigma \rho}{N_M KTM} = \frac{\sigma_0 \beta \sigma \rho}{RTM}$$

$$\therefore \quad \sigma = \frac{RTM}{\sigma_0 \beta \rho} a$$

$$\Rightarrow \frac{\sigma}{\sigma_0} = \frac{RTM}{\sigma_0^2 \beta \rho} a \longrightarrow ②$$

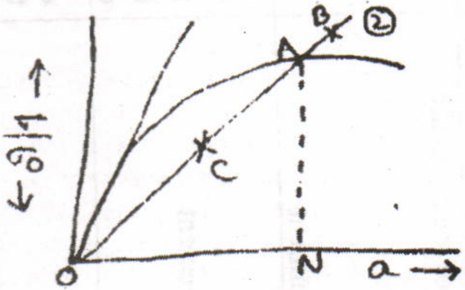


Fig 16.5

But $\frac{\sigma}{\sigma_0} = \text{Coth}\, a - \frac{1}{a}$.

The two equations for $\frac{\sigma}{\sigma_0}$ can be shown on the same graph

The two graphs interesct at two points, O and A. That means, the values of $\frac{\sigma}{\sigma_0}$ which satisfy both the equations are O and AN.

Since the spontaneous magnetisation is assumed for domains, the reasonable value for $\frac{\sigma}{\sigma_0}$ is only AN and not O. When the 'a' value is such that the value for $\frac{\sigma}{\sigma_0}$ is above AN, (that represented by B), the effect of molecular field decreases such tht the magnetisation is brought back to the equilibrium condition. Similarly, when 'a' is just more than zero, the molecular field increases and the magnetisation occurs so as to bring to the equilibrium position. Hence, only A represents the stable value of spontaneous magnetisation.

The slope of the line.(2) is $\frac{RTM}{\sigma_0^2\beta\rho}P$, which depends on temperature. At a particular temperature the slope becomes equal to that of the tangent drawn to the Langevin curve. Above that temperature, the tow curves will not interesect. So, there is no state of spontaneous magnetisation. Hence the condition for spontaneous magnetisation is the temperature, which must be such that $\frac{RTM}{\sigma_0^2\beta\rho} < \frac{1}{3}$

$\Rightarrow T < \frac{\sigma_0^2\beta\rho}{3RM}$ We know that $\frac{\sigma_0^2\beta\rho}{3RM} = \theta$. (curie point)

$\therefore$ The condition is $T < \theta$.

Hence below curie point, even in the absence of the applied field, the domains are magnetically saturated. Hence the condition for spontaneous magnetisation fo domains is that the temperature of the material must be less than the curie point. Above curie point, the spontaneous magnetisation fo the domeains is lost and the ferromagnetics become paramagnetics and obey Curie - Wiess law.

16.6 Anti ferromagnetism :

There are some substances in which the net spin magnetic moment is zero due to the fact that the antiparallel spin magnetic moments are equal. Those are called anti ferromagnetic materials. These substances have an important character that is susceptability vary with temperature and attaivs a maximum at a particular temperature and decreases with temperature as shown in the figure16.4. The temperature at which the susceptability attains maximum value is called Neel temperature. The small value of susceptability at O°K temp is due to possible perfect alignment of moments that are antiparalal. As temperature increases the disorder in the random behaviour for alignment of spin moments increases and results in a higher net magnetic moment in the presence of the external field.

At the Neel temperature the spin moments become essentially random and susceptability reaches maximum. Once the Neel temperature is crossed the susceptability decreases with increase of temperature and the substance behaves as paramagnetic.

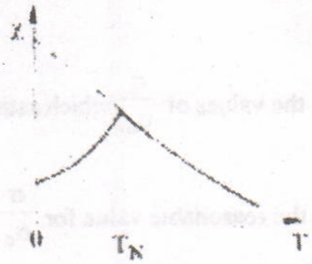


Fig 16.4

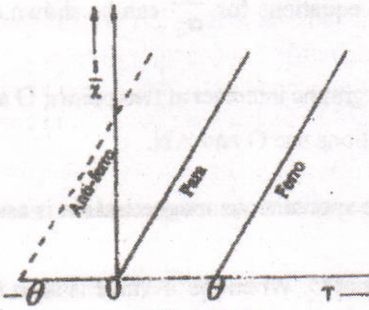


Fig 16.5

Fig 16.5 represents the varia_tion of $\frac{1}{\chi}$ verces T. It shows the comparison between Para, Ferro, and Anti ferro magnetic materials above the critical temparatures.

16.7 Ferrimagnetism :

In case of ferrimagnetic material the spins of different atoms or ions line up antiparallel but they donot cancel each other but there is a net moment. Below Neel temperature the Ferrimagnetic material behaves like a Ferromagnetic material and above θ_n it is para magnetic. The spontaneous magnetisation in these materials is due to antiparallel but unequal spins

Barium and strontium ferrites are generally used in the preperation of powerful magnets.

The Ferrite crystal structure can be thought of as a composite structure of two penetraling sublattices

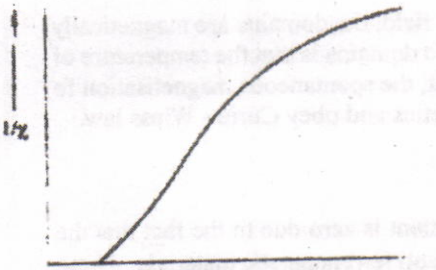


Fig 16.6

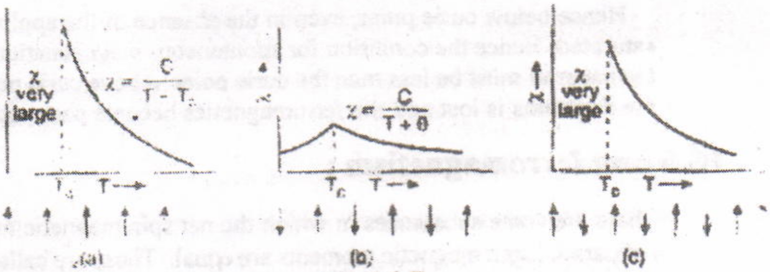


Fig 16.7

Fig.16.6 represents the variation of $\frac{1}{\chi}$ with temparature.

Fig. 16.7 shows χ verses T a) For ferro magnetic materials

b) For Anti ferro magnetic materials

c) For ferri magnetic materials.

16.8 Super conductivity :

In 1911 Kamerling Onnes was measuring the electrical resistivity of mercury at low temperatures. He observed that the electrical resistivity of pure mercury dropped abruptly to zero at about 4.2°K (boiling point of Helium). He concluded that at such low temperature mercury entered into a new state and called as superconducting state. The phenomenon is now referred to as superconductivity. As resistance is zero in such a state current can continue.

The particular temperature below which a material looses its resistance is called the critical temperature (T_c) or superconductive transition temperature.

16.9 Properties of superconducting materials :

Some of the properties of superconducting materials are given below.

1. In case of elements with different isotopes, the transition temperature T_c decreases with increasing atomic weight.
2. The property of super conductivity of an element is not lost by adding impurities but the critical temperature is found to decrease.
3. The thermal expansion and elastic properties do not change in the transition.
4. The crystal structure as studied by X-ray diffraction was found to have no chnage due to transition and thus superconductivity may be more connected with conduction electrons than with atoms as a whole.
5. All thermoelectric effects disapear in super conducting state.
6. Below T_c, the super conducting property is destroyed by the application of a strong magnetic field. At any temperature (below T_c) there is a corresponding critical value of magnetic field which can destroy superconductivity.
7. A super conductor pushes out the magnetic field so that magnetic induction B is equal to Zero inside the conductor. It is called Meissner effect.

16.10 Application of superconducting materials.

1. Using superconductors very strong magnetic are made
2. They are used in Medical field
3. They are used in Elecrtrical switching equipment
4. superconductors are used for windings in a tranformer and power transmission lines
5. Superconductors, because of levitation effects are used in frictionless bearings and highspeed trains.
6. Superconductors are used in SQUIDS (Super Conductring Quantum Interference Devices), Josephson devices Bolometers and Elecromagnetic shielding.
7. They are used in semiconductor-superconductor hybrids, optoelectronic devices and also in active super conducting devices like (FETs)

16.11 Summary

1. Magnetic and electrical phenomena have a close and inseparable link.
2. Magnetism is clasified as, Diamagnetism, Para magnetism, Ferromagnetism
3. Antiferromagnetism
4. Ferrimagnetision
5. In case of paramagnetic substance some resultant magnetic moment is found even in the absence of external magnetic field.
6. In Diamgnetic substances there are no un paired electrons. The two electrons in a pair give equal magnetic moments in opposite direction and hence the resultant magnetic moment is Zero in the absence of external field. When such material is subjected to external field there are changes in magnetic moments of the paired electrons caused by external field. That results in a net induced magnetic moment.
7. In Ferromagnetic materialism there are certain small regions, called domains in which all the magnetic dipoles are spontaveously aligned in a direction and gives saturation value to magnetic moment in that region. This magnetisation occuring in a domain is referred to as spontaneous magnetization.
8. In the absence of external field various donaius of a ferromapuetic material are randomly oriented such that the resultant magnitization is Zero.
9. Above a critical temperature the spontaneous magnetisation is lost and then the ferromagnetic material becomes paramagnetic. That temperature is called curie temperature.
10. In Antiferromagnetic materials the net spin magnetic moment is zero due to the fact that antiparallel spin magnetic moments are equal. The fundamental character of these materials is that the sesceptibility of these materials varies with temperature and attains a maximum and then decreases with increase of temperature.
11. In case of Ferrimagnetic materials the spins of different atoms or ions align antiparallel but do not cancel each other and the spontaneous magnetisation in these substances is due to antiparallel but unequal spins. They can be thought of as a composite structure of two penetrating sublattices. Above Neel temperature Ferrimagnetic material becomes paramagnetic.
12. At low temperatures certain materials are found to loose completely the electrical resistance and then the materials is said to be "Superconducting". This phenomenon of a substance becoming superconducting is called Superconductivity.

16.12 Key Words

Dia, Para , Ferro, Antiferro and ferrimagnetism, Ferrites, curie temperature Neel temperature, Super conductivity Meisner effect.

16.13 Self Assessment Questions

1. Explain Dia, para and ferromagnetism
2. Distinguish between Dia, Para and Ferromagnetism.
3. Explain in detail Weiss theory of Ferromagnetism.
4. Explain Antiferromagnetism
5. Explain Ferrimagnetism

16.14 Reference Books :

1.	Introduction to Solid State Physics.	Charles Kittel, John Wiley & Sons.
2.	Solid State Physics	S.O. Pillai, New Age International
3.	Solid State Physics	A.J. Dekkar, Mc.Millan India
4.	Solid State Physics	Dr. S.L. Gupta & Dr. V. Kumar K. Nath & Co, Merut.

LAB MANUAL (Paper-4)

INDEX

Expt No :1

e/m of an electron -J.J.Thomson Method

AIM : To determine the specific charge i.e the ratio of charge and man of an electron by J.J.Thomson method-using crossed electric and magnetic fields.

APPARATUS : Thomson's discharge tube, induction coil,D.C.supply of 100 to 220 volts,two long magnetometers,

scale and piece of chalk.

FORMULA : $\frac{e}{m} = \frac{X}{r.H^2}$ emu/gram.

Here X-the intensity of electric field

H-Magnetic field intensity to nullify the deflection of electron due to electric field.

r-radius of curvature of circular path in the magnetic field.

$X = v.10^8 / d$ emu.

Here V-potential difference between X1&X2 plates.

d-distance between plates

$$H = \frac{4\pi nI}{10} \text{ oersted}$$

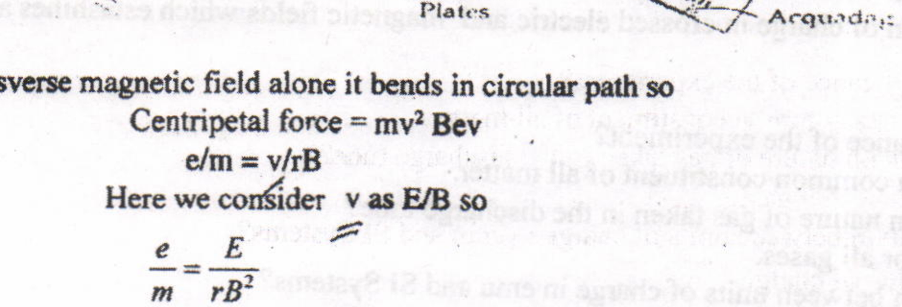
where n - no of turns in the solenoid

I-current in the solenoid

THEORY : A charged pariticle like an electron gets deflected in parabolic path in Transverse electric field and gets deflected in circular path in transverse magnetic field when both are applied at once and the deflection is made zero then

electric force = Ee = Bev (mag.force)

v = E/B



In Transverse magnetic field alone it bends in circular path so

Centripetal force = mv^2 Bev

e/m = v/rB

Here we consider v as E/B so

$$\frac{e}{m} = \frac{E}{rB^2}$$

In C.G.S. System we have taken B as H and the electric intensity as X so

$$\frac{e}{m} = \frac{X}{r.H^2}$$

EXPERIMENT:

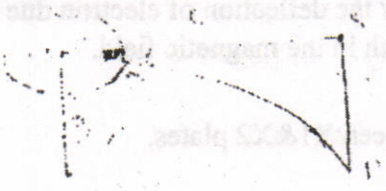
1.Keep the cathode ray tube along the magnetic meridian. Give D.C. voltage to electrodes.

2.When current is passed through the tube the electron beam is produced and it gives luminous spot on the screen. Read the potential appliec with the help of volt meter.

3.Using solenoid circuit the spot on the screen is again brought to original position.The current I passing through the solenoid is noted.

4.Without disturbing the solenoid circuit the spot non gets deflected under the influence of the magnetic field alone.

MEASUREMENT OF RADIUS:



$$Tan\theta = \frac{SP}{SG} = \frac{MB}{r..}$$

$$\therefore r = \frac{MN}{Tan\theta}$$

OBSERVATIONS AND CALCULATIONS:

1. Voltage applied across the mater in cathode ray tube=V
2. Distance between the plates $X_1 \& X_2 = d$
3. Current through the solenoid =I
4. Noof turns in the soleniod per unit length = x
5. Radius of circular path $r = MN/\tan\theta$

RESULT : The value of e/m=1.76 × 10^{11} coloumbs/kg.

VIVA QUESTIONS:

1.what is the principle in the experiment?

ANS: Study of motion of charge in crossed electric and magnetic fields which estashihes an electron has particle nature.

2.what is the significance of the experiment?

ANS:An electron is a common constituent of all matter.

3.Is e/m dependent on nature of gas taken in the discharge tube?

ANS:No.It is same for all gases.

4.What is the relation between units of charge in emu and SI Systems?

ANS:1col= 10^{-1} emu of charge.

5.What is the use of keeping dischargetube along the magnetic meridian?

ANS: To remove the effect of earth's magnetic field on the motion of electron..Because $F = e(v \times B)$=0. when v and B are same direction.

Expt No:2

TEMPERATURE CHARACTERISTICKS OF THERMISTOR

AIM : To determine the temprature coefficient of a thermistor with the help of temperature characteristicks.

APPARATUS : Thermistor,temprature bath ie.,a copper vessel with a liquid taken in a test tube,thermometer,connecting wires,multimeter.

FORMULA: $\log_{10} R = \log_{10}{}^{a} + 0.4343\frac{b}{T}$ and

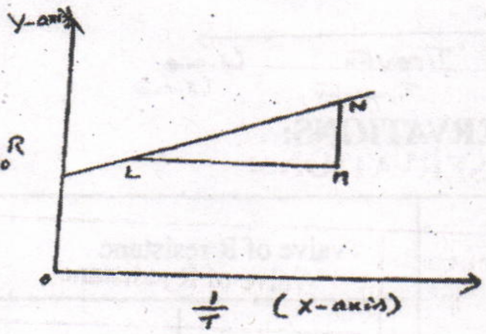
$$\alpha = \frac{-b}{T^{2}}$$

where R is the resistance

T is the absolute temprature

a and b are Thermistor constants(from graph)

THEORY : A graph is drawn taking the valves of resistance R and temperature in absolute scale which is as shown in the figure.

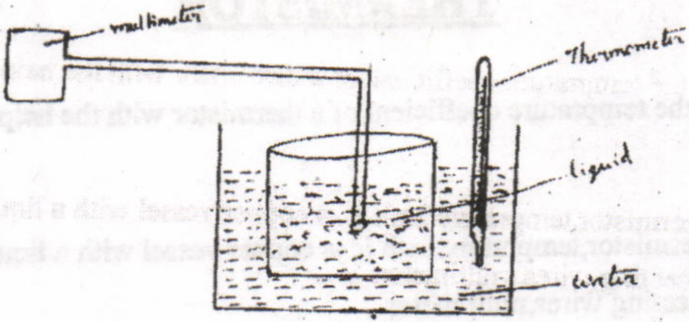


slope gives $\frac{NM}{LM}$ which is equal to 0.4343

The intercept on Y-axis ie., 'OA' gives $\log_{10} a$

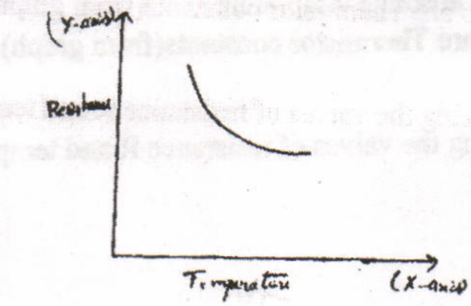
EXPERIMENT:The given thermistor is kept in the oil bath after connecting the wires to the multi-meter which is arranged to measure resistance of the thermistor.The initial temp of the oil bath is gradually increased and for every 5 C temp, the corresponding resistance is noted.The temperature is increased upto 100 C.Now twhile cooling again the resistance for every 5 C is noted.

Figure.



The average valve is taken as R for the temp t C.Now measure log 10 R and draw the graph between log 10 R and 1/T from which the constants a and b are determined using the equation ① the valve of temperature coefficient of the termistor can be determined.Another graph with temp and resistance can be drawn which is as shown in the figure.

Graph:



TABULAR FORM FOR OBSERVATIONS:

S.No.	Temperature		$\frac{1}{T}$	valve of R resistanc		R	$\log_{10} R$
	$t°c$	T=(t+273)		Temp increasing	Temp increassing		

CALCULATIONS AND RESULT:

(1)On the $\frac{1}{T}$-- $\log_{10} R$ graph the straight line obtained is extrapolated backwards to intersect Y-axis at A

OA= $\log_{10} R$ a=----------

(2)slope of the graph =NM/LM=0.4343b

b= ----------------

(3) $\alpha = \frac{-b}{T^2}$

and the valve of α can be deterined at 2 or 3 temperature.

PRECAUTIONS :

(1)Temperature are to be determined without taking the thermometer outside the oil bath.
(2)Dont operate the heating procedure beyond 100 C.
(3)Resistance range in the multimeter should be carefully adjusted.

VIVA - VOCE:

(1) What is a thermistor?
Ans: A thermistor is a sensitive semiconductor having large temp coefficient of resistance.
(2) How are thermistor made?
Ans: With the help of mixture of oxides like NiO2,Mn2O2 and Co2O3(cobalt oxide)
(3) What is the resistance range of a thermistor?
Ans: 100 ohms to 10 M ohms.
(4) How the temperature effects the resistance of a solid like conductor,semiconductor and alloys?
Ans: Resistances increases with increase of temp in conductors and deceases in semiconductors and remains almost same same in alloys like Mangnin and Constantan.

EXP NO:3

R.C COUPLED AMPLIFIER

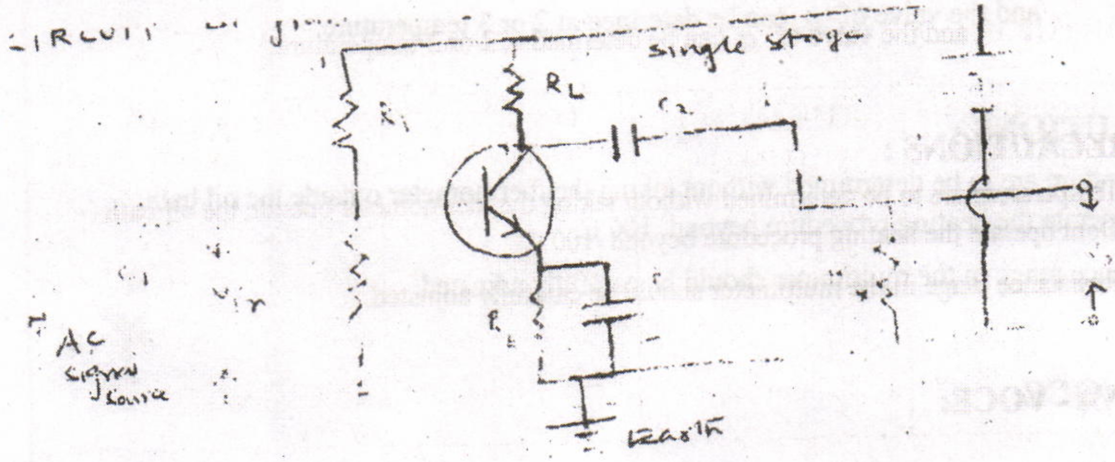
AIM

To draw the frequency response curve and also to measure the voltage gain for a single stage R.C Coupled amplifier

APPARATUS :

N P N tranister (BC 148), a signal generator (20 to 20,000 Hz) range ,capacitors,multimeter, 12v battery and connecting wires.

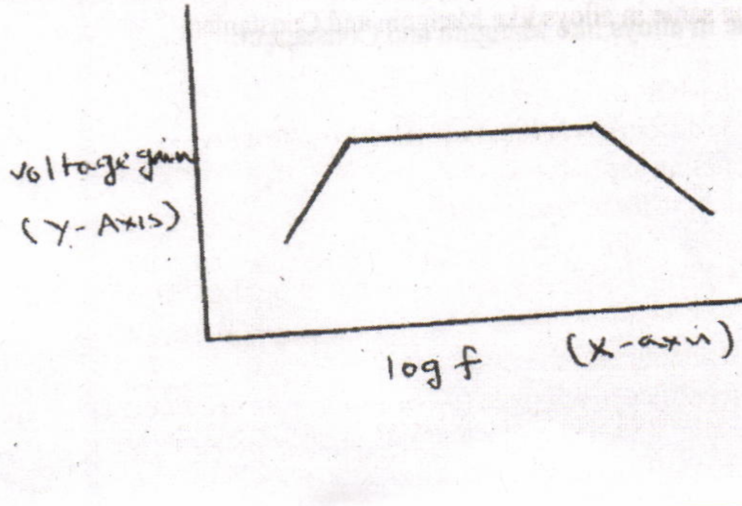
CIRCUIT DIAGRAM :



FORMULA:

$$\text{Voltage gain } (A_v) = \frac{\text{outputvoltage}}{\text{inputvoltage}} = V_o/V_i$$

GRAPH:



THEORY:

The positive terminal of 12v battery vcc is connected to the collector through the load resistance (R)=2K . the negative terminal is connected to the emitter through RE-CE combination.The audio frequency signal from a signal generator is applied between the base and the emitter through the coupleing capacitor c1 of 100 f and a resistor r1 of 50k and R2 of 22 k serving as potential divider. This arrangement provides the proper biasing to the emitter and the base. The capacitor c2 is also of 100 f as c1. After all connections are made the frequency oscillator is first kept at 100hz and the amplitude of the input signal is adjusted to be vi=20mv. This should be kept constant throughout the experiment while changing the frequency.Using multimeter vi and v0 are noted.

EXPERIMENT:

Changing the frequency as 200hz, 300hz--------------up to 100khz, The values of v0 are measured keeping vi as constant.

TABULAR FORM:

SNO	Frequency of input signal	input voltage vi=constant	output voltage	voltagegain *Vo / Vi*

PRECAUTIONS:

1.The input voltage vi should be kept constant .

2.Emitter junction is kept in forward bias and collector junction is in rivers bias.

Ans: they provide forward bias to the emitter base junction just by forming a potential divider with vcc.

RESULT :

A single stage R.C Coupled amplifier is constructed. it s voltage gain is calculated at different input frequencies. The frequency response curve is drawn.

VIVA -VOCE :

1.What care should be taken while Amplification ?

Ans:The signal should not be distorted while getting A mplified or enlarged.

2.what purpose does the coupling capacitor cc curve?

Ans: It couples the input signal to the input of the Ampifier.

3.What is the use of R1 and R2 transistors?

Ans: they provide forward bias to the emitter base junction just by forming a potential divider with Vcc.

4.What is the advantage of R-C coupled Amplifier?

Ans:It has uniform voltage amplificatin and there win be no distortior in the output.

Expt No:4 Verification of DEMORGAN'S THEOREMS

Aim: To verify DE morgan's theorems in Boolian Algebra.

1) $\overline{A+B} = \bar{A}.\bar{B}$

2) $\overline{A.B} = \bar{A}+\bar{B}$

Apparatus: OR gate , AND gate, NOT gate, batteris, bread board, connecting wires, D.C voltmeter.

Formula : 1. The complement of sum of two or more variables is equal to the product of the complement of the variables.

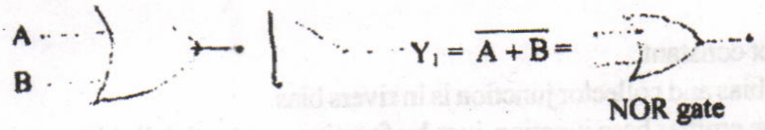
$$\overline{A+B} = \bar{A}.\bar{B}$$

2.The complement of product of two or more variables is equal to the sum of the complement of the variables.

$$\overline{A.B} = \bar{A}+\bar{B}$$

Circuit for verification of 1'st Law:

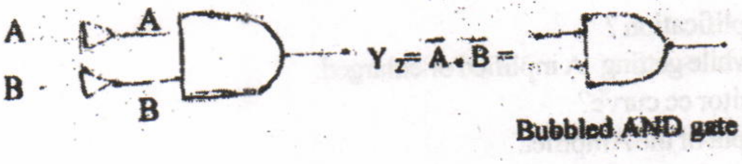
L.H.S.



A	B	A+B	$\overline{A+B}$
0	0	0	1
0	1	1	0
1	0	1	0
1	1	1	0

Fig. (a)

R.H.S.



A	B	$\bar{A}$	$\bar{B}$	$\bar{A}.\bar{B}$
0	0	1	1	1
0	1	1	0	0
1	0	0	1	0
1	1	0	0	0

Fig. (b)

Circuit for verification of 2'nd Law:

L.H.S.

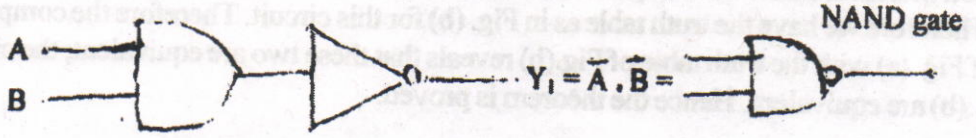


Fig. (c)

A	B	A.B	A.B
0	0	0	1
0	1	0	1
1	0	0	1
1	1	1	0

R.H.S.

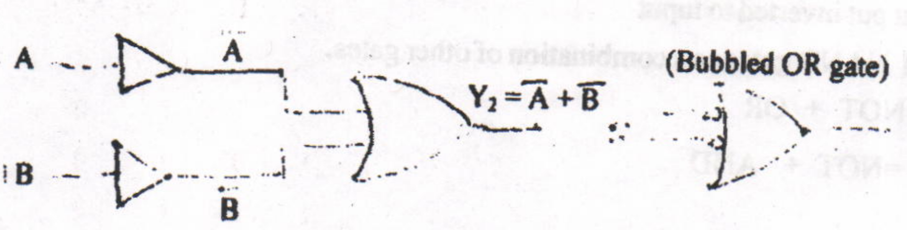


Fig. (d)

A	B	$\overline{A}$	$\overline{B}$	$\overline{A}+\overline{B}$
0	0	1	1	1
0	1	1	0	1
1	0	0	1	1
1	1	0	0	0

Experiment:

For 1 st Law:

Consider L.H.S i.e. It indicates a 2-input OR gate followed by a NOT gate that is a NOR gate as shown in fig (a). Fig (a) also shows its truth table. Similarly take the R.H.S of the theorem which is equal t $\overline{A}.\overline{B}$. This equation indicates that the two inputs A and B are inverted before they reach the AND gate a shown in Fig (b). Therefore we have the truth table as in Fig. (b) for this circuit. Therefore the comparison of the truth table of Fig .(a) with the truth table of Fig.(b) reveals that these two are equivalent; the circuits of Fig .(a) and Fig .(b) are equivalent. Hence the theorem is proved.

For the 2nd Law:

Left hand side of the theorem shown is a 2-input AND gate followed by a NOT gate i.e. a NAND gat having the circuit and truth table as shown in Fig (c). The right hand side of the equation shows an OR gate with two inverted inputs. The circuit and truth table is shown in Fig (d). Comparison of these two truth tabl reveals that they too are identical and equal. Therefore the theorem is proved.

VIVA - VOCE :

1)Which is a universal gate ? Why ?

Ans. NAND is a universal gate . Because by combining NAND gates we construct AND, OR, NOT etc. Sowe can carry any logic function using NAND gate alone.

2)Why is the NOT gate called an inverter ?

Ans. Because the out put inverted to input

3) Express NOR and NAND gates as a combination of other gates.

NOR gate = NOT + OR

NAND gate =NOT + AND

EXP NO : 5 PHASE SHIFT OSCILLATOR

AIM : To construct a phase shift oscillator which is semi conductor solid state bipolar -junction transistor and to check the out put frequency both by theoritical and experimental values.

APPARATUS :A p-n-p transistor, power supply CRO, suitable resistors and capacitors, multimeter, frequency meter connecting wires.

FORMULA : From theoritical considerations oputput frequeny

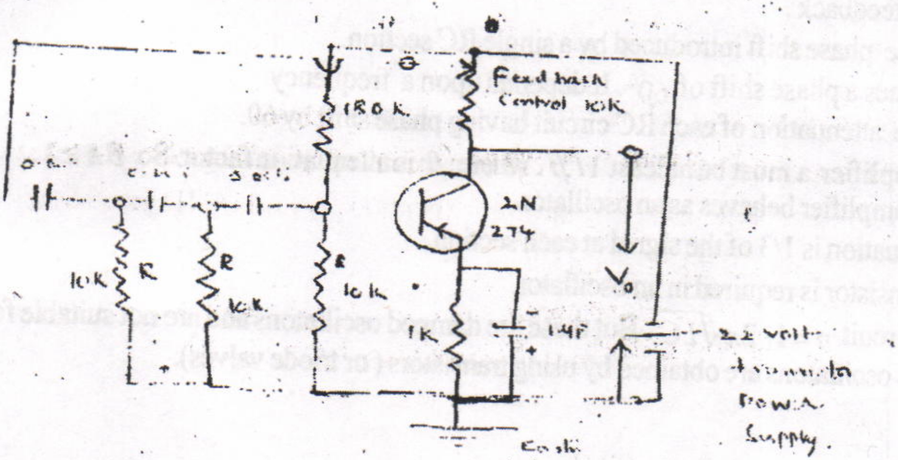
$$f_0 = 1/2\pi\sqrt{6}RC$$

From experimental observations

$$f_0 = 1/T$$

where T is the timeperiod from CRO

CIRCUIT DIAGRAM :



THEORY : An oscillator is a device that produces an out put signal that repeats a perticular pattern i.e sinewave squarewave sawtooth wave..etc.of current or voltage variations continoous with respect time. Usuing a D.C power source connected to the circuit, the oscillator gives output in the form opf A.C signal. this process can be concidered as a inverse of rectifications and an oscillator can be conceived of as aD.C to A.C converter.To maintain oscillatons, the signal losses with the waveforming network of the otherparts of the oscillator circuit.A part of the output signal is added to the signal that is being amplified.This is called feedback in to the input signal.

EXPERIMENT: By changing the values of either R or C on the breadboard waveforms of different amplitude can be observed on the CRO screen. So the corresponding time period can be measured directly from the screen using the scale on it. Othertwise theoutput frequency can be measured using a frequency meter.The theoritical value can be calculated using the formula for found to be nearly equal.There is also another method using Lissajous figures.which is given by

$$\frac{n_x}{n_y} = \text{No.of loops touching the Y-axis/No.of loops touching the x-axis}$$

PRECAUTIONS:

1.The polarity of the power supply and the emmiter by pass capacitor should be indicated in the diagram.

2.If gain is not atleast 29 we have to change the transistor.

VIVA-VOCE:

1. How does the phase shift oscillator work.

A.If couple the collcctor and the emmittershifts the phase by an addittional 180 so as to obtain a re generateive feedback .

2. What is the phase shift introduced by a single RC section.

A. It bproduces a phase shift of 60^0. It depends upon a frequency.

3.What is the attenuation of each RC circuit having phase shift by 60.

A. Of the amplifier a must be at least $1/\beta$. where β is attenuation factor. So $\beta A \geq 1$.

4. When an amplifier behaves as an oscillator.

A. The attenuation is 1/3 of the signal at each section.

5. Why a transistor is required in an oscillator.

A. For LC circuit $n = 1/2\pi\sqrt{LC}$. But these are damped oscillatons and are not suitable for transmission contionuous oscillatons are obtained by using transistors (or triode valves).

Expt No:6 Determination of Planck's Constant (Photo Cell)

Aim : To determine the Planck's Constant using a Photo Cell.

Apparatus : An in candescant lamp 100 W, a fine narrow slit, a covering lence , filters,galvano meter, Plng key, D.c Power supply (0-15V), veriable resistence R, connection wires.

Formula :

$$h=\frac{e(V_2-V_1)\lambda_1\lambda_2}{c(\lambda_1-\lambda_2)}$$

Where e - electronic charge

V_2- Stopping potential corresponding to wave length with filter one

V_1- Stopping potential corresponding to wave length with filter two

λ_1, λ_2 - wavelengths of light used

Theory :

Photo electric effect is an ideal example for Law of Conservation of energy. When E.M radiation of sufficiant energy is incident on alkali metals like Na, K, Li, Cs etc. the latter will emit Photo electrons. Since the electrons are bounded to the nucleans in an atom , some of the incident energy will be used to free the electrons, which is called work function.

$$h\upsilon = w + \frac{1}{2}mv^2$$

If V0 is the stopping potential of a particular colour of lifght then

$$\frac{1}{2}mv^2 = eV$$

$$\text{and } w = h\upsilon_0$$

which implies that $h\upsilon = h\upsilon_0 + eV$

$eV = h\upsilon - h\upsilon_0$

$$\therefore V = \frac{h}{e}\upsilon - \frac{h}{e}\upsilon_0$$

which is in the form Y= mx+c

So taking stopping potential value along Y-axis for different colours and their corresponding frequency along X-axis, if a graph is drawn it will be a straight line with an intercept. The slope of the graph which is a constant gives h/e.

Slop= h/e

Plank's constant h= slop × e

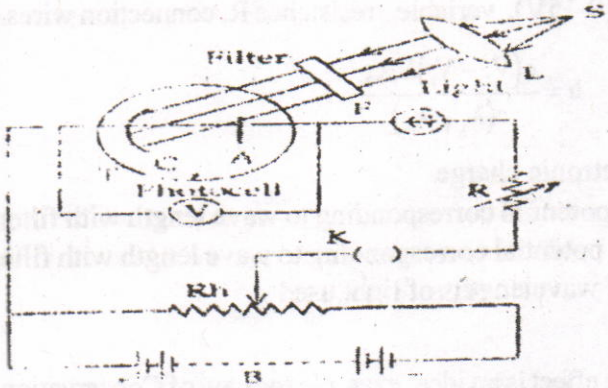
We can write $h\upsilon_1 = h\upsilon_0 + eV_1$ and $h\upsilon_2 = h\upsilon_0 + eV_2$ and $c = \upsilon\lambda$

$$\therefore h = \frac{e(V_2 - V_1)\lambda_1\lambda_2}{c(\lambda_1 - \lambda_2)}$$

substituting the values of λ_1, λ_2 and v_1, v_2 we can determine Plank's constant 'h'.

$$h = 6.625 \times 10^{-34} \text{ jouls. sec}$$

Circuit Diagram:



Experiment :

When white light is mace to incident on the Photo cell after passing through a filter, Photo electronis are ejected and Photo current is observed. When the emitter is given positive potential or the collector gradually decreases and at a particular stage it becomes zwro. Such a potential is called Stopping potential V1 for the colour of wavelength . The experiment is repeated for different colours and V2 , V3, V4 are noted against using any pair of readings the value of 'h' can be determined. Finally the average value can be measured.

Precautions :

1. **Care should be taken to see that filter choosen are monochromotic as far as possible.**
2. **The distance of the incandescent lamp framthe photo cell should not altered during the complete experiment.**

Viva Voce :

1. **Dose the Plank;s constant depend on the metal of Cathode or frequency of light incident?**

A. **No, it is independent of the factors and is a universal constant.**

2. **Who discovered Photo-electric effect?**

A. **Hertz.**

3. **What is the main source of error hear and how will it effect the result?**

A. **The surface of the Cathode.C will not be pure metal.Hence we don't get exact value of 'h'.**

4. **What are the other source of error in this experiment?**

A. **The filter may not be perfect and hence light coming out from it may not be pure monochromatic.**

5. **Wheredose 'h' arise? What is it's significance?.**

A. **'h' is predominaent and can be observed in all nuclear and atomic phenamena.It is more predominent than in mathematics.**

Exp. No:7 Rydberg constant-study of Hydrogenspectrum

AIM : To determine the Rydbergs constant for hydrogen by studying the hydrogen spectrom.

APPARATUS : Hydrogen discharge tube ,induction coin set up step up trasformer, diffraction grating spectrometer, spirit level, reading lens.

FORMULA :

$$\frac{1}{\lambda}=R\left(\frac{1}{n_1^{2}}-\frac{1}{n_2^{2}}\right)$$

Where $n_1 = 2$ are balmer series

$n_2 = 3,4,5$-----

λ = the wave length of corresponding spectral line

R = Rydbergs constant.

THEORY:

When an hydrogen atomis in exited state it radiates energy in the form of ultraviolet visible light .Infra red radiation since the Balmer series are electronjumps from high energy level to 2ndorbit .So when $n_1=2$, $n_2=3,4,5$--- we can see the spectral lines when $n_1=2$, $n_2=3$

$$\frac{1}{\lambda}=R\left(\frac{1}{4}-\frac{1}{9}\right)=\frac{5R}{36}$$

$$R=\frac{36}{5\lambda}$$

This spectral lines will be red in colour.

When $n_1=2$, $n_2=4$ we have

$$R_H=\frac{16}{3\lambda}$$

which is bluish green

When $n_1=2$, $n_2=5$ we have

$$R=\frac{100}{21\lambda}$$

which is blue colour

When $n_1=2$, $n_2=6$ we have

$$R=\frac{9}{2\lambda}$$

which is violet colour.

The unit of 'R' are cm^{-1} or m^{-1} .And

$$R = \frac{me^4}{8\varepsilon_0 ch^3}$$

whetre m = mass of electron
e = charge of electron
c = velocity of ligh
h = plank constant
ε_0 = permitivity of free space

The value of $R = 1.097 \times 10^{-7} m^{-1}$

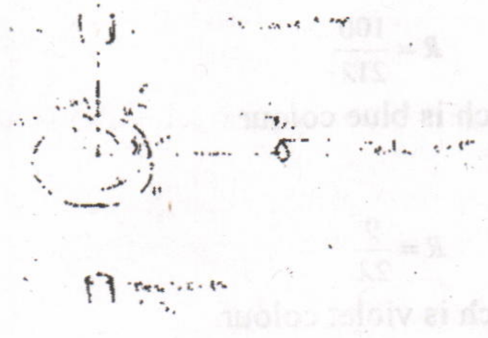
To calluculate the value of R using any one of the above equation we have to calculate λ accurately for that colour. So we are using grating plate for that perpose.

From grating plate

$$\lambda = \frac{\sin\theta}{Nn}$$

where θ - angle of diffraction
N - no. of linesw per centimete length of a grating.
n - order of spectrum.

<u>EXPERMENT</u>: After arrangement the hydrogen discharge tube in the actual set up mentioned for it with step up trasformer,priliminary adjustment to the spectrometer are made and the grating plate is fixed on its prism table .Now the adjust the grating to benormal to the incident light by bringing the collimeter infront of sodium vapour lampand the slit is illuminated as shown in figure and keep the grating in normal incidence.



Now white light from hydrogen discharge tube is made to incident on grating through collimeter .wewill have first order spectrum both on left andright sides of central maxima with colours violet blue,blueish green, red.Now coincide the cross wires of the telescope with violet colour then blue,blueish green , and red colours and note down the readings as R_1, R_2, R_3, R_4 .Now rotate the telescope to the right side end again note down the readings as R_1', R_2', R_3', R_4' corresding colours of the left side.Now the angle of diffraction

$$\theta = \frac{R_1' - R_1}{2}$$

for any grating using in laboratory

$$N = \frac{15000}{2.54} \text{ and } n = 1$$

so using $\lambda = \frac{\sin\theta}{Nn}$ **we can calaulate the wavelength of the corresponding colour which is required to calculate R using the equation**

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

TABLE

Spectral line colour	Left side			right side			θ
	M.S.R	V.S.R	Total R_1	M.S.R	V.S.R	Total R_2	$= \frac{R_1 \sim R_2}{2}$

PRECAUTIONS :

1.The grating should be vertical with itslines parallel to the slit and normal incident position for incident light.

2.Grating sould not be fourhead with hand .It should be handed only at the edges .

3.The spectrometer should becovered with cloth to eliminate any extraneous light ertering inciside the spectrometer

4 Priliminary adjustment to the spectrometer must be done care fully .

VIVA-VOCE:

1 Why should the telescope always face the ruled surface of the grating?

Ans:In such a cace only light falls normally on the grating plate enter it undiviated .Then at the ruled surface diffraction takes place and only the angle of diffraction is mensured.

2.To which class of diffraction this experiment belongs to ?

Ans. This is a Fraunhofer class of diffraction .Because the light rays coming out from the collimeter are parallal and the parallal beam is incident on the Grating.

3. What happens as the order of spectrum is increased ?

Ans: The intensity of spectral lines decreased and the distance between them increased.

4. Dose the grating spectrum depends upon the meterial ?

Ans. No. It is independent of meterial. Where as a prism spectrum is dependent on the meterial.

5. what are the reasons for the formation of spectum in prism and grating ?

Ans. In case of prism different colours have different refractive index. In caes of grating different colours get diffracted at different angles.

6. What is the differences in order of coloursof a grating and a prism spectrum ?

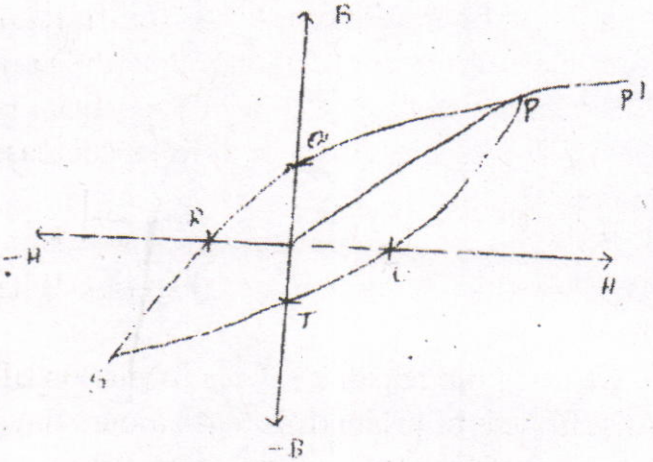
Ans. In case of grating violet is nearer to central maxima and red colour is the farther. In case of prism Red is nearer to undevided path and Violet is farther.

Expt No:8 8.HYSTERESIS CURVE OF TRANSFORMER CORE

AIM : To draw the hysteresis curve of a transformer core using a CRO and to find the energy loss per unit volume per cycle and the coerecivity and Retentivity of the material of core.

APPARATUS : A transformer core with primary (Np) and secondary (Ns) windings ;A step down transformer (3v to 10v and 100 mA), A low loss capacitor of 4 micro faraday capacitance , 2 resisters ,A.C main supply and CRO.

FORMULA :



The phenomenon by which magnetic induction (B) lags behind magnetising field H is called "Hysteresis"

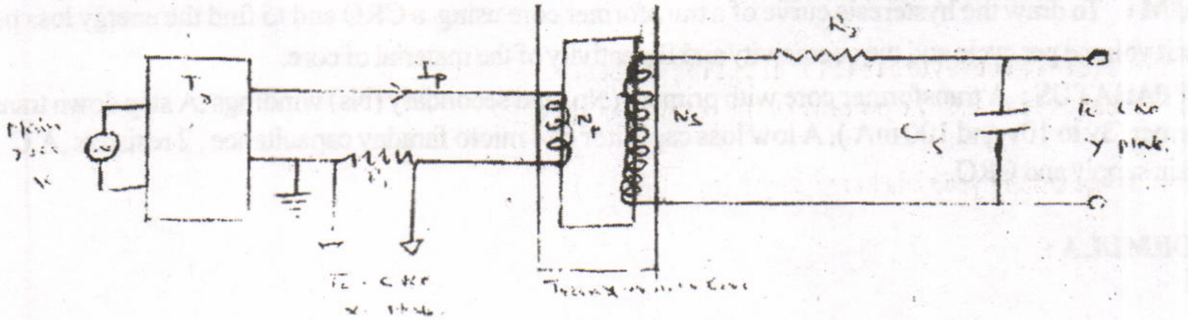
Hysteresis loss =Area of the curve PQRSTUP.

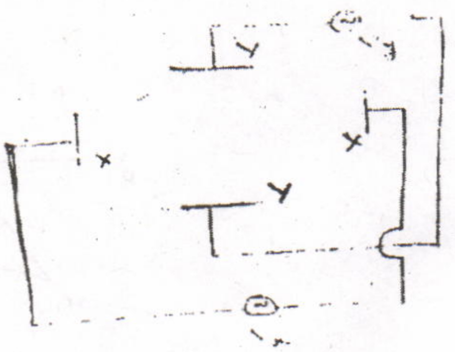
Retentivirty = OQ ________ units Tesla.

Coercivity = OR ________ units amp/meter.

THEORY : When external magnetic field H is applied the domains having their magnetisation parallel to the field grow at the expense of other domains.Thus initially magnetisation increases . This is shown by the curve OP .As and when all the domains get magnetised ,there is no further scope for increase in magnetisation and it is saturated as shown as PP'.Now let us gradually decrease the magnetising field H.Instead of coming back a long PO the curve retraces a long PQ.At Q even through the applied field H is completely removed ,there still remains certain magnetic field induction Br (=OQ).This Br is called retentivity. Now when the applied field is removed (-H) the magnetisation decreases and becoms zero at OR. OR is called coercivity.Further increases of H,the speciment gets magnetised in opposite direction and the process continuous up to saturation at S.When the negative field is gradually decreased the curve follows the path ST Where there is still magnetisation even when H=0 .B becoms zero when +H is increased upto U.with further increase of +H the curve follows up.The closed curve PQRSTUP is called the hysteresis curve.When we apply A>C the material gets magnetised and demagnetised during first half and see and haif of a cycle. Due to mechanical stress in material energy is wasted in the form of heat which is given under the area of the curve of hysteresis loop.

Eeperimental Arrangements :





Experimental procedure: the electrical connections are made as shown in figures a bove. The primary transformer is connected via the Resister R1 to step down transformer T which in turn is connected to the 220V-50HZ mains.The secandary of the transformer core is connected in series with the resister R2 and capacitor Cs.The voltage Vx acrossR1 is fed to the horizantal input XX plates of the CRO. the voltage Vy across Cs is fed to the vertical input YY plates of CRO. The horizantal and vertical gain central of the CRO are adjested to get a canvenient size of the hystersis curve of the material of the transformer core. Here Vx correspands to H and Vy correspands to B.Using a graph sheet trace the B-H curve appearing on the CRO screen by plotting point by point wise.

VIVA -VOCE :

(1) What is hystereies ? Inwhat type of materials we can find this behaviour?

Ans: A magnetic phenomenon in which magnetic induction (B) behind external magnetising force (or) field (H) is called hysterisis.Ferro magnetic materials like Iron, Cobalt,Nickel,Steel exhibit hysterisis.

(2) How curie law modified due to magnetic domain?

Ans: Due to spontaneous magnetisation of ferro magnetic domains curie law is modified as curie wiess law.

(3) What is the cause of hysterisis?

Ans: The phase difference between B and H is the cause of the hysterisis.The domain boundaries don't move all in one direction while magnetisation takes place.Also during demagnetisation all the boundaries of domains don't move completely back to their orginal position.

(4) What is the causes of hysterisis losses?

Ans: The tendency of domains to turn around in an external magnetic field gives rise to mechanical stress in the material.This gives rise to heating.Those heating losses result in hysterisis losses.

(5) What are the characteristicks of a transformer core?
Ans: The material should have (1)high permeability (2)low hysterisis loss (3)large specific resistance .These conditions are satisfied by Silicon-Iron.

(6) Can we use n electrolyte capacitor in this experiment?
Ans: No because for A.C the polarity of the plates will change.

(7) Which has small hysterisis loop?(a)soft iron (b)steel
Ans: Soft iron

Expt No:9 ABSORPTION SPECTRUM OF IODINE VAPOUR

Aim : To study the absorption spectrum of iodine vapour using difraction grating.

Apparatus : Incondanscent lamp glass tube length (one meter) with iodine grains,spectrometer diffraction gratting.

Formula: The energy levels of the iodine molecule can be calculated from $E = hc/\lambda$

Where λ is in meters and C is velocity of light.

This is messured using gratting

$$Sin\theta = Nn\lambda \Rightarrow$$

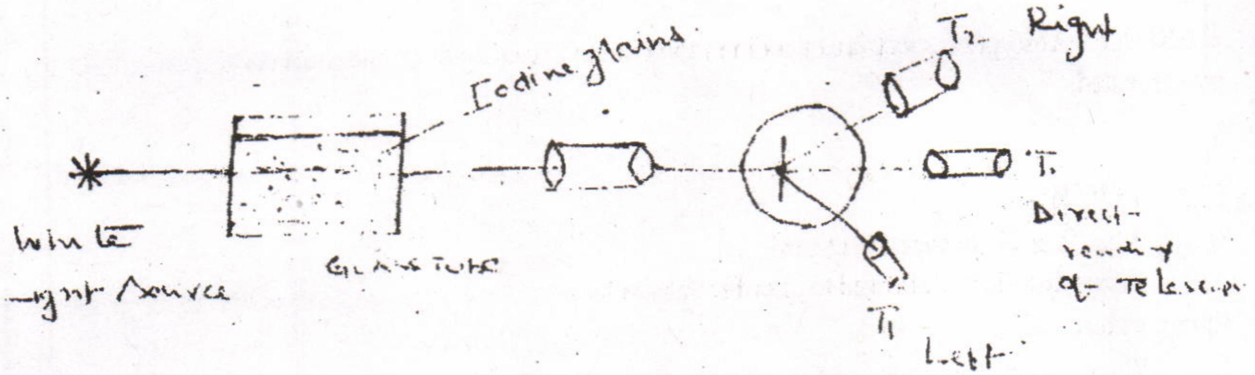
$$\lambda = \sin\theta / Nn$$

Here λ - is the angular position of the obsorption band of wave length

N - number of lines per centimeter length of grating

n- order of the spectrum

Arrangements:



Theory: Iodine even at room temperature is available in the form of a vapour. Where white light having different wavelenths is allowed in the glass tube, the molecular absorb energy and they have electron in existed state and they absorb radiation of wavelength . Which can be measured using diffraction grating formula given by $\sin\theta / Nn = \lambda$. The gratting should be adjusted in normal incident position. We will get a series of dark lines or more precisely bands which are dealing with iodine molecules.

Experiment: Due to the absorption of certain wavelength of white light by iodine molecule, dark bands are now observed through the telescope in a back ground of the continuous spectrum. Measurement are to be made from the farthest available band on the longer wavelength side because the successive bands are very close to each other count the farthest band as n in number take it's reading on the circular scale as T_1. Now came to the central part at equal intervals 5 bands each,counting them from the farthest n as n+5, n+10,n+15-------------,n+30, and take T_1 readings at each band. While going to the right of the centrel part of the experiment we have to count the bands as n+30,n+25,-------,n+5,n. and note the readings as T_2. Evidently $T_1 - T_2 / 2$ gives the angle of diffraction θ. Calculate the wavelength

$$\lambda = \sin\theta / Nn = hc / E \quad \text{for each band.}$$

Observations:

S.No	Reading when the telescope on left side R1		Reading when the telescope on right side R2		$\theta_1 = \frac{R_1 - R_2}{2}$ of V1	$\theta_2 = \frac{R_1 - R_2}{2}$ of V2	$\theta = \frac{\theta_1 + \theta_2}{2}$	$\lambda = \sin\theta / Nn$
	Vernier 1	vernier 2	Vernier 1	vernier 2				

RESULT: Absorption spectrum of iodine vapour is studied and wavelength and energies different bands are estimated.

VIVA - VOCE :

Q1. : What is an absorption spectrum?

Ans : When white light is allowed to pass through a substance in vapour state some of the colours in the light are absorbed by the material. So dark lines absorbed in the spectrum.

Q2. : Why we are using grating plate instead of a prism?

Ans : In grating plate the resolving power is large than that of prism. We have different orders spectra.

Q3. : Which spectral line is more sharp i.e, for grating or prism?

Ans. : In case of grating the spectral line are sharp.

Q4. : Is gratting spectrum dependent on nature of gratting material?

Ans. :No it is independent.

Expt No:10

ENERGY GAP OF AN INTRINSIC SEMI CONDUCTOR

AIM :

To determine the energy gap of an intrinsic semiconductor by determining the resistence at different temparatures.

APPARATUS :

Semiconductor with ohmic contact at both ends,Thermometer,Temprature bath, Multimeter,Connecting wires.

FORMULAE:

$$E_g = 4.6052 \times k \times slope of the graph$$

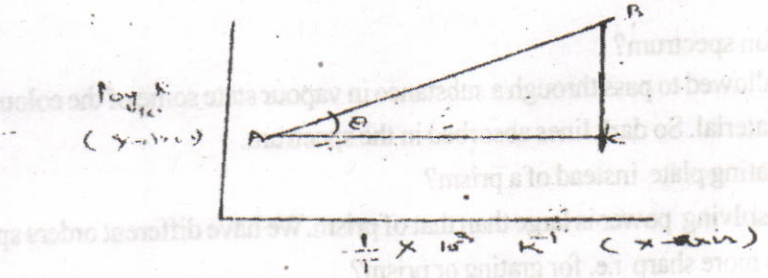
k = Boltzman Constant = 1.38×10^{-23} J/k

Slope - for graph $\log_{10} R$ and $\frac{1}{T}$

The energy gap in ev is given by

$$E_g = \frac{4.6052 \times k \times slope of the graph}{1.69 \times 10^{-19}}$$

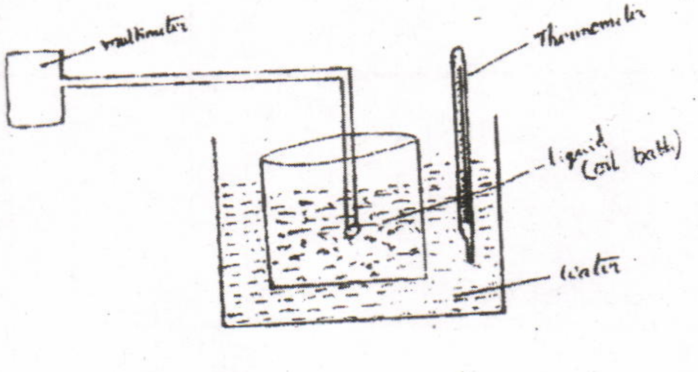
GRAPH:



$$\text{Slope } m = Tan\theta = \frac{BC}{AC}$$

A Graph is drawn between 1/T along X-axis and log along Y-axis.The slope is given by $Tan\theta = \frac{BC}{AC}$

CIRCUIT:



THEORY:

A Semiconductor will be having temparature coefficient as negative. The resistivity of the semiconductor is given by

$$\rho = Ce^{\frac{E_g}{2kT}}$$

Here Eg = Energy gap
k = Boltzman constant
T = Absolute temparature

So resistance $R = C^{1}e^{\frac{E_g}{2kT}}$

Here C and C^{1} are two different constants

$$\therefore \log_{10} R = \log_{10} C + \frac{1}{2.3026}\left(\frac{E_g}{2kT}\right)$$

$\frac{E_g}{4.6052k}$ = slope of $\log_{10} R \,\&\, \frac{1}{T}$ graph , $\therefore E_g = 4.6052k \times slope$

EXPERIMENT:

After connecting the semiconductor with multimeter,the room temparature of the liquid (oil bath) is measured and the corresponding resistance is noted .Now the temparature of bath is gradually increased in the steps of 5^0C and corresponding resistance is noted. The temparature is increased upto 90^0C . Now start cooling the oil bath and again the resistance is noted for every 5^0C fall of temparature.The readings are translated and then a graph is drawn between $\log_{10} R$ and $\frac{1}{T}$.

S.No	Temperature	1/T	Values of resistence		Resistence	$\log_{10}R$
			Temp incresing	Temr decreasing	$R = \frac{R_i + R_d}{2}$	

CALCULATION:

$E_g = 4.6052 \times k \times$ slope of graph = __________ J

In electron volts = $\frac{E_g}{1.6 \times 10^{-19}}$.

PRECAUTIONS:

(1) Don't operate above $90^0 C$

(2)Tempratures are to be determined carefully.

VIVA-VOCE :

(1) Is the energy is same at all tempratures?

Ans : No energy gap decreases with temprature.

(2) At what temparature Eg will be maximum.

Ans : At absolute zero temprature.

(3) What is meant by energy gap?

Ans. It is the energy difference between valence band and conduction band.

(4) At absolute zero how the semiconductor behaves?

Ans : At absolute zero it behaves like an Insulator. The valency band is completely filled with electrons.

Expt No:11

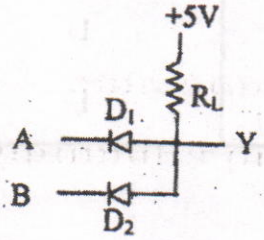
LOGIC GATES - AND, OR, NOT, EX - OR GATES

Aim : To construct too-input logic gates and to verify their truth tables.

Formula : A gate is a digital circuit with one or more input signals (voltages and currents) and only one output signal.

Electronic circuit and Truth table

AND-GATE



Circuit of AND gate

Fig . A

Truth Table

S.No	A	B	Out put A.B=Y
1.	0	0	0
2.	1	0	0
3.	0	1	0
4.	1	1	1

OR- GATE

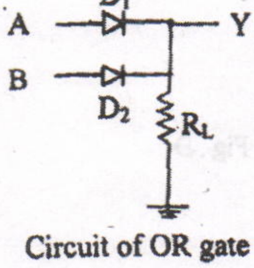


Fig. B

Circuit of OR gate

Truth Table

s.no	A	B	output A+B=Y
1.	0	0	0
2.	1	0	1
3.	0	1	1
4.	1	1	1

Not-Gate(Inverter)

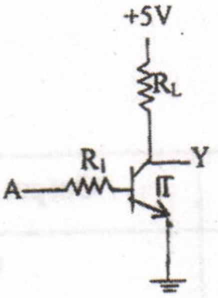


Fig. C

Truth Table

s.no	Input A	Output X= $\overline{A}$
1.	0	1
2.	1	0

X-OR Gate

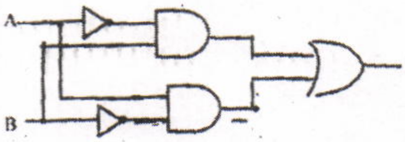


Fig . D

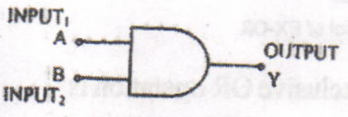
Truth Table

s.no	A	B	output A+B=Y
1.	0	0	0
2.	1	0	1
3.	0	1	1
4.	1	1	0

Theory :

(1) AND GATE

It has two inputs and only one out put.The inputs one A and B.and the output is Y

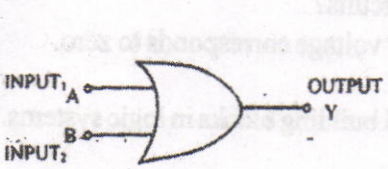


Logic Symbol of AND gate

The AND gate provides out put only when all the inputs are simultaneously present.
A.B = Y read as A AND B equals Y

(2) OR GATE

It has two or more inputs and only one out put. This is called OR gate because the out put will be true if any one or all of the inputs are true.

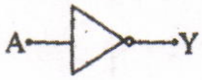


Logic Symbol of OR gate

Here A+B =Y. which is to be read as A or B equals Y.

(3) NOT GATE

This gate has only one input and one out put. The out put is 1 when onput is 0.similarly the output is o when ~~input is 1. Thus~~ an inversion takes place as the input passes through the NOT gate. The main purpose of an inverter gate is to complement its input value.



Y= $\overline{A}$ which is to be read as Y equals NOT A or Yis the complement of A

(4) EX-OR GATE (Exclusive OR gate)

These are used for addition lide half and full adders. For subtraction the circuits used are called half and full subtractors.

The out put of a two input Exclusive OR assucer the state 1 if one and only one input assumes the 1 state.

Logic Symbol of EX-OR gate

The Boolean expression for expression for exclusive OR opetation is

a. Y=(A+B) AB

Viva -Voce :

(1) What type of transistor is used in NOT circuit?

Ans : A silican n-p-n transistor is used.

(2) What is a digital signal?

Ans : A signal that is characterized by only two digits ziro and one with discrete values or lexels is called a digital signal.

(3) How can you count 0 and 1 in electronic circuits?

Ans : A high voltage corresponds to 1 and low voltage corresponds to zero.

(4) What is the advantage of EX-OR gate?

Ans : It is one of the most important conceptual building blocks in logic systems. It employed with the arthimatic section of a computer.

Expt No:12

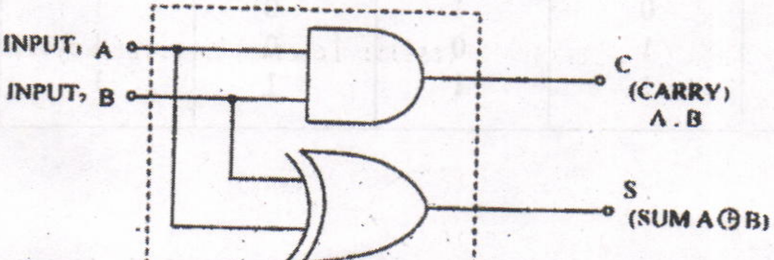
HALF ADDER - FULL ADDER

AIM : To verify the truth tables of half and full adders by designing them in the laboratory.

APPARATUS : (1) One AND-gate IC 7408.
One X-OR gate IC 7486 and LED.
(2) Two AND-gate IC 7408,
Two X-OR gates IC 7486 and,
oneOR gate IC 7432 and LED.

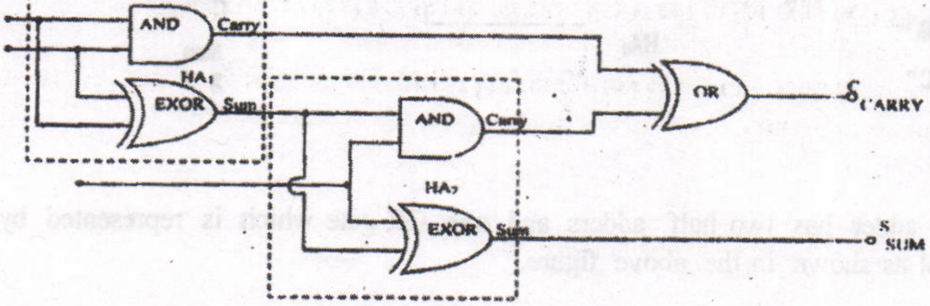
ELECTRANIC CIRCUIT :

Half adder:



S.No	A	B	sum	carry	Result
1.	0	0	0	0	ok
2.	0	1	1	0	ok
3.	1	0	1.	0	ok
4.	1	1	0	1	ok

Full adder:



Truth Table:

S.No	A	B	C	sum	carry	Result
1.	0	0	0	0	0	ok
2.	0	0	1	1	0	ok
3.	0	1	0	1	0	ok
4.	0	1	1	0	1	ok
5.	1	0	0	1	0	ok
6.	1	0	1	0	1	ok
7.	1	1	0	0	1	ok
8.	1	1	1	1	1	ok

HALF ADDER : It is an electanic logic circuit that adds two single bits to produce a sum and a carry to be usedm in the next higher position. In a half adder, there is no possibility for a carry input (Q) and as a conseqence, a half adder can be used for addition of the lower most bit only. since it is not accepting acarry in (Q) from the previous addition it is called a half adder. In order to achieve a carry in from previouS addition, we have to construct a 3 input adder which is called a full adder.

FULL ADDER : A full adder is an electronic logic circuit that add three bits, two bits to be added and a carry bit from (lower column) previous addition resulting in a sum and a carry. actuvally in a full adder two half adders and one OR-gate are cascaded.

Actuvally a full adder has two half adders and one OR-gate which is represented by a standord symbol as shown in the above figure.

Expt. No. 13

ABSORPTION OF ALPHA AND BETA RAYS

AIM: To study the absorption of alpha -rays and beta -rays and find the respective mass absorption coefficient.

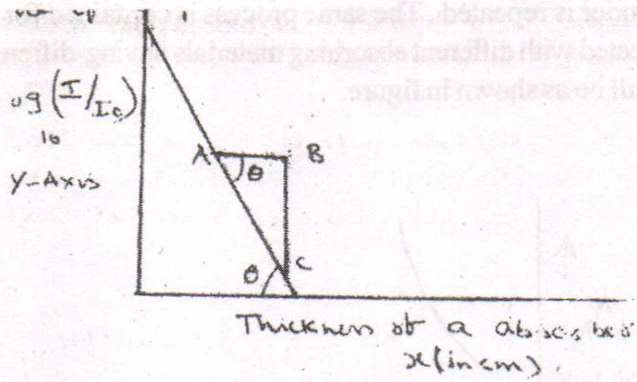
APPARATUS: A G.M counter tube (end window type) with a counting system ,an alpha source like rador a beta -source like thalium 204 (81 th 204) stand for alpha or beta source and absorbers as well with shelves ,aluminium foils (absorbers) of uniform thikness t,lead castle.

FORMULA:

$$I = I_0 e^{-\mu x}$$

here μ the linear absorption coeficent in units of per centimeter . Here μ_m in the ratio of $\frac{\mu}{\rho}$ here ρ is the density of material.

GRAPH: A graph is drawn between thikness of absorption X in centemeter and $\log_{10}\left(\frac{I}{I_0}\right)$ along Y-axis . The slope of the curve given the valuve of $\mu = 0.4343$



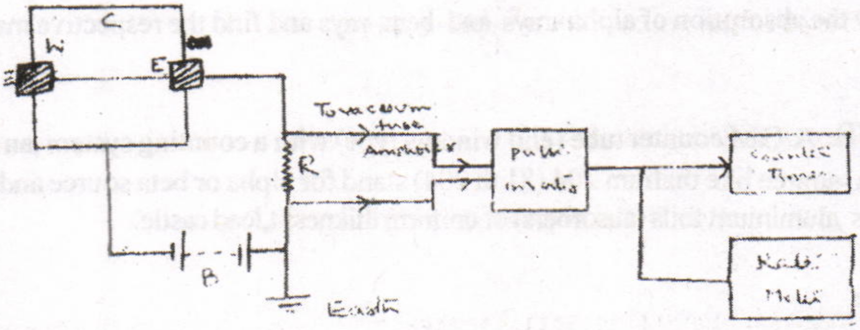
Slope $m = \frac{BC}{AB}$ gives the value of $\mu = 0.4343$

This is becuase $\log_{10} M = 0.4343 \log_e M$

hence $\mu = m \times 2.3026 \, {cm^2}/{mg}$

and $\mu_m = \frac{\mu}{\rho}$ can be easily caluted .

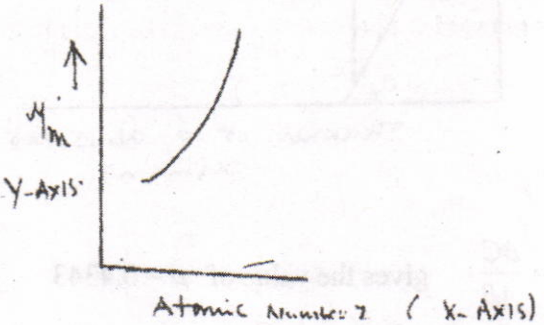
EXPERIMENTAL ARRANGEMENT:



Itcosits of a central electrode of tungsten wire w of about diameter of 0.01 cm. The outer electrode is a metal tube which can be contained inside a glass envelope . The metal tube is filed in well insulated brass the central electrode . the tube is filled with a mixture of 90% argon gas and 10% alcohol gas at apresure of 10cm of Hg. The applied voltage is in the neighbourhood of 1000 voits .The experimental circuit contains a high peak resistance R,the out put fram which is connected to a vacuum tube amplifier. the out put from the amlifier is connected to a pulse invertr and from this to counter meter and rate meter as shown in the above figure.

EXPERIMENT: The aluminium foil is iserted between the source and the window of the G.M tube. The counting rate I is noted per the same preset time and thickness t of the one alluminium foil i.e x = t Next ,second aluminium foil of same thickness is placed in the first foil so that now the total thickness will be x=2t and the same procuder is repeated . The same process is contained for x=3t, 4t,5t---- The same experiment isnow repeated with different absorbing materials having different atomic number (z). the graph between and z will be as shown in figure.

GRAPH:



OBSERVATIONS:

Thickness x	t	2t	3t	4t	5t	6t
count rate I						
value of log (I/						

CALCULATIONS:

$$\text{Slope of the graph} \quad m = \frac{BC}{AB} = 0.4343$$

$$\mu = m \times 2.3026 = \text{----------------}/\text{cm}$$

$$\text{Density of the material } \rho = \text{----------------mg}/$$

$$\text{Mass absorbtion coefficient } \mu_m = \frac{\mu}{\rho} = \text{......} \, {cm^2}/{mg}$$

ans: Electron of very high energoies loose their energy in the form of radiation due to inelastic collisior with the coulomb's field of the atomic nuclei,which is called Brenstrang lung

PRECAUTIONS:

1. UP to 1000 counts/minute , one minite interval is to be allowed
2. the thickness of the counter window and the equivalent thickness of air space between the source and the window are also to be considered.

VIVA–VOCE:

1. What id Bremstrang lung?
Ans: Electron of very high energoies loose their energy in the form of radiation due to inelastic collision with the coulomb's field of the atomic nuclei,which is called Brenstrang lung
2. What is the cause of the absorption of either -rays or -rays
ans: the absorption is due to the loss of energy of these rays through Ionization and also Bremstrang lung in the case of -rays
3. At what voltage is the counter operated
ans: The counter is to be ooperated at about 100 v above the Geiger thresold.

Expt No: 14 HALL PROBE

Aim :

To measure the magnetic field using Hall Probe Methode.

Apparatus:

Hall probe, a crystal of bismuts,1.5V battery , Rheostat of 10 k resistence, ammeter, voltmeter, electro magnet, key, screw gauge.

Formula:

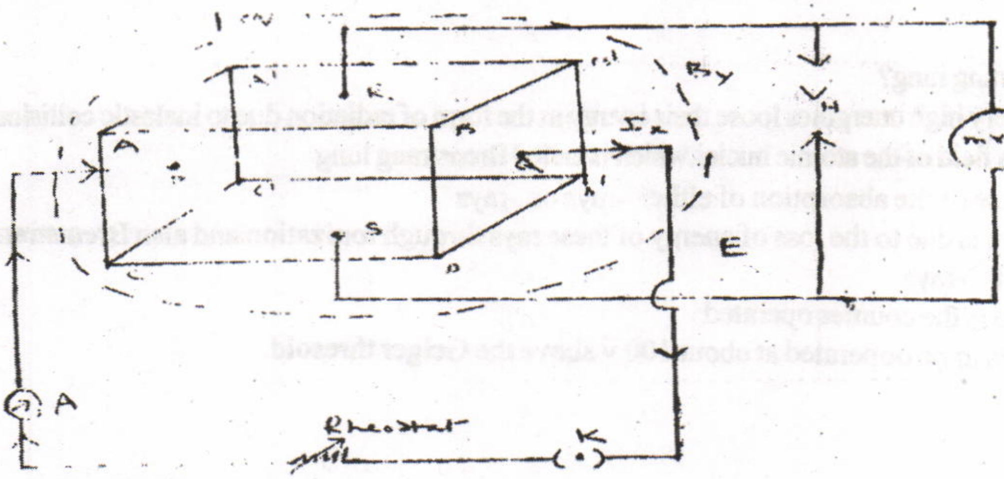
The Hall coefficiant of speciman is given by

$$R_H = \left(\frac{V_H}{I_X}\right)\frac{b}{B_Y} \quad \frac{m^3}{coloumb}$$

BY $B = \left(\frac{V_H}{I_X}\right)\frac{b}{R_H}$ Tesla

Experiment:

The circuit diagrame and arrangement for the experiment is as shown in the following figure.



B_y is the Y-direction.

V_H is the Z-direction.

I_x is the X-direction.

AA'=BB'=b

AC=BD=d

ABCD, A'3'C'D' is the speciman. In place of mV we may hear a potentiometer arrangement to measure V_H.

Experiment Procedure:

The breadth b of the hall probe is measured with a screwgauge and readings are tabulated.

Table:

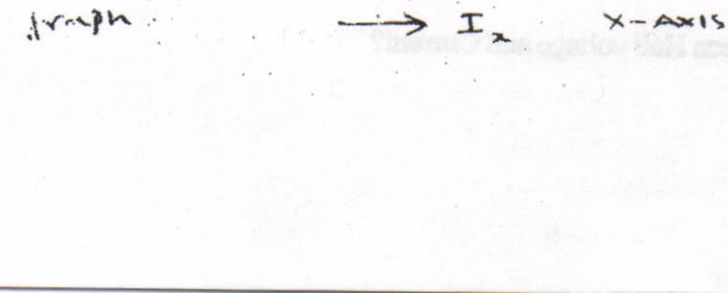
S.No	Pitch scale reading	Head scale reading		b=n.L.C	Bredth
		observed	corrected		

Without changing the magnetic field strenth without changing current through the magnetic coils the current gradually in steps of 10mA and each time and at each step the corresponding Hall voltage is measured (V_H).

Table:

S.No	current Ix in amp	Hall voltage VH in volts

Graph:



$$m = \frac{V_H}{I_x} = \frac{CB}{AB} = Tan\theta = \frac{volt}{Amp}$$

Calculation:

1. Hall coefficiant of the speciman

$$R_H = \underline{\hspace{3cm}} \frac{m^3}{col}$$

2. Breadth of the Speciman

b = ________________ cm

3. Slope of V_H- I_x curve

$$m = \underline{\hspace{3cm}} \frac{volt}{amp}$$

4. Magnetic field

$$B_y = \left(\frac{V_H}{I_x}\right)\frac{b}{R_H} \text{ Tesla}$$

Precautions:

1. Magnetic poles should not be distubed through out the experiment.
2. Current fluctuations should be checked from time to time while taking readings.
3. The voltage from the power supply should be increased slowly and gradually other wise the rectifier may be damaged.

Viva-Voce:

1. What ia Hall effect?

A. When a magnetic field is appied perpenducular to a current carrying condecter , a potential difference is devoloped between the opposite sides of the condector.

2. On what factors dose the direction of the Hall voltage depend upon?

A. The direction of Hall voltage depends upon the nature of Charge carries.

3. What is the Cause of Hall voltage?

A. It is the Lorentz-force acting as a charge moving in electric and magnetic fields. It is of order few milli or micro volts.

4. What is the nature of the graph drawn between Hall voltage and Current?

A. It is a Strait line passing through the origin.

Expt No. 15

ENERGY GAP OF A SEMICONDUCTOR USING A JUNCTION DIODE

AIM : To determine the band (energy gap) in a semiconductor using a p-n junction diode.

APPARATUS : A p-n junction diode,a thermometer, a multimeter, connecting wires,plug key,heating arrangement.

FORMULA :

$I_s = Ae^{-Eg/kT}$ where

Is----reverse saturation current

Eg---energy gap of the diode in joules

K---boltzmann constant=1.38*10-23 J/K

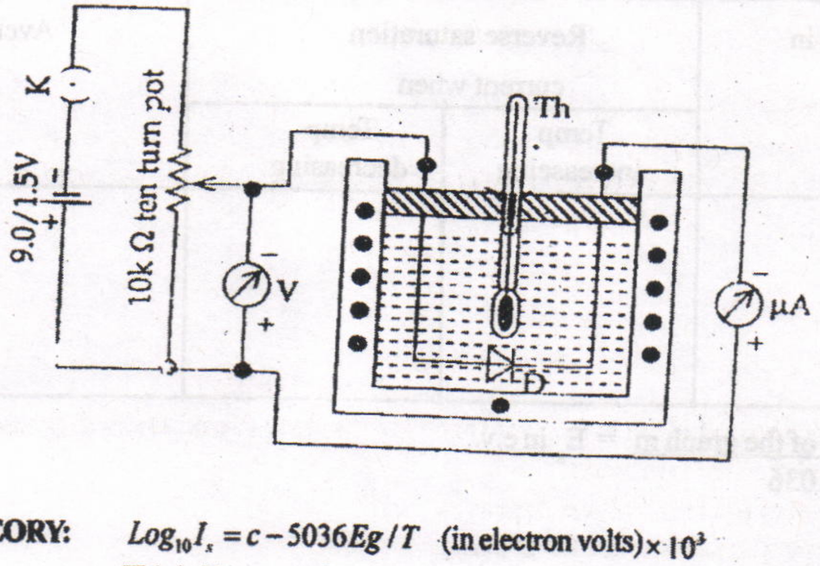
T---absolute temperature

$$Log_{10} I_s = \log_{10} A - 0.4343 E_g / KT$$

subtracting the value of K and expressing Eg in electran volts we get

$$Log_{10} I_s = \log_{10} A - 5036 E_g / T$$

Circuit Diagram:

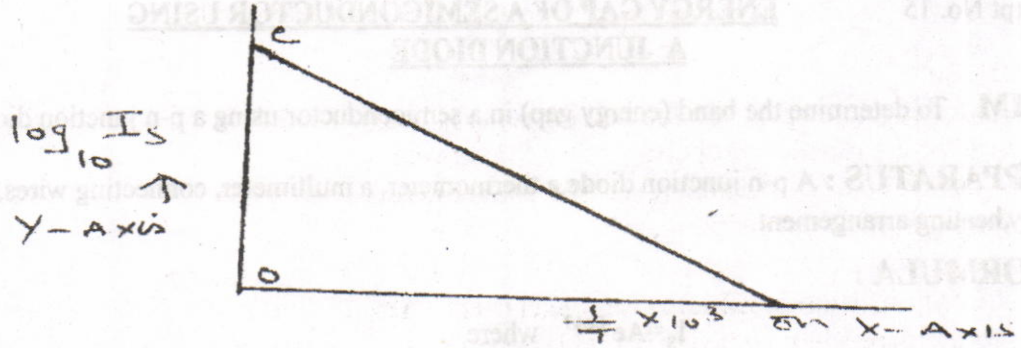


THEORY: $Log_{10} I_s = c - 5036 Eg / T$ (in electron volts) $\times 10^3$

This is Y=-mx+c form

so the graph between Log Is on Y-axis and $1/T \times 10^3$ on X-axis gives a straight line and the slope is divided by 5.036 it gives the valve of Eg in electron volts.

GRAPH:



$$\Delta \log_{10} I_s = \log_{10} I_s \text{ at } T_2 - \log I_s \text{ at } T_1$$

$$\Delta\left(\frac{1}{T}\right) = \frac{1}{T_2} - \frac{1}{T_1} \text{ and } E_g = \frac{m}{5.036}$$

$$\text{with} \quad m = \frac{\Delta \log_{10}(I_s)}{\Delta\left(\frac{1}{T}\right) \times 10^3}$$

OBSERVATIONS: Max. permissable reverse voltage that can be applied to the p-n junction diode=_______ volts

S.No	Temp in 0^0C	Temp in 0^0C	Reverse saturation current when		Average I_S
			Temp increaseing	Temp decreasing	

CALCULATIONS: $\frac{\text{Slope of the graph m}}{5.036} = E_g$ in e.v.

PRECAUTIONS:

(1) The diode should be properly reverse biased.It should be carefully and scrupulously observed.

(2) The heating temp is below 75 C when diode is made up with germanium.

(3) The reverse voltage should be quite below the breakdown voltage.

(4) Readings of temprature and Is should be taken only after Ts attains a steady valve

VIVA VOCE:

1) If the diode is made up of Ge the heating temp is balow 75 C why?

Ans: Otherwise the junction properties will be destroyed.

2) Is=A e-Eg/nKT What are the valves of n for germanium and silicon?

Ans:For germanium n=1 for silicon n=2.

(3) Why the reverse saturation current depends on temprature ?

Ans:Is is due to diffusion of minority charge carriers.These are thermally generated.The diffusion is also temprature dependent.Hence Is is highly sensitive to temprature changes.

(4) Why should the reverse bias be kept well below the breakdown voltage?

Ans: Then only the reverse saturation currrent Is remains constant.

(5) Which shows greater temperature variation of the reverse saturation current out of germanium and silicon diodes?

Ans: It is germanium which shows greater temperature variation.

(6) Why the reverse bias current is called reverse saturation current?

Ans: Because the reverse current become saturated quickly with increase in the reverse bias.

(కత్తిరించి పంపవలెను)

అధ్యాపకుల, విద్యార్థుల సలహాలు, సూచనలు :

అధ్యాపకులు, విద్యార్థులు ఈ స్టడీ మెటీరియల్‌కు సంబంధించిన సలహాలు, సూచనలు, ముద్రణ దోషాలు తెలియపరచినచో, పునర్ముద్రణలో తగు చర్యలు తీసుకొనగలము. తెలియపరచవలసిన చిరునామా : డిప్యూటీ డైరెక్టర్, దూరవిద్యా కేంద్రం, ఆచార్య నాగార్జున విశ్వవిద్యాలయం, నాగార్జున నగర్ - 522 510.

Course	**Year**	**Paper No. & Title**
B.Sc. Physics	3rd Year	Paper - IV, Modern Physics

(కత్తిరించి పంపవలెను)

(కత్తిరించి పంపవలెను)

(కత్తిరించి పంపవలెను)