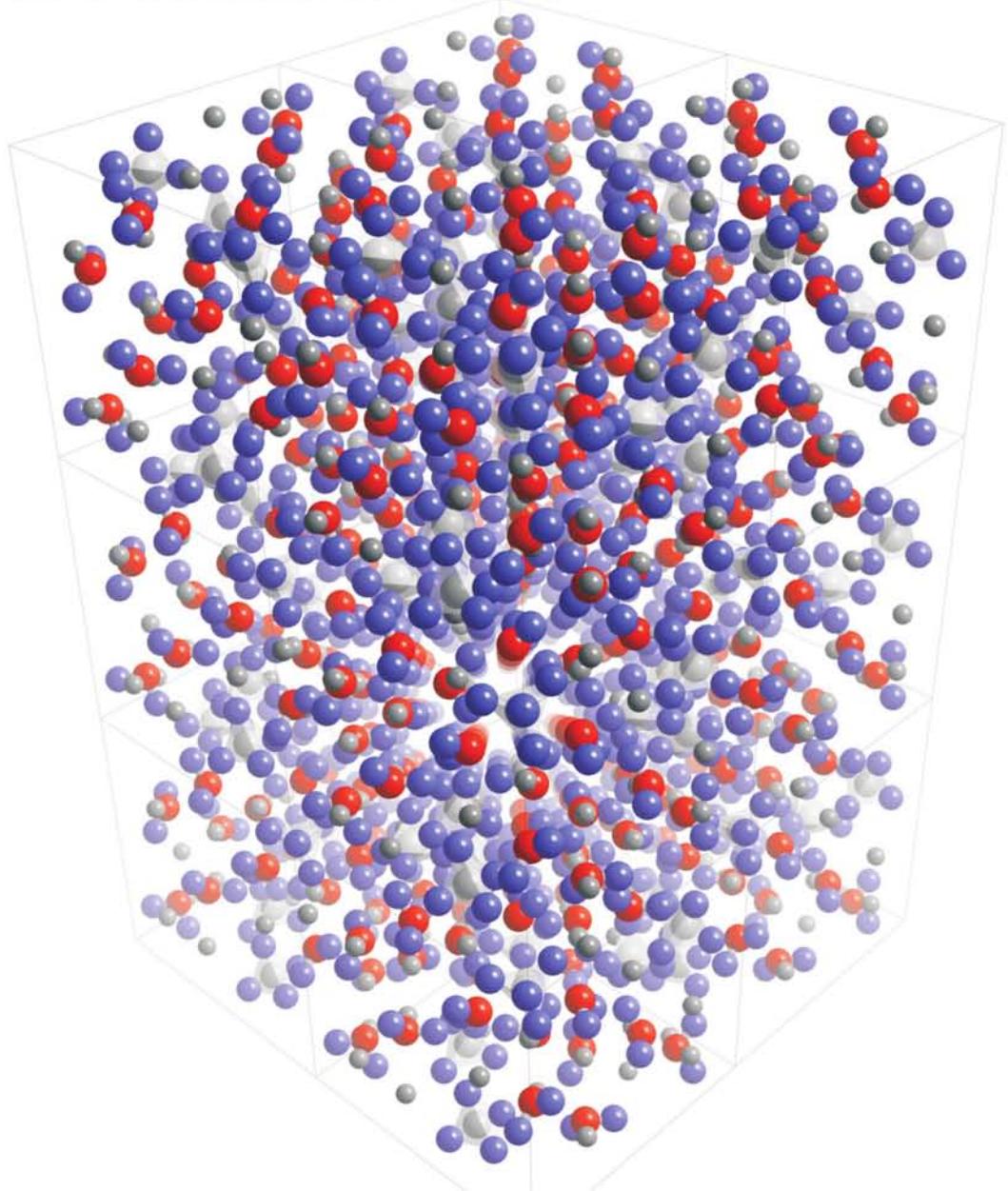


# APPLIED PHYSICS

S. MANI NAIDU



A text book of

# APPLIED PHYSICS

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A text book of

# APPLIED PHYSICS

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**Dr. S. Mani Naidu**

M.Sc., Ph.D., P.G.D.C.A.

Associate Professor of Physics

Sree Vidyanikethan Engineering College

Tirupati, Andhra Pradesh

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# Contents

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<b>Foreword</b>	<b>xiv</b>
<b>Preface</b>	<b>xv</b>
<b>Acknowledgements</b>	<b>xvi</b>
<b>Road Map to the Syllabus – JNTU Hyderabad</b>	<b>xvii</b>
<b>Chapter 1 Bonding in Solids</b>	<b>1.1</b>
1.1 Different types of bonding in solids	1.1
1.2 Cohesive energy and estimation of cohesive energy of ionic solids	1.4
1.3 Estimation of cohesive energy of NaCl molecule in a solid	1.8
1.4 Madelung constant	1.9
Formulae	1.10
Solved Problems	1.11
Multiple Choice Questions	1.14
Answers	1.16
Review Questions	1.16
<b>Chapter 2 Crystal Structures</b>	<b>2.1</b>
2.1 Introduction	2.1
2.2 Space lattice (or) crystal lattice	2.2
2.3 The basis and crystal structure	2.3

## Contents

2.4	Unit cell and lattice parameters	2.3
2.5	Crystal systems and Bravais lattices	2.4
2.6	Structure and packing fractions of simple cubic [SC] structure	2.8
2.7	Structure and packing fractions of body-centred cubic structure [BCC]	2.9
2.8	Structure and packing fractions of face-centred cubic [FCC] structure	2.10
2.9	Diamond cubic structure	2.11
2.10	NaCl crystal structure	2.12
2.11	Caesium chloride [CsCl] structure	2.13
2.12	Zinc sulphide [ZnS] structure	2.14
2.13	Stacking sequence in metallic crystals	2.14
2.14	Calculation of lattice constant	2.15
	Solved Problems	2.16
	Multiple Choice Questions	2.18
	Answers	2.21
	Review Questions	2.21

### **Chapter 3 Crystal Planes, X-ray Diffraction and Defects in Solids**

**3.1**

3.1	Crystal planes, directions and Miller indices	3.1
3.2	Distance of separation between successive $hkl$ planes	3.4
3.3	Imperfections in crystals	3.7
3.4	Energy for the formation of a vacancy and number of vacancies at equilibrium concentration	3.10
3.5	Diffraction of X-rays by crystal planes and Bragg's law	3.14
3.6	Powder Method	3.16
3.7	Laue Method	3.17
	Formulae	3.18
	Solved Problems	3.19
	Multiple Choice Questions	3.25
	Answers	3.30
	Review Questions	3.31

**Chapter 4 Elements of Statistical Mechanics  
and Principles of Quantum**

<b>Mechanics</b>	<b>4.1</b>
4.1 Introduction	4.1
4.2 Phase space	4.1
4.3 Maxwell–Boltzmann distribution	4.1
4.4 Fermi–Dirac distribution	4.3
4.5 Bose–Einstein distribution	4.5
4.6 Comparison of Maxwell–Boltzmann, Fermi– Dirac and Bose–Einstein distributions	4.7
4.7 Photon gas	4.7
4.8 Concept of electron gas and Fermi energy	4.7
4.9 Density of electron states	4.8
4.10 Black body radiation	4.10
4.11 Waves and particles—de Broglie hypothesis— Matter waves	4.12
4.12 Relativistic correction	4.14
4.13 Planck’s quantum theory of black body radiation	4.17
4.14 Experimental study of matter waves	4.19
4.14 Schrödinger’s time-independent wave equation	4.25
4.15 Heisenberg uncertainty principle	4.28
4.16 Physical significance of the wave function	4.30
4.17 Particle in a potential box	4.31
Formulae	4.39
Solved Problems	4.41
Multiple Choice Questions	4.46
Answers	4.51
Review Questions	4.51

**Chapter 5 Electron Theory of Metals**

<b>5.1</b>	
5.1 Introduction	5.1
5.2 Classical free electron theory of metals	5.2
5.3 Relaxation time, mean free path, mean collision time and drift velocity	5.5
5.4 Fermi-Dirac distribution	5.7
5.5 Quantum free electron theory of electrical conduction	5.8

## Contents

5.6	Sources of electrical resistance	5.11
5.7	Band theory of solids	5.12
5.8	Bloch theorem	5.19
5.9	Origin of energy bands formation in solids	5.21
5.10	Velocity and effective mass of an electron	5.21
5.11	Distinction between metals, semiconductors and insulators	5.24
	Formulae	5.26
	Solved Problems	5.27
	Multiple Choice Questions	5.34
	Answers	5.38
	Review Questions	5.38
<b>Chapter 6 Dielectric Properties</b>		<b>6.1</b>
6.1	Introduction	6.1
6.2	Dielectric constant	6.1
6.3	Internal or local field	6.2
6.4	Clausius–Mosotti relation	6.4
6.5	Orientational, ionic and electronic polarizations	6.7
6.6	Frequency dependence of polarizability: [Dielectrics in alternating fields]	6.12
6.7	Piezoelectricity	6.17
6.8	Ferroelectricity	6.18
6.9	Frequency dependence of dielectric constant	6.20
6.10	Important requirements of insulators	6.21
	Formulae	6.23
	Solved Problems	6.23
	Multiple Choice Questions	6.29
	Answers	6.33
	Review Questions	6.33
<b>Chapter 7 Magnetic Properties</b>		<b>7.1</b>
7.1	Magnetic permeability	7.1
7.2	Magnetization ( $M$ )	7.2

7.3	Origin of magnetic moment – Bohr magneton – electron spin	7.2
7.4	Classification of magnetic materials	7.5
7.5	Classical theory of diamagnetism (Langevin theory)	7.6
7.6	Theory of paramagnetism	7.9
7.7	Domain theory of ferromagnetism	7.12
7.8	Hysteresis curve	7.16
7.9	Anti-ferromagnetic substances	7.17
7.10	Ferrimagnetic substances [Ferrites]	7.19
7.11	Soft and hard magnetic materials	7.20
7.12	Applications of ferrites	7.21
	Formulae	7.22
	Solved Problems	7.22
	Multiple Choice Questions	7.25
	Answers	7.29
	Review Questions	7.29

## **Chapter 8 Semiconductors and Physics of Semiconductor Devices**

**8.1**

8.1	Introduction	8.1
8.2	Intrinsic semiconductors – carrier concentration	8.1
8.3	Electrical conductivity of a semiconductor	8.10
8.4	Extrinsic semiconductors	8.14
8.5	Carrier concentration in extrinsic semiconductors	8.17
8.6	Minority carrier life time	8.19
8.7	Drift and diffusion currents	8.22
8.8	Einstein's relations	8.24
8.9	Continuity equation	8.25
8.10	Hall effect	8.29
8.11	Direct and indirect band gap semiconductors	8.31
8.12	Formation of p-n junction	8.33
8.13	Energy band diagram of p-n diode	8.36
8.14	Diode equation	8.37
8.15	p-n junction biasing	8.37

**Contents**

8.16 V-I characteristics of p-n diode	8.39
8.17 p-n diode rectifier	8.41
8.18 Light emitting diode [LED]	8.46
8.19 Liquid crystal display (LCD)	8.49
8.20 Photodiodes	8.51
Formulae	8.53
Solved Problems	8.55
Multiple Choice Questions	8.63
Answers	8.69
Review Questions	8.69

**Chapter 9 Superconductivity 9.1**

9.1 Introduction	9.1
9.2 General features of superconductors	9.3
9.3 Type-I and Type-II superconductors	9.7
9.4 Penetration depth	9.9
9.5 Flux quantization	9.10
9.6 Quantum tunneling	9.11
9.7 Josephson's effect	9.13
9.8 BCS theory	9.15
9.9 Applications of superconductivity	9.18
Formulae	9.21
Solved Problems	9.22
Multiple Choice Questions	9.24
Answers	9.27
Review Questions	9.27

**Chapter 10 Lasers 10.1**

10.1 Introduction	10.1
10.2 Characteristics of laser radiation	10.1
10.3 Spontaneous and stimulated emission	10.2
10.4 Einstein's coefficients	10.4
10.5 Population inversion	10.6

10.6	Helium–Neon gas [He–Ne] laser	10.8
10.7	Ruby laser	10.10
10.8	Semiconductor lasers	10.12
10.9	Carbon dioxide laser	10.15
10.10	Applications of lasers	10.18
	Formula	10.20
	Solved Problems	10.20
	Multiple Choice Questions	10.21
	Answers	10.23
	Review Questions	10.24

## Chapter 11 Fibre Optics 11.1

11.1	Introduction	11.1
11.2	Principle of optical fibre, acceptance angle and acceptance cone	11.1
11.3	Numerical aperture (NA)	11.3
11.4	Step index fibres and graded index fibres—transmission of signals in them	11.5
11.5	Difference between step index fibres and graded index fibres	11.8
11.6	Differences between single mode fibres and multimode fibres	11.8
11.7	Attenuation in optical fibres	11.9
11.8	Optical fibres in communication	11.11
11.9	Advantages of optical fibres in communication	11.12
11.10	Fibre optic sensing applications	11.13
11.11	Applications of optical fibres in medical field	11.15
	Formulae	11.16
	Solved Problems	11.16
	Multiple Choice Questions	11.21
	Answers	11.23
	Review Questions	11.23

<b>Chapter 12 Holography</b>	<b>12.1</b>
12.1 Introduction	12.1
12.2 Basic principle of holography	12.1
12.3 Recording of image on a holographic plate	12.1
12.4 Reconstruction of image from a hologram	12.2
12.5 Applications of holography	12.3
Multiple Choice Questions	12.3
Answers	12.4
Review Questions	12.4
<b>Chapter 13 Acoustics of Buildings and Acoustic Quieting</b>	<b>13.1</b>
13.1 Introduction to acoustics of buildings	13.1
13.2 Reverberation and time of reverberation	13.1
13.3 Sabine's empirical formula for reverberation time	13.2
13.4 Sabine's reverberation theory for reverberation time	13.2
13.5 Absorption coefficient of sound and its measurement	13.7
13.6 Basic requirements of an acoustically good hall	13.8
13.7 Factors affecting architectural acoustics and their remedies	13.8
13.8 Acoustic quieting	13.10
13.9 Methods of quieting	13.11
13.10 Quieting for specific observers	13.12
13.11 Muffler (or silencer)	13.12
13.12 Sound proofing	13.13
Formulae	13.14
Solved Problem	13.14
Multiple Choice Questions	13.14
Answers	13.16
Review Questions	13.16
<b>Chapter 14 Nanotechnology</b>	<b>14.1</b>
14.1 Basic principle of nanoscience and nanotechnology	14.1
14.2 Physical properties	14.4

14.3	Chemical properties	14.6
14.4	Fabrication	14.7
14.5	Production of nanoparticle	14.9
14.6	Carbon nanotubes	14.10
14.7	Application of nanotechnology	14.13
	Multiple Choice Questions	14.15
	Answers	14.19
	Review Questions	14.19

<b>Appendix A Hexagonal Close Pack (HCP) Structure</b>	A.1 – A.4
<b>Appendix B Surface Defects</b>	A.5 – A.8
<b>Dictionary of Selected Terms</b>	D.1 – D.14
<b>Question Papers</b>	Q.1 – Q.26
<b>Index</b>	I.1 – I.8

# Foreword

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This book is well-written. The theories, concepts and their explanations have been presented in a simple and lucid style by the author, based on his vast experience of teaching physics to engineering students. The book's layout, as well as the quality of its production, is excellent. In each chapter, the author has included review questions, solved problems, and ample multiple-choice questions to assist students in facing internal assessments and term-end examinations.

This book will be immensely useful to all first year B.Tech. students of the Jawaharlal Nehru Technological University (JNTU) and its affiliated colleges. The topics are dealt with in such a way as to enhance the student's understanding of the subject.

I whole-heartedly recommend this book for the study of topics covered under Applied Physics syllabus prescribed by JNTU for first year engineering students.



**Dr M. Krishnaiah**  
Professor of Physics  
S.V. University  
Tirupati

# Preface

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The contents of *Applied Physics* have been designed to cater to the needs of B.Tech. students at the freshman level in colleges affiliated to the Jawaharlal Nehru Technological University (JNTU), Hyderabad. The book follows a simple narrative style with emphasis on clarity. The concepts are treated rigorously to help students gain a deep-seated understanding of the key elements intrinsic to the subject. To this end, a list of important formulae, solved problems, multiple-choice questions and review questions have been included at the end of each chapter. These pedagogical elements would prepare the student-reader to face both internal tests and term-end examinations with ease. Further, a glossary of useful terms and a collection of previous years' university question papers are included to enhance the book's value as an undergraduate text.

Applied physics deals with the physics of substances that are of practical utility. This book focuses on the changes in properties of materials arising from the distribution of electrons in metals, semiconductors and insulators. It also covers topics on crystallography, free electron theory of metals, principles of quantum mechanics, superconductivity, properties of dielectric and magnetic materials, lasers, fibre optics, holography and nanotechnology.

I hope this book will be beneficial to both students and teachers of physics at various engineering colleges under JNTU, as well as other engineering colleges. Comments, feedback and suggestions for the improvement of this book are welcome. Any error that may have crept into the book inadvertently may kindly be brought to my notice, or to that of the publisher.

Mani Naidu

# Acknowledgements

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I thank Dr M. Mohan Babu, cine artiste, former M.P. and Chairman, Sree Vidyanikethan educational institutions, for providing a congenial atmosphere and encouraging me to write this book.

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I appreciate the contribution of the team at Pearson Education, especially that of Thomas Mathew Rajesh, M. E. Sethurajan, Sojan Jose and M. R. Ramesh in bringing this work to fruition.

I am indebted to my guide, Dr M. Krishnaiah, Professor of physics, S. V. University, Tirupati, for his valuable suggestions to enhance the worth of this book. I am also grateful to all my students and colleagues at SVEC for evincing keen interest in the making of this book.

Last, but not the least, I am eternally thankful to the goddess Sree Sallapuramma for granting me the perseverance and commitment to complete this book.

Mani Naidu

# Road Map to the Syllabus

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APPLIED PHYSICS  
JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY  
HYDERABAD

## UNIT I

**BONDING IN SOLIDS:** Ionic bond – Covalent bond – Metallic bond – Hydrogen bond – Vander-Waal's bond – Calculation of cohesive energy.

 REFER

CHAPTER 1

**CRYSTALLOGRAPHY AND CRYSTAL STRUCTURES:** Space lattice – Unit cell, lattice parameters – Crystal systems: Bravais lattices, Miller indices – Crystal planes and directions – Inter planar spacing of orthogonal crystal systems – Atomic radius, Co-ordination number and packing factor of sc, bcc, fcc, diamond and hcp structures – Structures of NaCl, ZnS, CsCl.

 REFER

CHAPTER 2

## UNIT II

**X-RAY DIFFRACTION:** Basic principles – Bragg's law – Laue method – Powder method – Applications of X-ray diffraction.

 REFER

CHAPTER 3

**DEFECTS IN CRYSTALS:** Point defects – Vacancies, substitutional, interstitial, Frenkel and Schottky defects – Qualitative treatment of line (edge and screw dislocations) defects – Burger's vector – Surface defects and volume defects.

 REFER

CHAPTER 3

## UNIT III

**ELEMENTS OF STATISTICAL MECHANICS:** Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac Statistics (qualitative treatment) – Photon gas – Wein's law, Rayleigh-Jeans law, Planck's law of black body radiation – Concept of electron gas – Fermi energy – Density of states.

 REFER

CHAPTER 4

**PRINCIPLES OF QUANTUM MECHANICS:** Waves and particles, de Broglie hypothesis – Matter waves, Davisson and Germer's experiment, G. P. Thomson experiment, Heisenberg's uncertainty principle – Schrödinger's time-independent wave equation – Physical significance of the wave function - Particle in a one-dimensional potential box.

 REFER

## CHAPTER 4

### UNIT IV

**BAND THEORY OF SOLIDS:** Electron in a periodic potential – Bloch theorem – Kronig-Penny model (qualitative treatment) – Origin of energy band formation in solids – Classification of materials into conductors, semiconductors and insulators – Concept of effective mass of an electron and hole.

 REFER

## CHAPTER 5

### UNIT V

**SEMICONDUCTORS:** Fermi level in intrinsic and extrinsic semiconductors – Intrinsic semiconductors and carrier concentration – Extrinsic semiconductors and carrier concentration – Equation of continuity – Direct and indirect band gap semiconductors – Hall effect.

 REFER

## CHAPTER 8

**PHYSICS OF SEMICONDUCTOR DEVICES:** Formation of PN junction – Open circuit PN junction – Energy diagram of PN diode – I-V characteristics of PN junction – PN diode as a rectifier (forward and reverse bias) – Diode equation – LED, LCD and photo diodes.

 REFER

## CHAPTER 8

### UNIT VI

**DIELECTRIC PROPERTIES:** Electric dipole – Dipole moment – Dielectric constant – Polarizability – Electric susceptibility – Displacement vector – Electronic, ionic and orientation polarizations – Calculation of polarizabilities – Internal fields in solids – Clausius–Mossotti equation – Piezo-electricity, pyro-electricity and ferro-electricity.

 REFER

## CHAPTER 6

**MAGNETIC PROPERTIES:** Permeability – Field intensity – Magnetic field induction – Magnetization – Magnetic susceptibility – Origin of magnetic moment – Bohr magneton – Classification of dia, para and ferro magnetic materials on the basis of magnetic moment – Domain theory of ferro magnetism – Basis of the hysteresis curve – Soft and hard magnetic materials – Properties of anti-ferro and ferri magnetic materials – Ferrites and their applications – Concept of perfect diamagnetism – Meissner effect – Magnetic levitation – Applications of superconductors.

 REFER

## CHAPTER 7 AND 9

## UNIT VII

**LASERS:** Characteristics of lasers – Spontaneous and stimulated emission of radiation – Meta-stable state – Population inversion – Lasing action – Einstein's coefficients and relation between them – Ruby laser, Helium–neon laser, Carbon dioxide laser, Semiconductor diode laser – Applications of lasers.

 REFER

CHAPTER 10

**FIBER OPTICS:** Principle of optical fiber – Acceptance angle and acceptance cone – Numerical aperture – Types of optical fibers and refractive index profiles – Attenuation in optical fibers – Application of optical fibers.

 REFER

CHAPTER 11

## UNIT VIII

**ACOUSTICS OF BUILDINGS AND ACOUSTIC QUIETING:** Basic requirement of an acoustically good hall – Reverberation and time of reverberation – Sabine's formula for reverberation time (qualitative treatment) – Measurement of absorption coefficient of a material – Factors affecting architectural acoustics and their remedies – Acoustic quieting – Aspects of acoustic quieting – Methods of quieting – Quietling for specific observers – Mufflers – Sound-proofing.

 REFER

CHAPTER 13

**NANOTECHNOLOGY:** Origin of nanotechnology – Nano scale – Surface-to-volume ratio – Quantum confinement – Bottom-up fabrication: sol-gel, precipitation, combustion methods – Top-down fabrication: chemical vapour deposition, physical vapour deposition, pulsed laser vapour deposition methods – Characterization (XRD and TEM) and Applications.

 REFER

CHAPTER 14

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## CHAPTER

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# 1

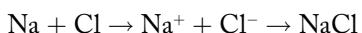
## Bonding in Solids

### 1.1 Different types of bonding in solids

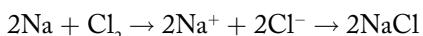
A crystal consists of atoms or molecules bound by interatomic forces or bonds. The interatomic forces are basically electrostatic in nature. These forces consist of both attractive and repulsive forces. Attractive forces are between negatively and positively charged particles and repulsive forces are between same kinds of particles. The different types of bonds are due to the differences in electronic structure of the atoms. Depending on strength and directionality, bonds are divided into two types: (1) primary and (2) secondary bonds. Primary bonds are interatomic in nature whereas secondary bonds are intermolecular in nature. Primary bond is a direct consequence of the transfer or sharing of valence electrons so as to obtain eight [or two] electrons in the outermost orbit for stability. The primary bonds are ionic, covalent and metallic bonds. In a solid crystal, atoms are bound together with certain amount of energy called bonding energy or cohesive energy. It is defined as the amount of energy required to separate atoms to infinite distance or the amount of energy evolved when a bond is formed. The bond strength generally depends on its melting and boiling points. Now, we will study the various types of bonds, as described below.

**(i) Interatomic bonds:** They are as follows:

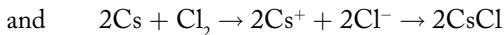
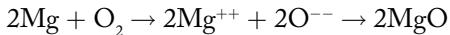
**(a) Ionic bond:** A bond formed by transfer of electron [or electrons] from one atom to another atom is called an ionic bond. Ionic bonding occurs between electropositive atoms [elements on the left side of the periodic table] and electronegative atoms [elements on the right side of the periodic table]. Examples for ionic substances are NaCl, KBr, MgO, etc. In the formation of NaCl crystal, each Na atom readily gives its valence electron [due to low ionization energy] to Cl atom and the Cl atom takes electron [due to high electron affinity] from Na atom. As a result,  $\text{Na}^+$  and  $\text{Cl}^-$  ions are formed because of opposite charge; these ions attract strongly and form a bond called an ionic bond. During this process, energy is released. This reaction is represented as:



Since chlorine exists as molecules, the chemical reaction is represented as:



Similarly, ionic bonding in other substances can be represented as:

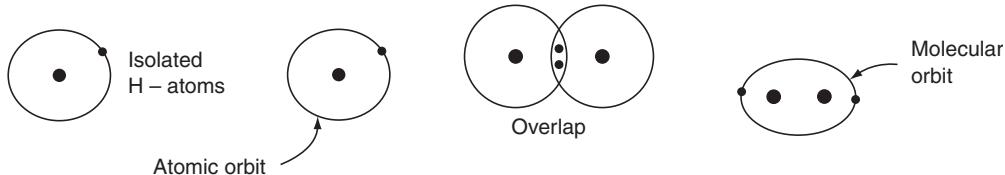


Some other examples are: KI, K<sub>2</sub>O, LiH, etc.

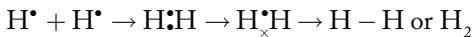
### Properties of ionic solids:

- (i) Ionic crystals are rigid, so they possess high melting and boiling points.
- (ii) Pure and dry ionic compounds are insulators, whereas in solution they conduct electricity due to the movement of charged ions.
- (iii) They are easily soluble in polar solvents like water [because of high dielectric constant] and insoluble in non-polar solvents like benzene [C<sub>6</sub>H<sub>6</sub>], carbon tetrachloride [CCl<sub>4</sub>], etc. [because of very low dielectric constant].
- (iv) When subjected to stresses, they cleave (break) along certain planes of crystal.

**(b) Covalent Bonds:** Covalent bonds are formed by sharing pairs of electrons among atoms. The covalent bond formation in hydrogen molecule can be explained in the following way: when two isolated H atoms approach each other, then their 1s orbits begin to overlap and the 1s electrons are attracted by the other nucleus and the overlap increases [provided the spin of the electrons is opposite]. The atomic orbits merge to form a single molecular orbit. In the molecular orbit, the two electrons are attracted by both the nuclei. The overlapping of atomic orbits will be stopped if the repulsive forces between the nuclei is balanced by the attractive force between electrons and opposite atom nucleus and a molecule is formed at a separation of 0.074 nm. The stability of the molecule is greater than that of the two isolated atoms.



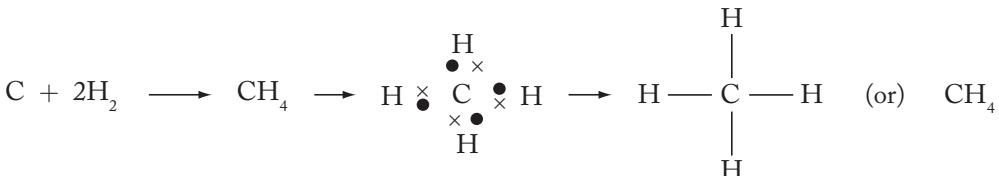
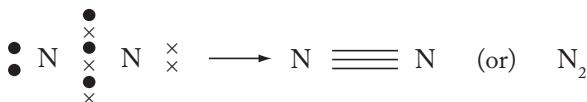
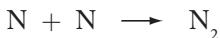
In the molecular orbit, the two electrons are equally shared between the nuclei and hence electron density is large between the nuclei. If  $N$  electrons are present in the valence shell of an atom, then it makes  $(8 - N)$  covalent bonds with the surrounding atoms to obtain an octet. A covalent bond is represented by putting two electrons between the symbols of atoms. For hydrogen, it is represented as H:H to make clear that an electron belongs to a particular atom; it can be represented as H<sup>.</sup><sub>x</sub>H, so that the dot electron belongs to left H – atom and  $x$  electron belongs to the right H – atom. The actual bond is represented as H – H. Thus:



In case of chlorine, each atom has seven electrons in the outermost shell. When two chlorine atoms combine to form chlorine molecule, one electron from each atom is shared with the other.



Other examples are:



### Properties of covalent compounds:

- (i) Covalent compounds are mostly gases and liquids. Covalent crystals are hard and brittle and incapable of an appreciable bending since the bonds are directional.
- (ii) Most of the covalent substances are insulators because of the non-availability of free electrons and ions.
- (iii) They are insoluble in polar solvents like  $\text{H}_2\text{O}$  and soluble in non-polar solvents like benzene, carbon disulphide, etc.

**(c) Metallic bond:** A collective bond formed between the positive ions and free electrons of a metal is called metallic bond. In metallic bonding, each atom of a metal gives one or two valence electrons to the crystal, which hold the atoms together and are not bound to individual atoms but move freely throughout the whole metal. In metals, the ionization energies are low so that metallic atoms give their valence electrons to the crystal. These valence electrons will form an electron cloud or electron gas (say), that occupy throughout the metal space. The positive ions are held together by the electrostatic forces due to free electrons. The electrostatic interaction between the positive ions and the electron gas hold the metal together.

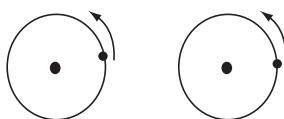
### Properties of metallic substances:

- (i) The free electrons in metals can easily migrate through large distances in crystal so that metals have high electrical and thermal conductivities.
- (ii) Metals may deform without fracture.
- (iii) Metals are opaque to light, since light energy is absorbed by free electrons.
- (iv) Their melting points range from moderate to high. Examples are Cu, Na, Ag, Al, etc.

**(ii) Intermolecular bonds:** The bonds formed with intermolecular forces are known as Vander Waals bonds. These forces unite the molecules in a solid. The secondary bonds are formed as a result of dipole attractions. The dipoles are formed due to uneven distribution of electrons in symmetric molecules. There are three types of intermolecular bonds. They are: (a) dispersion bonds, (b) dipole bonds and (c) hydrogen bonds.

**(a) Dispersion bonds:** These bonds are formed due to the variation of centres of positive and negative charges in a molecule. This has been explained in the hydrogen molecule. As shown in Fig. 1.1, the  $\text{H}_2$  molecule is

**Figure 1.1** Dispersion effect in a  $\text{H}_2$  molecule

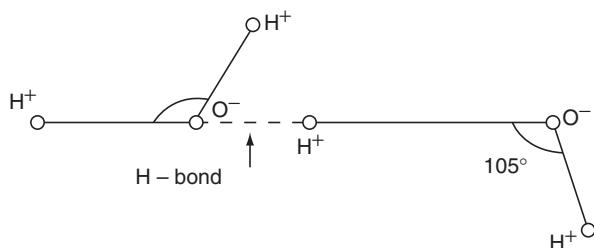


instantaneously charged negatively on the right end and positively on the left end because the revolving electrons around the nuclei tend to keep in phase. This fluctuating charge on one molecule tends to interact with the fluctuating charge on a neighbouring molecule. This results in a net attraction. The strength of the bond depends on the extent to which one atom can influence the other. Inert gases atoms are also held together by dispersion forces when the gases are solidified. The weak interatomic attractive forces are known as Vander Waals forces.

**(b) Dipole bond:** Dipole bonds are formed due to the variation in electron-sharing strengths of bonded atoms in a molecule. For example in  $\text{HCl}$  gas molecules, covalent bonds exist. Chlorine atoms share bonding electrons and are slightly larger than  $\text{H}$  atoms, as a result, chlorine atom acquires slightly negative charge and  $\text{H}$  – atom acquires slightly positive charge. Because of these charges, a dipole exists in  $\text{HCl}$  molecule. So, adjacent  $\text{HCl}$  molecules attract each other by means of the electrostatic attraction between their oppositely charged ends. The dipole bonds are considerably stronger than dispersion bonds. Examples for dipole bonds are  $\text{HBr}$ ,  $\text{SO}_2$  and  $\text{HCN}$ .

**(c) Hydrogen bonds:** This bond is similar to the dipole bond, but it is considerably stronger. Hydrogen bonds occur in those substances in which hydrogen atom is covalently bonded to a relatively larger atom such as nitrogen, oxygen, fluorine, etc. In these molecules, permanent dipoles exist because electron cloud is pulled more towards the heavier atom of molecule so that hydrogen atom gets more positive charge. A bond may exist between hydrogen of one molecule and a heavy atom of another molecule. Hydrogen bond in  $\text{H}_2\text{O}$  molecules is shown in Fig. 1.2.

**Figure 1.2** Hydrogen bond between two water molecules



## 1.2 Cohesive energy and estimation of cohesive energy of ionic solids

**Cohesive energy:** The amount of energy evolved when a crystalline solid is formed from infinitely separated atoms or the amount of energy required to separate atoms in a crystalline solid to infinite distance is known

as cohesive or binding energy of the crystal. The interatomic forces which hold the atoms together in a solid are responsible for crystal formation. So, the energy of the crystal is lower than that of the free atoms by an amount equal to the energy required to pull the atoms to an infinite distance. This energy is called the binding energy of the crystal.

**Force between atoms:** When atoms are at infinite separation, then there is no interaction between them. As we bring the atoms from infinite separation to close proximity to form a solid, there exist two types of forces between the atoms. (i) attractive forces and (ii) repulsive forces. When two atoms are present at a separation ' $r$ ' then:

$$\begin{aligned} \text{The attractive force } (F_A) &\propto \frac{1}{r^M} \\ &= \frac{A}{r^M} \quad \text{--- (1.1)} \end{aligned}$$

where ' $A$ ' is proportionality constant and  $M$  is usually 2 as per Coulomb's law.

$$\begin{aligned} \text{The repulsive force } (F_R) &\propto \frac{1}{r^N} \\ &= \frac{B}{r^N} \quad \text{--- (1.2)} \end{aligned}$$

where  $B$  is proportionality constant and  $N$  is usually in between 7 and 10.

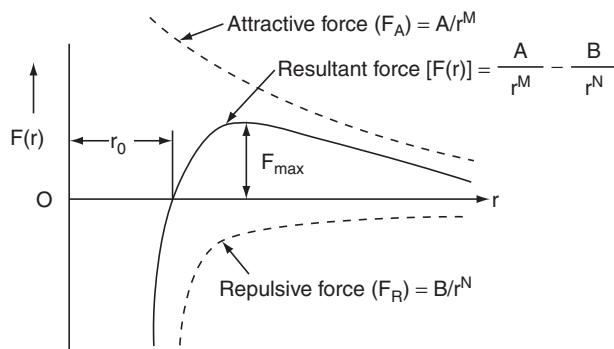
When the atoms are present in equilibrium with equilibrium separation ' $r_0$ ', then the magnitudes of  $F_A$  and  $F_R$  are equal and opposite. So, the resultant force between the atoms is zero. If the distance between the atoms is less than  $r_0$ , then repulsive force dominates and if the distance between atoms is larger than  $r_0$  then attractive force dominates. The sum of attractive and repulsive forces,  $F(r)$  at a separation ' $r$ ' is:

$$F(r) = \frac{A}{r^M} - \frac{B}{r^N} \quad \text{--- (1.3)}$$

The second term is negative because of the repulsive force.

The variation of  $F_A$ ,  $F_R$  and  $F(r)$  with respect to the separation between atoms ' $r$ ' is represented in Fig. 1.3.

**Figure 1.3 Variation of force with distance between atoms**



**At equilibrium separation ' $r_0$ :**

$$\text{i.e. } r = r_0, F(r) = 0$$

From Equation (1.3), we have:

$$0 = \frac{A}{r_0^M} = \frac{B}{r_0^N} \quad \text{or}$$

$$\frac{A}{r_0^M} = \frac{B}{r_0^M} \quad \text{or} \quad r_0^{N-M} = \frac{B}{A}$$

$$r_0 = \left( \frac{B}{A} \right)^{\frac{1}{N-M}} \quad \text{--- (1.4)}$$

### Calculation of Cohesive energy of Ionic Crystals:

The potential energy between the atoms  $U(r)$  can be obtained by integrating Equation (1.3) w.r.t. ' $r$ '. Thus:

$$U(r) = \int F(r) dr = \int \left[ \frac{A}{r^M} - \frac{B}{r^N} \right] dr$$

$$= \int \left[ Ar^{-M} - Br^{-N} \right] dr$$

$$= \frac{Ar^{1-M}}{1-M} - \frac{Br^{1-N}}{1-N} + c$$

where ' $c$ ' is the constant of integration

$$= - \left[ \frac{A}{M-1} \right] \left[ \frac{1}{r^{M-1}} \right] + \left[ \frac{B}{N-1} \right] \left[ \frac{1}{r^{N-1}} \right] + c$$

$$\text{Let } \frac{A}{M-1} = a; \quad \frac{B}{N-1} = b; \quad M-1 = m \quad \text{and} \quad N-1 = n$$

$$\text{then } U(r) = \frac{-a}{r^m} + \frac{b}{r^n} + c \quad \text{--- (1.5)}$$

where  $a$  and  $b$  are attractive and repulsive force constants respectively, and  $m$  and  $n$  are positive integers. The value of ' $c$ ' can be obtained by applying boundary conditions on Equation (1.5).

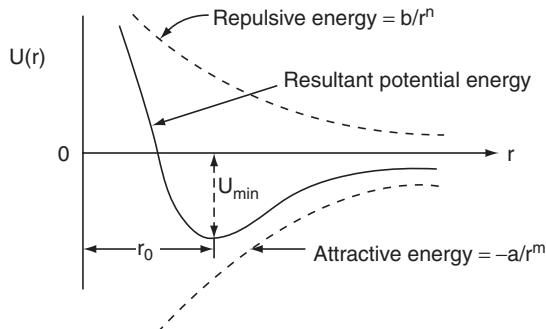
When  $r = \infty$ ,  $U(r) = 0$  and  $c = 0$

$$\text{so, } U(r) = \frac{-a}{r^m} + \frac{b}{r^n} \quad \text{--- (1.6)}$$

In Equation (1.6), the quantity  $\frac{-a}{r^m}$  represents attractive potential energy and  $\frac{b}{r^n}$  represents repulsive potential energy. The variation of potential energy  $U(r)$  with ' $r$ ' is shown in Fig. 1.4.

The potential energy is minimum [ $U_{\min}$ ] for a separation of  $r_0$ . This spacing  $r_0$  is called equilibrium spacing of atoms. At  $r = r_0$ , potential energy is negative, hence a positive amount of energy  $U_{\min}$  is needed to separate

**Figure 1.4 Variation of potential energy with distance between atoms**



the atoms. When the atoms are at equilibrium, then the potential energy between the atoms is minimum [ $U_{\min}$ ] and it is represented as  $U(r_0)$ .

$$\text{So } U(r_0) = U_{\min} = \frac{-a}{r_0^m} + \frac{b}{r_0^n} \quad (1.7)$$

where  $r_0$  is the equilibrium separation between the atoms. This energy ( $U_{\min}$ ) is called bonding energy or cohesive energy or dissociation energy of the atoms because this is the energy with which the two atoms bond together and that amount of energy required to separate them.  $U(r_0)$  is calculated by the following way.

Differentiating Equation (1.6) with respect to 'r' gives:

$$\frac{dU}{dr} = \frac{am}{r^{m+1}} - \frac{bn}{r^{n+1}} \quad (1.8)$$

At equilibrium separation, Equation (1.8) becomes:

$$\left( \frac{dU}{dr} \right)_{r=r_0} = \frac{am}{r_0^{m+1}} - \frac{bn}{r_0^{n+1}} = 0$$

$$\text{or } \frac{am}{r_0^{m+1}} = \frac{bn}{r_0^{n+1}}$$

$$\text{or } r_0^n = r_0^m \left( \frac{b}{a} \right) \left( \frac{n}{m} \right) \quad (1.9)$$

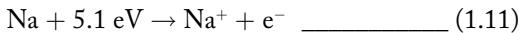
Substituting Equation (1.9) in (1.7), we get:

$$\begin{aligned} U_{\min} &= \frac{-a}{r_0^m} + \frac{b}{r_0^m} \left( \frac{a}{b} \right) \left( \frac{m}{n} \right) = \frac{-a}{r_0^m} + \frac{a}{r_0^m} \left( \frac{m}{n} \right) \\ &= \frac{-a}{r_0^m} \left( 1 - \frac{m}{n} \right) \end{aligned} \quad (1.10)$$

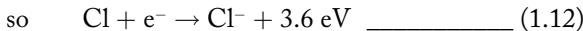
This is the expression for cohesive energy of a molecule containing two atoms in a molecule.

### 1.3. Estimation of cohesive energy of NaCl molecule in a solid

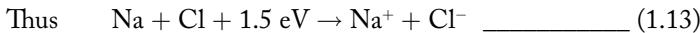
It is defined as the amount of energy released when a NaCl molecule is formed from isolated Na and Cl atoms. The cohesive energy of NaCl molecule is calculated as follows. The ionization energy or the amount of energy needed to remove the outermost valence electron from Na atom is 5.1 eV. That is:



The electron affinity of Cl atom is 3.6 eV; i.e., the amount of energy released when an electron is added to Cl atom is 3.6 eV.



The net amount of energy required to form  $\text{Na}^+$  and  $\text{Cl}^-$  ions at infinite separation is  $[5.1 \text{ eV} - 3.6 \text{ eV}] = 1.5 \text{ eV}$ .



As the ions possess opposite charge, so there exists an electrostatic attractive force between them, and this brings atoms to the equilibrium distance. At equilibrium distance, the potential energy is minimum. This indicates that energy is released in the formation of NaCl molecule. This energy is equal to the cohesive or bonding energy of NaCl molecule. The potential energy ( $V$ ) at equilibrium is:

$$(V) = \frac{-e^2}{4\pi\epsilon_0 r_0}$$

The equilibrium spacing ( $r_0$ ) in NaCl molecule is 0.24 nm. So,

$$\begin{aligned} (V) &= \frac{-[1.6 \times 10^{-19}]^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 2.4 \times 10^{-10}} \text{ J} \\ &= \frac{-[1.6 \times 10^{-19}]^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 2.4 \times 10^{-10} \times 1.6 \times 10^{-19}} \text{ eV} \cong -6 \text{ eV} \end{aligned}$$

The energy released in the formation of NaCl molecule from atoms at infinite separation is equal to  $5.1 \text{ eV} - 3.6 \text{ eV} - 6 \text{ eV} = -4.5 \text{ eV}$ . This is equal to cohesive or bond energy of NaCl molecule.

The Coulomb potential energy of an ion in a molecule is different as in case of a crystalline solid. In a crystalline solid, each ion is surrounded by oppositely charged ions, further surrounded by the same kind of ions and so on. In such cases, the Coulomb potential energy is  $V = \frac{-\alpha_M e^2}{4\pi\epsilon_0 r_0}$ , where  $\alpha_M$  is called Madelung constant.

Following Born the lattice energy for the univalent alkali metal halides is given by  $U_{r_0} = \frac{-\alpha_M e^2 N_A}{4\pi\epsilon_0 r_0} \left( \frac{n-1}{n} \right)$

Hence the cohesive energy of a molecule is

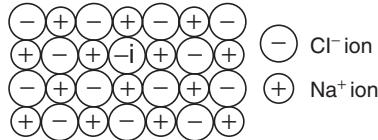
$$\frac{U_{r_0}}{N_A} = \frac{-\alpha_M e^2}{4\pi\epsilon_0 r_0} \left( \frac{n-1}{n} \right).$$

## 1.4 Madelung constant

In ionic crystals, the effect of interaction of all the ions on an ion has been represented by Madelung constant,  $\alpha_M$ . In ionic crystals, individual atoms do not exist. Every ion is surrounded by some number of opposite ions, i.e., an anion is surrounded by certain number of cations and vice versa. The Madelung constant has been explained by considering one of the ionic crystals [say NaCl]. As shown in Fig. 1.5, let  $u_{ij}$  is the interaction energy between a particular ion ' $i$ ' and another ion ' $j$ ' [ $j$  is a variable], so that the separation between these ions is  $r_{ij}$ . The  $i^{\text{th}}$  ion makes an interaction with a number of surrounding ions in pair-wise. The net interaction energy  $u_i$  is the sum of all pair-wise interaction energies with the  $i^{\text{th}}$  ion so that:

$$u_i = \sum_j u_{ij} \quad i \neq j$$

**Figure 1.5 Ionic crystal [NaCl]**



The interaction energy does not depend on the position of the reference ion in the crystal and irrespective of whether it is positive or negative. Usually, the interaction energy  $u_{ij}$  is of coulombic in nature, given as:

$$u_{ij} = \frac{-z_i z_j e^2}{4\pi \epsilon_0 r_{ij}}$$

where  $Z_i$  and  $Z_j$  are the charges on  $i^{\text{th}}$  and  $j^{\text{th}}$  ions and one of these two ions is negative.

Suppose  $r_{ij} = \alpha_{ij} r_0$ , where  $r_0$  is the shortest distance between unlike ions in the crystal. Then the total electrostatic energy between the  $i^{\text{th}}$  ion and other ions in the crystal is:

$$\begin{aligned} u_i &= \sum_j \left[ \frac{-z_i z_j e^2}{4\pi \epsilon_0 \alpha_{ij} r_0} \right] = - \sum_j \frac{1}{\alpha_{ij}} \times \frac{z_i z_j e^2}{4\pi \epsilon_0 r_0} \\ &= \frac{-z_i z_j e^2 \alpha_M}{4\pi \epsilon_0 r_0} \end{aligned}$$

where  $\alpha_M = \sum_j \frac{1}{\alpha_{ij}}$ . The constant  $\alpha_M$  is called Madelung constant.

As shown in Fig. 1.5, if we consider the ions on either side of the reference ion ' $i$ ' in a row, then the interaction energies are:

$$u_{i+1} = \frac{-e^2}{4\pi \epsilon_0 r_0} \quad \text{and} \quad u_{i-1} = \frac{-e^2}{4\pi \epsilon_0 r_0}$$

so that the net energy is  $\frac{-2e^2}{4\pi\epsilon_0 r_0}$

The interaction energy on the  $i^{\text{th}}$  ion due to the next two ions on either side is  $\frac{2e^2}{4\pi\epsilon_0 2r_0}$ .

Again the interaction energy on the  $i^{\text{th}}$  ion due to the next two ions on either side is  $\frac{-2e^2}{4\pi\epsilon_0 3r_0}$ . This process can be extended up to the end of the row.

$$\text{Then } \frac{\alpha_M}{r_0} = 2 \left[ \frac{1}{r_0} - \frac{1}{2r_0} + \frac{1}{3r_0} - \frac{1}{4r_0} + \dots \right]$$

The multiplier 2 in the above equation is due to the two ions; one present on the left side and the other present on the right side at equal distances from the  $i^{\text{th}}$  ion.

$$\text{Hence, } \alpha_M = 2 \left[ 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \dots \right] = 2l_n 2$$

This is the Madelung constant for a row of atoms. This concept can be extended to the three-dimensional space. For NaCl crystal, each  $\text{Na}^+$  ion is surrounded by 6  $\text{Cl}^-$  ions at equilibrium separation  $r_0$  and is surrounded by 12 same kind of ions ( $\text{Na}^+$ ) at a distance of  $\sqrt{2}r_0$ ; also 8  $\text{Cl}^-$  ions at a distance of  $\sqrt{3}r_0$  and 6  $\text{Na}^+$  ions at a distance of  $\sqrt{4}r_0$  and so on. Hence, the Madelung constant for NaCl crystal is:

$$\alpha_M = \left[ \frac{6}{\sqrt{1}} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} + \dots \right]$$

The Madelung constant for NaCl is 1.75 and for CsCl is 1.76.

## Formulae

$$1. \quad F(r) = \frac{A}{r^N} - \frac{B}{r^M}$$

$$2. \quad r_0 = \left( \frac{B}{A} \right)^{\frac{1}{N-M}}$$

$$3. \quad U(r) = \int F(r) dr = \int \left[ \frac{A}{r^M} - \frac{B}{r^N} \right] dr$$

$$4. \quad U(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

$$5. \quad U_{\min} = \frac{-a}{r_0^m} \left( 1 - \frac{m}{n} \right)$$

$$6. \quad V = \frac{-e^2}{4\pi\epsilon_0 r_0}$$

$$7. \quad \frac{U_{r_0}}{N_A} = \frac{-\alpha_M e^2}{4\pi\epsilon_0 r_0} \left( \frac{n-1}{n} \right)$$

## Solved Problems

1. Estimate the bond energy for the  $\text{NaCl}$  molecule as formed from sodium and chlorine atoms. The interionic equilibrium distance is 236 pm. Born constant is 8. The ionization energy of sodium is 5.14 eV and electron affinity of chlorine is 3.65 eV.

(Set-2-May 2004), (Set-4-Nov. 2004), (Set-2-May 2003)

**Sol:** The equilibrium separation of the ions ( $r_0$ ) = 236 pm =  $236 \times 10^{-12}$  m

The potential energy at this separation is:

$$\begin{aligned} V &= \frac{-e^2}{4\pi\epsilon_0 r_0} = \frac{-[1.6 \times 10^{-19}]^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 236 \times 10^{-12}} \\ &= \frac{-1.6 \times 1.6 \times 10^{-14}}{\frac{88}{7} \times 8.85 \times 236} \text{ J} = \frac{-1.6 \times 1.6 \times 10^{-14}}{\frac{88}{7} \times 8.85} \\ &= -6.094 \text{ eV} \quad [\text{energy released during the formation of molecule from ions}] \end{aligned}$$

Ionization energy of Na = 5.14 eV      [energy supplied to remove an electron]

Electron affinity of chlorine = -3.65 eV

[energy released when an electron is added to chlorine atom]

$\therefore$  Bonding energy of  $\text{NaCl}$  molecule =  $5.14 \text{ eV} - 3.65 \text{ eV} - 6.09 \text{ eV}$

$$= -4.6 \text{ eV}$$

2. The Madelung constant of  $\text{KCl}$  is 1.75. Its neighbour separation is 0.314 nm. Find the cohesive energy per atom. [Given that the Repulsive exponent value = 5.77; Ionization energy of potassium = 4.1 eV; Electron affinity of chlorine = 3.6 eV]

(Set-3, Set-4-May 2008)

**Sol:** The madelung constant of  $\text{KCl}$ , A = 1.75

Separation between ion pair,  $r_0$  = 0.314 nm

Repulsive exponent value,  $n$  = 5.77

Ionization energy of potassium = 4.1 eV

Electron affinity of chlorine = 3.6 eV

$$\text{Potential energy or cohesive energy per molecule of KCl} = \frac{-Ae^2}{4\pi\epsilon_0 r_0} \left(1 - \frac{1}{n}\right)$$

$$= \frac{-1.75 \times (1.602 \times 10^{-19})^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 0.314 \times 10^{-9}} \times \left(1 - \frac{1}{5.77}\right) \text{ J}$$

$$= \frac{-1.75 \times 1.602 \times 10^{-19} \times 7}{4 \times 22 \times 8.85 \times 10^{-12} \times 0.314 \times 10^{-9}} \times 0.82669 \text{ eV}$$

$$= -6.6342 \text{ eV}$$

$$\text{Cohesive energy per atom} = \frac{-6.6342}{2} = -3.3171 \text{ eV}$$

But the energy needed to form ion pair from atoms is equal to

= Ionizational energy of K – electron affinity of Cl

$$= 4.1 \text{ eV} - 3.6 \text{ eV} = 0.5 \text{ eV}$$

$$\therefore \text{Contribution to cohesive energy per atom} = \frac{0.5 \text{ eV}}{2}$$

$$= 0.25 \text{ eV}$$

$$\therefore \text{Total cohesive energy per atom} = -3.3171 \text{ eV} + 0.25 \text{ eV} = -3.0671 \text{ eV}$$

3. Calculate the cohesive energy of NaCl from the following data:

Equilibrium separation between the ion pair = 0.281 nm

Ionization energy of Na = 5.14 eV

Electron affinity of Cl = 3.61 eV

Born repulsive exponent = 9

Madelung constant = 1.748

(Set-4–June 2005)

**Sol:** The given data are

$$r_0 = 0.281 \text{ nm} = 0.281 \times 10^{-9} \text{ m}$$

$$n = 9$$

$$\alpha_M = 1.748$$

$$\begin{aligned} \text{Cohesive energy per molecule of NaCl} &= \frac{-\alpha_M e^2}{4\pi \epsilon_0 r_0} \left( 1 - \frac{1}{n} \right) \\ &= \frac{-1.748 \times (1.602 \times 10^{-19})^2 \times 8/9}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 0.281 \times 10^{-9}} \\ &= -0.12755 \times 10^{-17} \text{ J} \\ &= \frac{-0.12755 \times 10^{-17}}{1.602 \times 10^{-19}} \text{ eV} \\ &= -7.96 \text{ eV} \end{aligned}$$

4. Calculate the potential energy of the system of  $\text{Na}^+$  and  $\text{Cl}^-$  ions when they are 0.25 nm apart.

(Set-4–Sept. 2007)

**Sol:** Separation between  $\text{Na}^+$  and  $\text{Cl}^-$  ions  $r_0 = 0.25 \text{ nm}$

$$= 2.5 \times 10^{-10} \text{ m}$$

The expression for P.E. is

$$\text{P.E.} = \frac{-e^2}{4\pi \epsilon_0 r_0}$$

$$\epsilon = 1.6 \times 10^{-19} \text{ C}$$

$$\epsilon_0 = 8.85 \times 10^{-12} \text{ F/m}$$

$$\therefore \text{P.E.} = \frac{-(1.6 \times 10^{-19})^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 2.5 \times 10^{-10}} \text{ Joules}$$

$$= \frac{-(1.6 \times 10^{-19})^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 2.5 \times 10^{-10} \times 1.6 \times 10^{-9}} \text{ eV}$$

$$= 5.75 \text{ eV}$$

5. Calculate the cohesive energy of NaCl from the given data: The equilibrium separation of  $\text{Na}^+$  and  $\text{Cl}^-$  ions = 0.281 nm,  $a = 1.748 \times 10^{-28} \text{ J-m}^2$ ,  $n = 9$ ,  $m = 1$ .

**Sol:** Cohesive energy  $(U_{r_0}) = \frac{-a}{r_0^m} \left(1 - \frac{m}{n}\right)$

Given data are:  $r_0 = 0.281 \text{ nm} = 0.281 \times 10^{-9} \text{ m}$

$$a = 1.748 \times 10^{-28} \text{ J-m}^2$$

$$n = 9, m = 1$$

$$\begin{aligned} \therefore U_{r_0} &= \frac{-1.748 \times 10^{-28}}{0.281 \times 10^{-9}} + \left(1 - \frac{1}{9}\right) \text{ J} \\ &= \frac{-1.748 \times 10^{-28}}{0.281 \times 10^{-9}} + \frac{\left(1 - \frac{1}{9}\right)}{1.6 \times 10^{-9}} \text{ eV} = -3.46 \text{ eV} \end{aligned}$$

6. Calculate the cohesive energy of NaCl, when the equilibrium separation between  $\text{Na}^+$  and  $\text{Cl}^-$  ions is 0.281 nm. The ionization energy of Na atom is 5.14 eV and electron affinity of Cl atom is 3.61 eV.

**Sol:** Equilibrium separation ( $r_0$ ) = 0.281 nm =  $0.281 \times 10^{-9} \text{ m}$

Ionization energy of Na = 5.14 eV

Electron affinity of Cl = -3.61 eV

$$\begin{aligned} \text{Potential energy at equilibrium separation } (V) &= \frac{-e^2}{4\pi\epsilon_0 r_0} \\ &= \frac{-(1.6 \times 10^{-19})^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 0.281 \times 10^{-9}} \text{ J} \\ &= \frac{-(1.6 \times 10^{-19})^2}{4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times 0.281 \times 10^{-9} \times 1.6 \times 10^{-19}} \text{ eV} \\ &= \frac{-1.6 \times 10^{-19} \times 7}{88 \times 8.85 \times 0.281 \times 10^{-21}} \text{ eV} = -5.12 \text{ eV} \end{aligned}$$

Cohesive energy =  $[5.14 - 3.61 - 5.12] \text{ eV} = -3.59 \text{ eV}$

## Multiple Choice Questions

1. Basically, interatomic forces are: ( )

(a) electrostatic in nature (b) gravitational forces  
(c) magnetic forces (d) short-range forces

2. Primary bonds are \_\_\_\_\_ in nature ( )

(a) intermolecular (b) interatomic  
(c) Vanderwaals forces (d) none

3. Primary bonds are: ( )

(a) ionic bonds (b) covalent bonds (c) metallic bonds (d) all

4. Bonding or cohesive energy is defined as: ( )

(a) the amount of energy required to separate atoms to an infinite distance  
(b) the amount of energy evolved when a bond is formed  
(c) a and b  
(d) none

5. Examples for ionic crystals are: ( )

(a) NaCl and KBr (b) MgO and KI  
(c) K<sub>2</sub>O and LiH (d) all

6. Ionic crystals ( )

(a) are rigid and possess high melting and boiling points  
(b) in solution conduct electricity  
(c) are easily soluble in polar solvents like water  
(d) all

7. Covalent bond is formed by: ( )

(a) sharing of pair of electrons between atoms  
(b) transfer of electrons from one atom to another  
(c) evaporation of electrons from atoms  
(d) none

8. Covalent compounds are: ( )

(a) hard and brittle  
(b) most of them are insulators  
(c) they are insoluble in polar solvents like H<sub>2</sub>O  
(d) all

9. Metals ( )

(a) possess high electrical and thermal conductivities  
(b) may deform without fracture  
(c) are opaque to light  
(d) all

10. Intermolecular bonds are: ( )

(a) dispersion bonds (b) dipole bonds  
(c) hydrogen bonds (d) all

11. When the atoms are present in equilibrium with equilibrium separation  $r_0$ , then the resultant force between the atoms is: ( )  
(a) zero (b) positive (c) negative (d) very large

12. The amount of energy with two atoms bond together and the same amount of energy required to separate them is called \_\_\_\_\_ of atoms. ( )  
(a) bonding energy (b) cohesive energy  
(c) dissociation energy (d) all

13. The cohesive or bond energy of NaCl molecule is: ( )  
(a) 3.6 eV (b) 6 eV (c) 4.5 eV (d) 5.1 eV

14. In a crystal, atoms or molecules are bonded by \_\_\_\_\_ forces. ( )  
(a) interatomic (b) Vanderwaals (c) adhesive (d) cohesive

15. Secondary bonds are \_\_\_\_\_ in nature. ( )  
(a) interatomic (b) intermolecular (c) adhesive (d) none

16. Ionic bond occurs between \_\_\_\_\_ atoms and \_\_\_\_\_ atoms. ( )  
(a) electropositive, electronegative (b) electropositive, electropositive  
(c) electronegative, electronegative (d) none

17. If  $N$  electrons are present in the valence shell of an atom, then it makes \_\_\_\_\_ covalent bonds. ( )  
(a)  $N$  (b)  $8 - N$  (c)  $N - 8$  (d) none

18. Covalent compounds are soluble in non-polar solvents like ( )  
(a) benzene (b) carbon disulphide  
(c) both a and b (d) none

19. Each atom of a metal gives one or two \_\_\_\_\_ to the crystal. ( )  
(a) valence electrons (b) bounded electrons  
(c) both a and b (d) none

20. Dispersion bonds are formed due to \_\_\_\_\_ of positive and negative charges in a molecule. ( )  
(a) centres (b) variation of centres  
(c) both a and b (d) none

21. \_\_\_\_\_ bonds are formed due to the variation in electron-sharing strengths of bonded atoms in a molecule. ( )  
(a) covalent (b) ionic (c) hydrogen (d) dipole

22. \_\_\_\_\_ bond is similar to dipole bond but considerably stronger than it ( )  
(a) hydrogen (b) covalent (c) ionic (d) none

23. The energy of the crystal is lower than that of the free atoms by an amount called ( )  
(a) interatomic energy (b) intermolecular energy  
(c) cohesive energy (d) none

24. When the atoms are at equilibrium, then the potential energy between the atoms is: ( )  
(a) maximum (b) minimum (c) both a and b (d) none

## Answers

1. a      2. b      3. d      4. c      5. d      6. d      7. a      8. d      9. d      10. d      11. a  
12. d     13. c     14. a     15. b     16. a     17. b     18. c     19. a     20. b     21. d     22. a  
23. c     24. b     25. a     26. b

# Review Questions

- What are ionic crystals? Explain the formation of an ionic crystal and obtain an expression for its cohesive energy.  
(Set-4–June 2005)
  - Explain the forces between two interacting atoms when they are brought nearer to form a molecule.  
(Set-1–May 2008), (Set-2–May 2006), (Set-1–May 2004),  
(Set-2–Nov. 2004), (Set-1–May 2003)
  - Derive an expression for the equilibrium spacing of two atoms for which the potential energy is minimum and hence obtain the dissociation energy.  
(Set-1–May 2008), (Set-2–May 2006), (Set-1–May 2004),  
(Set-2–Nov. 2004), (Set-1–May 2003)
  - Plot and explain the variation of: (i) attractive potential energy (ii) repulsive potential energy and (iii) resultant potential energy with interatomic distance, when two atoms are brought nearer.  
(Set-3–May 2008), (Set-2–May 2004), (Set-4–Nov. 2004), (Set-2–May 2003)
  - Explain various types of bondings in solids with suitable examples.  
(Set-4–May 2008)
  - Explain the bonding in NaCl  
(Set-4–Sept. 2007)
  - Calculate the bond energy for NaCl molecule  
(Set-4–Sept. 2007)
  - Explain the formation of an ionic crystal, with suitable example.  
(Set-2–Sept. 2008)
  - Derive an expression for the cohesive energy of an ionic crystal.  
(Set-2–Sept. 2008)
  - Explain with suitable examples the ionic, covalent, metallic and molecular type of bonds in solids.
  - What is cohesive energy? Assuming a suitable model for interatomic forces, derive an expression for the cohesive energy.
  - Explain the formation of an ionic bond. Calculate the cohesive energy of NaCl molecule.
  - Explain the different types of bondings in solids with suitable examples. Compare their bond energies.
  - Illustrate graphically the variation of: (i) interatomic forces and (ii) potential energy with the spacing between two atoms.
  - Write short notes on binding energy of NaCl molecule.

16. Define cohesive energy of a molecule and derive an expression for it as a function of equilibrium atomic separation and attractional or repulsive interaction exponents.
17. Prove that the value of Madelung constant for an FCC crystal is 1.75.
18. Draw a diagram that depicts the variation of interatomic force as a function of spacing in terms of its attractional and repulsive components. Derive an expression for equilibrium spacing.
19. Derive an expression for the lattice energy in ionic crystals and prove that the Madelung constant for molecule in NaCl like ionic crystal is  $2 \ln 2$ .

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## CHAPTER

# 2

## Crystal Structures

### 2.1 Introduction

Matter exists in three different states; they are gaseous, liquid and solid states. In gaseous and liquid states, the atoms or molecules of the substance move from one place to other, and there is no fixed position of atoms in the substance. In solids, the positions of the atoms or molecules are fixed and may or may not be present periodically at regular intervals of distance. If the atoms or molecules in a solid are periodical at regular intervals of distances in three-dimensional space, then that solid is known as crystalline solid. If the atoms or molecules do not have such a periodicity in a solid, then that solid is known as amorphous solid. When the periodicity of atoms or molecules is extended throughout the solid, then the solid is known as single crystalline solid. If the periodicity of atoms or molecules is extended up to small regions called grains and if these grains are very large in number, and are of different sizes in the solid, such a material is known as polycrystalline solid. The study of geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams constitute the science of crystallography.

### Distinction between crystalline and amorphous solids

Crystalline Solids	Amorphous Solids
1. The atoms or molecules of the crystalline solids are periodic in space.	1. The atoms or molecules of the amorphous solids are not periodic in space.
2. Some crystalline solids are anisotropic i.e., the magnitude of physical properties [such as refractive index, electrical conductivity, thermal conductivity, etc.,] are different along different directions of the crystal.	2. Amorphous solids are isotropic i.e., the magnitude of the physical properties are same along all directions of the solid.
3. Crystalline solids have sharp melting points.	3. Amorphous solids do not possess sharp melting points.

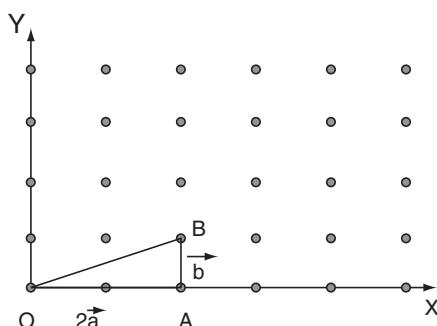
- |   |  |
|---|--|
| 4. Breaks are observed in the cooling curve of a crystalline solid.<br>5. A crystal breaks along certain crystallographic planes. | 4. Breaks are not observed in the cooling curve.<br>5. When an amorphous solid breaks, the broken surface is irregular because it has no crystal planes. |
|---|--|

## 2.2 Space lattice (or) crystal lattice

In a solid crystalline material, the atoms or molecules are arranged regularly and periodically in three dimensions. To explain crystal symmetries easily, it is convenient to represent an atom or a group of atoms that repeats in three dimensions in the crystal as a unit. If each such unit of atoms or atom in a crystal is replaced by a point in space, then the resultant points in space are called space lattice. Each point in space is called a lattice point and each unit of atoms or atom is called basis or pattern. A space lattice represents the geometrical pattern of crystal in which the surroundings of each lattice point is the same.

If the surroundings of each lattice point is same or if the atom or all the atoms at lattice points are identical, then such a lattice is called Bravais lattice. On the other hand, if the atom or the atoms at lattice points are not same, then it is said to be a non-Bravais lattice. Figure 2.1 shows a two-dimensional lattice.

**Figure 2.1** Two-dimensional lattice

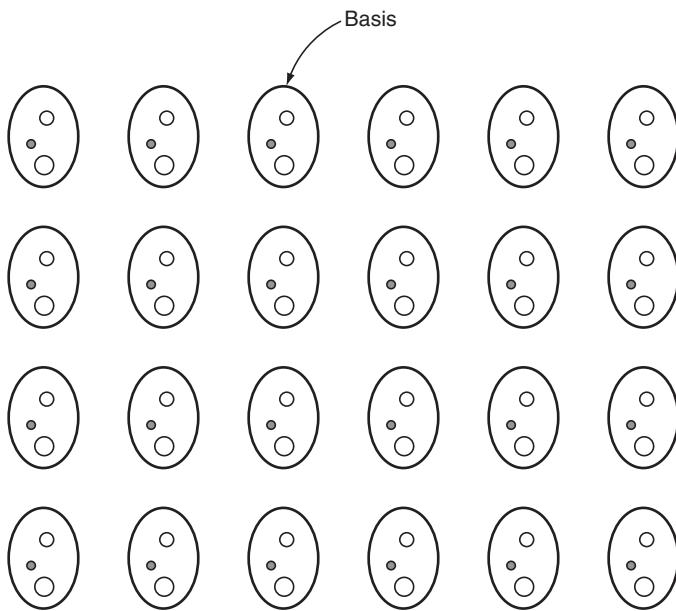


To represent translational vectors or basis vectors, consider a co-ordinate system with its origin at the lattice point 'O'. Let  $\vec{OA} = 2\vec{a}$  and  $\vec{AB} = \vec{b}$ , such that  $\vec{OB} = 2\vec{a} + \vec{b}$ . where  $\vec{a}$  and  $\vec{b}$  are called translational or basis vectors along X and Y directions. The position vector  $\vec{R}$  of any lattice point can be represented as  $\vec{R} = n_1\vec{a} + n_2\vec{b}$ . where  $n_1$  and  $n_2$  are integers, their values depend on the position of the lattice point under consideration with respect to the origin. In three dimensions, the position vector of a point can be expressed as  $\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$ , where  $\vec{a}$ ,  $\vec{b}$  and  $\vec{c}$  are the translational or basis vectors along X, Y and Z directions, respectively. They are also called translational primitives.

## 2.3 The basis and crystal structure

The crystal structure is formed by associating every lattice point with an assembly of atoms or molecules or ions, which are identical in composition, arrangement and orientation, is called as the basis. The atomic arrangement in a crystal is called crystal structure. If the basis is substituted for the lattice points, then the resulting structure is called crystal structure as shown in Fig. 2.2. Thus lattice + basis = crystal structure. The basis shown in Fig. 2.2 contains three different atoms. In copper and sodium crystals the basis is single atoms; in NaCl, the basis is diatomic and in CaF<sub>2</sub>, the basis is triatomic.

**Figure 2.2** Two-dimensional crystal structure

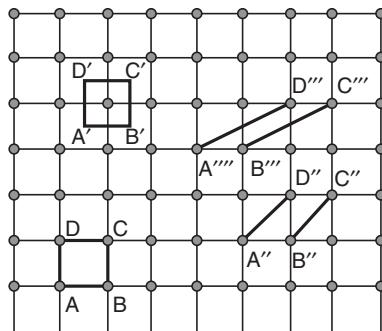


## 2.4 Unit cell and lattice parameters

Unit cells for most of the crystals are parallelopipeds or cubes having three sets of parallel faces. A unit cell is the basic structural unit or building block of the crystal. A unit cell is defined as the smallest parallelopiped volume in the crystal, which on repetition along the crystallographic axes gives the actual crystal structure or the smallest geometric figure, which on repetition in three-dimensional space, gives the actual crystal structure called a unit cell. The choice of a unit cell is not unique but it can be constructed in a number of ways; Fig. 2.3 shows different ways of representing unit cells in a two-dimensional lattice. A unit cell can be represented as ABCD or A'B'C'D' or A''B''C''D'', etc.

To define the lattice parameters, first we define crystallographic axes. These axes are obtained by the intersection of the three non-coplanar faces of the unit cell. The angle between these faces or crystallographic

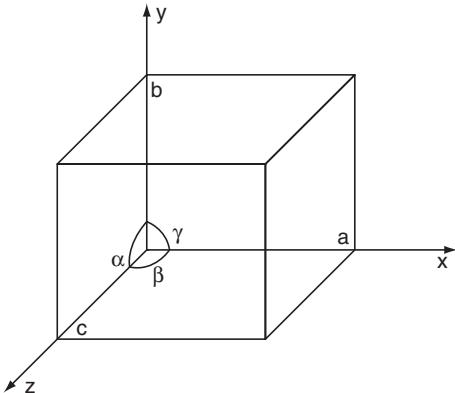
**Figure 2.3** Unit cells in crystal lattice



axes are known as interfacial or interaxial angles. The angles between the axes Y and Z is  $\alpha$ , between Z and X is  $\beta$  and between X and Y is  $\gamma$ . The translational vectors or primitives  $a$ ,  $b$ ,  $c$  of a unit cell along X, Y, Z axes and interaxial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  are called cell parameters. These cell parameters are shown in Fig. 2.4.

The cell parameters determine the actual size and shape of the unit cell. The unit cell formed by primitives is called a primitive unit cell. A primitive unit cell contains only one lattice point. If a unit cell contains more than one lattice point, then it is called non-primitive or multiple cells. For example, BCC and FCC are non-primitive unit cells.

**Figure 2.4** Unit cell parameters



## 2.5 Crystal systems and Bravais lattices

For representing the type of distribution of lattice points in space, seven different co-ordinate systems are required. These co-ordinate systems are called crystal systems. The crystal systems are named on the basis of geometrical shape and symmetry. The seven crystal systems are: (1) Cubic (2) Tetragonal (3) Orthorhombic (4) Monoclinic (5) Triclinic (6) Rhombohedral (or Trigonal) and (7) Hexagonal. Space lattices are classified according to their symmetry. In 1948, Bravais showed that 14 lattices are sufficient to describe all crystals. These 14 lattices are known as Bravais lattices and are classified into 7 crystal systems based on cell parameters.

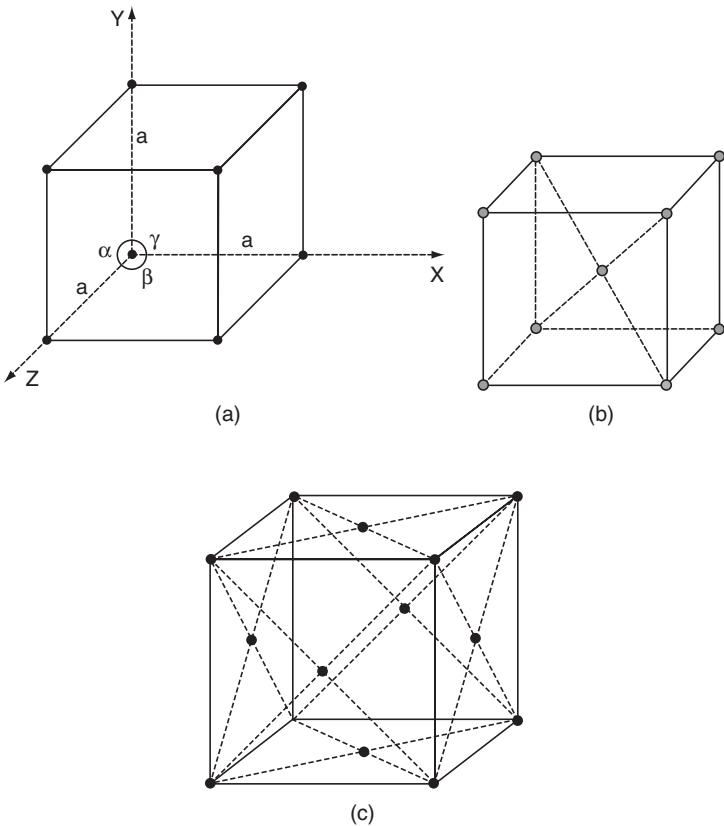
The Bravais lattices are categorized as primitive lattice (P); body-centred lattice (I); face-centred lattice (F) and base-centred lattice (C). These seven crystal systems and Bravais lattices are described below.

**1. Cubic crystal system:** In this crystal system, all the unit cell edge lengths are equal and are at right angles to one another i.e.,  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$ . In cubic system, there are three Bravais lattices; they are simple (primitive); body-centred and face-centred. Examples for cubic system are Au, Cu, Ag, NaCl, diamond, etc.

In simple cubic lattice, lattice points or atoms are present at the corners of the cube. In body-centred cube, atoms are present at the corners and one atom is completely present at the centre of the cube. In the case of face-centred cube, atoms are present at corners and at the centres of all faces of cube.

Figure 2.5

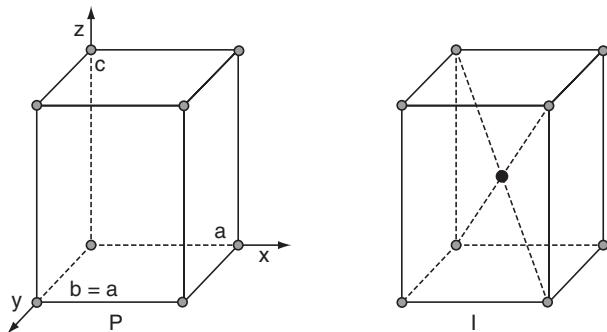
Cubic crystal system: (a) Simple cubic (P); (b) Body-centred cube (I) and (c) Face-centred cube (F)



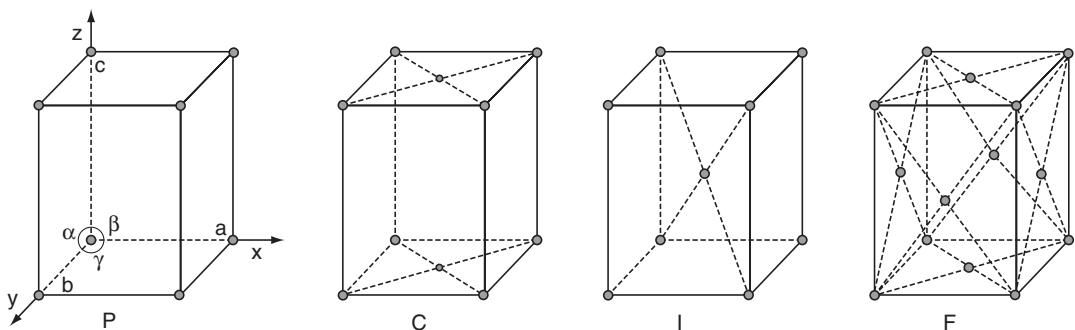
**2. Tetragonal crystal system:** In this crystal system, two lengths of the unit cell edges are equal whereas the third length is different. The three edges are perpendicular to one another i.e.,  $a = b \neq c$  and  $\alpha = \beta = \gamma = 90^\circ$ . In tetragonal system, there are two Bravais lattices; they are simple and body-centred. These are shown in Fig. 2.6. Examples for tetragonal crystal systems are  $TiO_2$ ,  $SnO_2$ , etc.

**3. Orthorhombic crystal system:** In this crystal system, unit cell edge lengths are different and they are perpendicular to one another i.e.,  $a \neq b \neq c$  and  $\alpha = \beta = \gamma = 90^\circ$ . There are four Bravais lattices in this

**Figure 2.6** Tetragonal crystal system



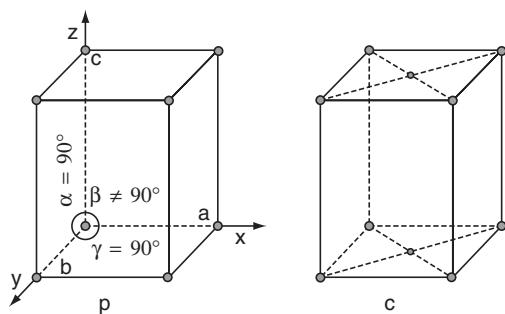
**Figure 2.7** Orthorhombic crystal system



system. They are simple, face centred, body centred and base centred. These are shown in Fig. 2.7. Examples for orthorhombic crystal system are  $\text{BaSO}_4$ ,  $\text{K}_2\text{SO}_4$ ,  $\text{SnSO}_4$ , etc.

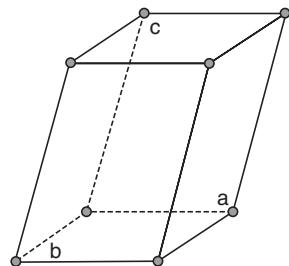
**4. Monoclinic crystal system:** In this crystal system, the unit cell edge lengths are different. Two unit cell edges are not perpendicular, but they are perpendicular to the third edge i.e.,  $a \neq b \neq c$ ;  $\alpha = \gamma = 90^\circ \neq \beta$ . This crystal system has two Bravais lattices; they are simple and base centred. These are shown in Fig. 2.8. Examples for Monoclinic crystal system are  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$  (gypsum),  $\text{Na}_3\text{AlF}_6$  (cryolite), etc.

**Figure 2.8** Monoclinic crystal system



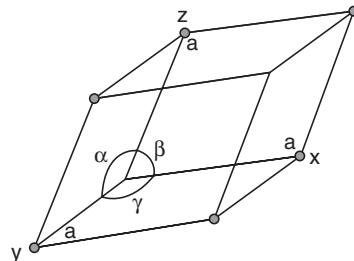
**5. Triclinic crystal system:** In this crystal system, the unit cell edge lengths are different and are not perpendicular i.e.,  $a \neq b \neq c$  and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$  and all the angles are different. This crystal exists in primitive cell only. This is shown in Fig. 2.9. Examples for triclinic crystal system are  $K_2Cr_2O_7$ ,  $CuSO_4 \cdot 5H_2O$ , etc.

Figure 2.9 Triclinic crystal system



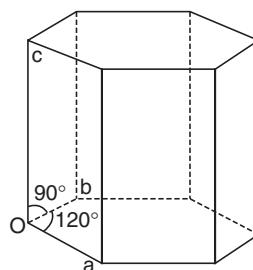
**6. Rhombohedral [Trigonal] crystal system:** In this crystal system, all the lengths of unit cell edges are equal. The angles between the axes are equal but other than  $90^\circ$  i.e.,  $a = b = c$  and  $\alpha = \beta = \gamma \neq 90^\circ$ . The Bravais lattice is simple only as shown in Fig. 2.10. Examples for Rhombohedral crystal system are As, Bi, Sb, etc.

Figure 2.10 Rhombohedral crystal system



**7. Hexagonal crystal system:** In this crystal system, two sides of the unit cell edge lengths are equal and the angle between these edges is  $120^\circ$ . These two edges are perpendicular to the third edge, and not equal in length i.e.,  $a = b \neq c$  and  $\alpha = \beta = 90^\circ$ ;  $\gamma = 120^\circ$ . The Bravais lattice is primitive only. This is shown in Fig. 2.11. The atoms in this crystal system are arranged in the form of a hexagonal close pack. This is dealt with in more detail in Appendix A.

Figure 2.11 Hexagonal crystal system



The 14 Bravais lattices of 7 crystal systems are shown in the table below.

Sl. No	Crystal System	Types of Bravais Lattices	No. of Bravais Lattices	Relation between Lengths and Angles
1	Cubic	P, I, F	3	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
2	Tetragonal	P, I	2	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
3	Orthorhombic	P, I, F, C	4	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
4	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$
5	Triclinic	P	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
6	Rhombohedral (Trigonal)	P	1	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$
7	Hexagonal	P	1	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

## 2.6 Structure and packing fractions of simple cubic [SC] structure

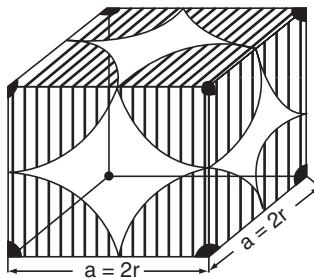
The unit cell edge lengths of this structure along the crystallographic axes and interaxial angles are equal [i.e.,  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$ ]. Atoms are present only at the corners of this unit cell. A corner atom is shared by eight unit cells, so that the contribution of a corner atom to a unit cell is  $1/8$ . The cube has eight corners, hence the contribution of eight corner atoms to a unit cell or the number of atoms per unit cell  $= \frac{1}{8} \times 8 = 1$ . Let ' $r$ ' be the radius of an atom. The surfaces of the atoms touch along the cube edges. So, the distance between the centres of two neighbouring atoms or the nearest neighbour distance ( $2r$ ) is equal to the lattice constant ' $a$ '. In simple cubic cell, the number of nearest neighbour atoms to an atom or co-ordination number is six. Since atoms are present at a distance of ' $a$ ' along  $\pm X$ ,  $\pm Y$  and  $\pm Z$  directions. The number of nearest equidistant neighbouring atoms to an atom in the structure is called co-ordination number. Figure. 2.12 shows the simple cubic structure. Next, we find the fraction of the unit cell volume occupied by the atoms. The simple cubic structure contains only one atom per unit cell.

$$\text{The volume occupied by atoms in the unit cell } (v) = 1 \times \frac{4}{3} \pi r^3 \text{ and}$$

$$\text{The volume of unit cell } (V) = a^3. \text{ Hence, the packing factor or density of packing in the unit cell } (\text{PF}) = \frac{v}{V}$$

$$= \frac{\frac{4}{3} \pi r^3}{a^3} = \frac{4}{3} \frac{\pi r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 \text{ or } 52\%$$

**Figure 2.12 Simple cubic structure**

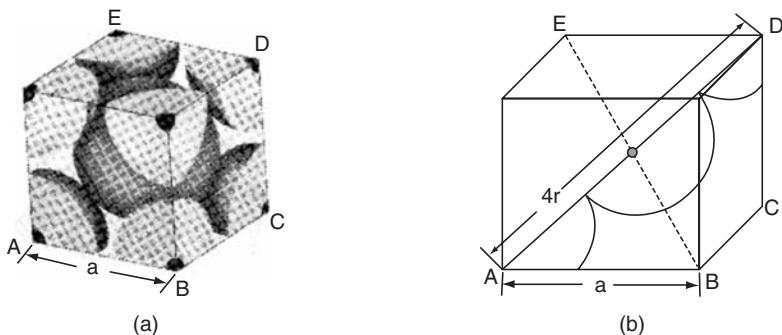


Atomic packing factor is defined as the fraction of the space occupied by atoms in the unit cell or it is the ratio of the volume occupied by atoms in the unit cell to the unit cell volume. An example for simple cubic structure is polonium crystal.

## 2.7 Structure and packing fractions of body-centred cubic structure [BCC]

For this unit cell, atoms are present at the corners of the cube and one atom is completely present at the centre of the unit cell. The centre of the unit cell is defined as the intersecting point of two body diagonals [AD and BE as shown in Fig. 2.13]. A corner atom is shared by eight unit cells so that the contribution of a corner atom to a unit cell is  $1/8$ . Therefore, the number of atoms per unit cell  $= (1/8) \times 8 + 1 = 2$ . The centre atom is surrounded by eight corner atoms, so the coordination number is 8. The surfaces of unit cell corner atoms may not touch, but they are in contact with the centre atom i.e., the surfaces of atoms are in contact along a body diagonal of the unit cell. Half the distance between the centres of a corner atom and central atom is equal to the radius ( $r$ ) of an atom. The relation between unit cell edge length ( $a$ ) and radius ( $r$ ) of an atom can be obtained with reference to Fig. 2.13(b).

**Figure 2.13 Body-centred cubic structure**



The length of the body diagonal AD =  $4r$

$$\therefore AD^2 = AC^2 + CD^2 = AB^2 + BC^2 + CD^2 = a^2 + a^2 + a^2 = 3a^2$$

$$(4r)^2 = 3a^2$$

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

$$(\text{or}) \quad a = \frac{4}{\sqrt{3}}r$$

$$\text{Lastly, Packing factor (PF)} = \frac{\text{volume of all atoms in unit cell}}{\text{volume of unit cell}} = \frac{v}{V}$$

$$\begin{aligned} &= \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{8\pi r^3}{3a^3} = \frac{8\pi r^3 3\sqrt{3}}{3(4r)^3} \\ &= \frac{\sqrt{3}\pi}{8} = 0.68 \text{ or } 68\%. \end{aligned}$$

The elements like tungsten, chromium, sodium, potassium, etc. possess bcc structure.

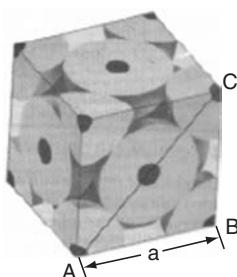
## 2.8 Structure and packing fractions of face-centred cubic [FCC] structure

Atoms are present at the corners and at the face centres of this cubic structure. The intersection of face diagonals represent face centre of the cube. A corner atom is shared by eight unit cells and a face-centred atom is shared by two unit cells. The cube has eight corners and bounded by six faces; so, the number of atoms per unit cell =  $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$ .

Let  $r$  be the radius of an atom. The surfaces of atoms do not touch along unit cell edges but the surfaces of atoms along face diagonals of this structure are in contact. The unit cell structure is shown in Fig. 2.14. Half of the nearest neighbour distance along the face diagonal is equal to radius of an atom.

The relation between the radius of an atom and unit cell edge length of a unit cell can be obtained with reference to Fig. 2.14.

**Figure 2.14** FCC structure



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

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

$$4r = \sqrt{2}a \quad \text{or} \quad a = 2\sqrt{2}r$$

The co-ordination number is 12, and this can be explained in following way:

A face-centred atom of the cubic structure is surrounded by four corner atoms of the face of a unit cell, four surrounding face-centred atoms of the unit cell and four surrounding face-centred atoms of the adjacent unit cell. Therefore, the co-ordination number is 12. The packing factor PF of the unit cell:

$$= \frac{\text{volume occupied by all the atoms in a unit cell}}{\text{unit cell volume}}$$

$$= \frac{v}{V} = \frac{4 \times \frac{4}{3}\pi r^3}{a^3} = \frac{16\pi r^3}{3(2\sqrt{2}r)^3}$$

$$= \frac{16\pi r^3}{3 \times 8 \times 2\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ or } 74\%$$

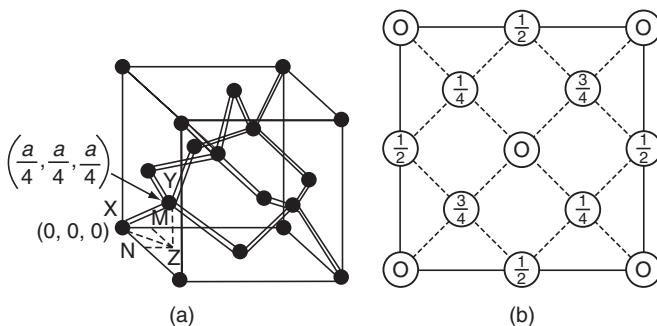
The packing factor of FCC structure is 74%. Examples for this structure are Cu, Ag, Al, etc.

## 2.9 Diamond cubic structure

The structure of diamond crystal unit cell is considered as the interpenetration of two FCC carbon unit cells along their body diagonals by a distance of  $\frac{1}{4}$ th the diagonal length. The origin of one unit cell is at (000) and the origin of another unit cell is at  $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$ . The diamond lattice structure and the projection of lattice points on bottom face of the cube are shown in Fig. 2.15. The fractions denote height of lattice points above the bottom face, in terms of cube edge.

**Figure 2.15**

(a) Diamond lattice structure; (b) Projection of diamond lattice points on bottom face



In diamond, each carbon atom is bonded covalently with other surrounding four carbon atoms so that the number of nearest neighbours or the co-ordination number is four. The surfaces of diamond unit cell corner and nearest diagonal atoms touch, half the distance of a corner and the nearest diagonal atom distance is equal to radius of the atom. The relation between radius of an atom and unit cell edge length ' $a$ ' can be given with reference to Fig. 2.15(a).  $XY = 2r$ .

$$(XY)^2 = (XZ)^2 + (ZY)^2 = (XN)^2 + (NZ)^2 + (ZY)^2$$

$$(2r)^2 = \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 = 3\left(\frac{a}{4}\right)^2$$

$$2r = \sqrt{3} \frac{a}{4} \quad (\text{or}) \quad a = \frac{8r}{\sqrt{3}}$$

The number of atoms in the unit cell can be estimated in the following way: Atoms are present at 8 corners of the cube, at 6 face centres of the cube and 4 atoms are completely present in the unit cell along the body diagonal at a distance of 1/4th diagonal distance from the face diagonal opposite atoms of the bottom face and the other two corners from the top face into the cube. Therefore, the total number of atoms per unit cell =  $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 = 8$  .

$$\text{Finally, PF} = \frac{\text{volume occupied by all atoms of the unit cell } (v)}{\text{volume of unit cell } (V)}$$

$$= \frac{8 \times \frac{4}{3} \pi r^3}{a^3} = \frac{32}{3} \frac{\pi r^3}{\left(\frac{8r}{\sqrt{3}}\right)^3} = \frac{32\pi r^3 3\sqrt{3}}{3 \times 8 \times 8 \times 8r^3}$$

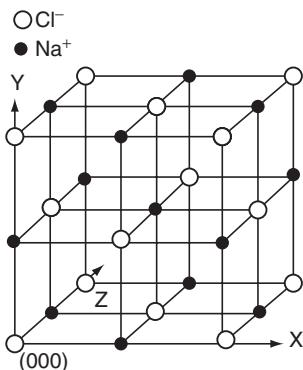
$$\frac{\pi\sqrt{3}}{16} = 0.34 \text{ or } 34\%.$$

This is a loosely packed structure; C, Ge and Si crystallize in this form.

## 2.10 NaCl crystal structure

The Bravais lattice of NaCl crystal is a face-centred cube as shown in Fig. 2.16. NaCl is an ionic crystal. It consists of two FCC sub-lattices, one of  $\text{Cl}^-$  ions having origin at (000) and the other of  $\text{Na}^+$  ion having origin at one half of the body diagonal of the unit cell. The  $\text{Na}^+$  and  $\text{Cl}^-$  ions are present at equilibrium distances in the crystal. The attractive force between  $\text{Na}^+$  or  $\text{Cl}^-$  ions in the crystal is balanced by the repulsive forces between them due to same type of charges. In this crystal, either  $\text{Na}^+$  or  $\text{Cl}^-$  ions could occupy the corner and face-centre positions with the ions of the opposite type occupying the alternate positions in between them. Each ion is surrounded by six other type ions so that the co-ordination number is six. There are 12 next nearest neighbours of the same kind as the reference ion. If  $\text{Cl}^-$  ions occupy corners of the unit cell, one corner is taken as the origin and the co-ordinates of ions are expressed in fractions of the edge length of the cube. The co-ordinates of  $\text{Cl}^-$  ions are  $000, \frac{1}{2}0\frac{1}{2}, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}\frac{1}{2}0$ . In the same coordinate system, the co-ordinates of the four  $\text{Na}^+$  ions are  $\frac{1}{2}\frac{1}{2}\frac{1}{2}, \frac{1}{2}00, 0\frac{1}{2}0, 00\frac{1}{2}$ .

**Figure 2.16** NaCl lattice structure



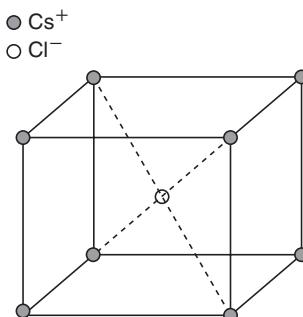
The unit cell of NaCl crystal contains four sodium and four chlorine ions. Therefore, the unit cell contains four NaCl molecules. The other crystals, which show this type of structure, are KCl, KBr, MgO, AgBr, etc.

## 2.11 Caesium chloride [CsCl] structure

The Bravais lattice of CsCl is a simple cube. It is an ionic compound. It is considered as the interpenetration of two simple cubic lattices of caesium and chlorine ions along half the body diagonal of a unit cell. The relative positions of the two cube systems are such that, each ion of one type occupies the centre of the cube formed by ions of the other type and vice versa. If caesium ion is present at the origin (000), then chlorine ion is present at the centre point  $\left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right)$  of the cube as shown in Fig. 2.17. The co-ordinates of caesium ions are

000, 100, 010, 001, 011, 101, 110 and 111. In this unit cell, each kind of ion is surrounded by eight other kinds of ions so that the co-ordination number is 8. The unit cell contains one CsCl molecule. Other examples of this type of structure are RbCl, LiHg, CuZn (brass), AgMg and AlNi.

**Figure 2.17** Caesium chloride structure



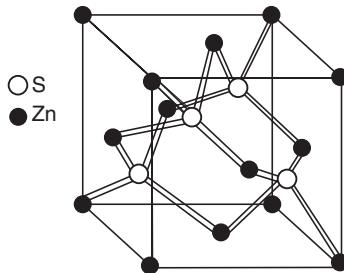
## 2.12 Zinc sulphide [ZnS] structure

This is an ionic compound. This structure consists of two different types of atoms. The Bravais lattice of ZnS is a face-centred cube. The crystal structure of ZnS is considered as the interpenetration of two FCC sub-lattices along the body diagonal such that the origin of one sub-lattice is at a distance of 1/4th the body diagonal from the origin along the body diagonal. One sub-lattice contains Zn atoms and other sub-lattice contains S atoms. The ZnS crystal structure is similar to diamond crystal structure. The unit cell contains four ZnS molecules. Each atom is surrounded by four other kind of atoms at the corners of a regular tetrahedron.

The co-ordinates of S atom is  $\frac{1}{4} \frac{1}{4} \frac{1}{4}$  and that of Zn atoms co-ordinates are  $000, \frac{1}{2} 0 \frac{1}{2}, \frac{1}{2} \frac{1}{2} 0$  and  $0 \frac{1}{2} \frac{1}{2}$ .

Other examples of this structure are CdS, InSb, CaCl, GaAs, GaP, etc.

**Figure 2.18 ZnS Crystal Structure**



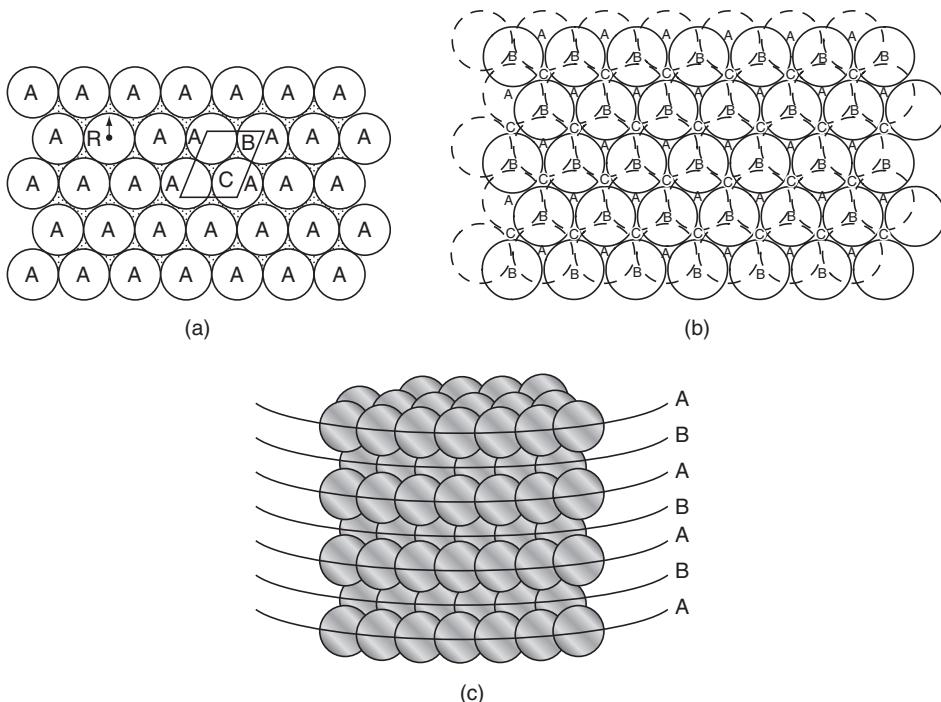
## 2.13 Stacking sequence in metallic crystals

To minimize the potential energy of a metallic crystal, the atoms in it are very closely packed. A close packing is a way of arranging equidimensional objects in space so that the available space is filled very effectively. In metallic crystals, the atoms are assumed to be hard, incompressible spheres. If we have equal-sized spheres, then a closest packing of like spheres is that the arrangement in which each sphere to form an intimate contact with a large number of its neighbours, occupying the available space most efficiently.

A closest packed layer of equal-sized atoms is shown in Fig. 2.19(a), the sites of atoms are represented as 'A', each sphere has six nearest neighbours in a closest packed layer and 12 nearest neighbours in three-dimensional closest packing. As shown in Fig. 2.19, each row of atoms is placed in the space between the adjacent atoms of upper and lower rows such that the surfaces of atoms are in contact. This layer of atoms has several interesting features: (a) each sphere is surrounded by six spheres, (b) each sphere is surrounded by six voids and (c) each void is surrounded by three spheres. As shown in Fig. 2.19(a), on an average two triangular voids belong to each sphere. The apex of one triangular void is pointing up and the other triangular void apex is pointing down. To distinguish the two kinds of voids, they are labelled as B and C, respectively.

As shown in Fig. 2.19(b), if the spheres (atoms) in a hexagonal closest packed layer are all moved from their original sites i.e., from 'A' to new sites 'B', another hexagonal closest packed layer results. Similarly, if all the 'C' sites are occupied by equal spheres, another hexagonal closest packed layer is again obtained. It is obvious that in the stacking of layers to form a closest packing, a hexagonal closest packed layer can occupy only the sites A or B or C. If a layer is named as A, B or C accordingly as the spheres in that layer occupy A, B or C sites, then a two-fold choice exists in placing one hexagonal closest packed layer one above the other. If the

**Figure 2.19** A two-dimensional closest packed layer of atoms



first layer be an 'A' layer, then the next layer can be either a 'B' layer or a 'C' layer; say that it is a 'B' layer. The next layer above can now be either an 'A' layer or a 'C' layer and so forth. So, the stacking sequence of hexagonal closest packed layers can be designated by representing the layers in a sequence by the letters A, B and C.

In stacking successive layers, a finite translation period normal to the layers is limited. The hexagonal closest packing contains the simple two different layers stacking in the sequence ... ABAB ... as shown in Fig. 2.19(c) and the cubic closest packing consisting of three different layers stacked in the sequence ... ABC ABC ... .

## 2.14 Calculation of lattice constant

The unit cell edge length of a cubic system is calculated using the density of the crystal. Let 'a' be the edge length (or primitive) of a cubic unit cell and 'ρ' be the density of the crystal.

$$\text{The mass of the unit cell} = \rho a^3 \quad (2.1)$$

Let 'M' be the molecular weight and  $N_A$  be the Avogadro number (i.e., number of molecules per kg mole of the substance) of the crystal.

$$\text{Then, mass of each molecule} = \frac{M}{N_A}$$

If each unit cell contains  $n$  molecules (or lattice points),

$$\text{Then the mass of unit cell} = n \frac{M}{N_A} \quad (2.2)$$

From Equation (2.1) and (2.2), we have:

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

$$a^3 = \frac{nM}{\rho N_A} \quad \text{or} \quad a = \left( \frac{nM}{\rho N_A} \right)^{1/3}$$

## Solved Problems

---

1. Chromium has BCC structure. Its atomic radius is 0.1249 nm. Calculate the free volume/unit cell.

(Set-4-May 2007), (Set-4-Sept. 2006)

**Sol:** Given data are

Atomic radius of chromium,  $r = 0.1249 \text{ nm}$ .

Free volume/unit cell = ?

If ' $a$ ' is the BCC unit cell edge length, then the relation between ' $a$ ' and ' $r$ ' is

$$a = \frac{4}{\sqrt{3}}r = \frac{4}{\sqrt{3}} \times 0.1249 \text{ nm}$$

$$= 0.28845 \text{ nm}.$$

$$\text{Volume of unit cell, } V = a^3 = (0.28845)^3 \text{ nm}^3$$

$$= 0.024 \text{ nm}^3$$

Number of atoms in BCC unit cell = 2

$$\text{Hence volume of atoms in unit cell, } v = \frac{4}{3}\pi r^3 \times 2 = 0.01633 \text{ nm}^3$$

$$\text{Free volume/unit cell} = V - v = 0.00767 \text{ nm}^3$$

2. Lithium crystallizes in BCC structure. Calculate the lattice constant, given that the atomic weight and density for lithium are 6.94 and  $530 \text{ kg/m}^3$  respectively.

(Set-4-Nov. 2003)

**Sol:** Lithium crystallizes in BCC structure, so the number of atoms per unit cell,  $n = 2$

Atomic weight,  $M = 6.94$

Density,  $\rho = 530 \text{ Kg/m}^3$

Lattice constant,  $a = ?$

$$a^3 = \frac{nM}{\rho N_A}, \text{ where } N_A = \text{Avogadro's number}$$

$$a^3 = \frac{2 \times 6.94}{530 \times 6.02 \times 10^{26}}$$

$$= 43.50 \times 10^{-30}$$

$$\therefore a = 3.517 \times 10^{-10} \text{ m}$$

$$= 3.517 \text{ \AA}$$

3. Iron crystallizes in BCC structure. Calculate the lattice constant, given that the atomic weight and density of iron are 55.85 and 7860 kg/m<sup>3</sup>, respectively.

(Set-3–Sept. 2006), (Set-1–Nov. 2003)

**Sol:** Atomic weight of iron,  $M = 55.85$

Density of iron,  $\rho = 7860 \text{ kg/m}^3$

Find lattice constant,  $a$  in BCC iron

Number of atoms in BCC unit cell,  $n = 2$

We know that:

$$a = \left( \frac{nM}{\rho N_A} \right)^{1/3}$$

$$\left[ \frac{2 \times 55.85}{7860 \times 6.02 \times 10^{26}} \right]^{1/3} = 2.87 \times 10^{-10} \text{ m} = 2.87 \text{ \AA}$$

4. If the edge of the unit cell of a cube in the diamond structure is 0.356 nm, calculate the number of atoms/m<sup>3</sup>.

(Set-3–Nov. 2003)

**Sol:** The lattice constant of diamond,  $a = 0.356 \text{ nm} = 0.356 \times 10^{-9} \text{ m}$

The number of carbon atoms per unit cell,  $n = 8$

$$\text{The number of unit cells in } 1 \text{ m}^3 = \frac{1 \text{ m}^3}{a^3}$$

$$\text{and the number of atoms per } \text{m}^3 = \frac{1 \text{ m}^3}{a^3} \times 8 = \frac{1 \text{ m}^3 \times 8}{(0.356 \times 10^{-9} \text{ m})^3}$$

$$= \frac{8 \times 10^{27}}{(0.356)^3} = 177.3 \times 10^{27} \text{ atoms/m}^3$$

5. A metal in BCC structure has a lattice constant 3.5 \AA. Calculate the number of atoms per sq. mm area in the (200) plane.

**Sol:** Lattice constant,  $a = 3.5 \text{ \AA}$

The (200) plane is perpendicular to X-axis and passes through the centre of the unit cell. So, this plane contains only the central atom.

$$\therefore \text{The area per atom} = a^2 = 3.57 \text{ \AA} \times 3.5 \text{ \AA} = 12.25 \text{ \AA}^2$$

$$\text{Number of atoms per sq. mm} = \frac{1 \text{ mm} \times 1 \text{ mm}}{12.25 \text{ \AA}^2}$$

$$= \frac{10^7 \text{ \AA} \times 10^7 \text{ \AA}}{12.25 \text{ \AA}^2} = 8.16 \times 10^{12} \quad [\text{since } 1 \text{ mm} = 10^7 \text{ \AA}]$$

6. Germanium crystallizes in diamond (form) structures with 8 atoms per unit cell. If the lattice constant is 5.62 Å, calculate its density.

**Sol:** Number of atoms per unit cell,  $n = 8$

Lattice constant,  $a = 5.62 \text{ \AA} = 5.62 \times 10^{-10} \text{ m}$

Atomic weight of Ge,  $M = 72.59$

Density,  $\rho = ?$

We know that  $a^3 = \frac{nM}{\rho N_A}$ , where  $N_A$  = Avogadro's number

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

$$= \frac{8 \times 72.59}{[5.62 \times 10^{-10}]^3 \times 6.02 \times 10^{26}} \text{ Kg/m}^3$$

$$= 5434.5 \text{ kg/m}^3.$$

## Multiple Choice Questions

8. Tetragonal crystal system is represented by ( )
- |  |   |   |   |
|--|---|---|---|
| (a) $a = b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$ | (b) $a \neq b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$ | (c) $a \neq b = c$<br>$\alpha = \beta = \gamma \neq 90^\circ$ | (d) $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ |
|--|---|---|---|
9. Monoclinic crystal system is represented by ( )
- |  |  |   |  |
|--|--|---|--|
| (a) $a \neq b \neq c$<br>$\alpha \neq \beta \neq \gamma \neq 90^\circ$ | (b) $a \neq b \neq c$<br>$\alpha = \gamma = 90^\circ$<br>$\beta \neq 90^\circ$ | (c) $a = b = c$<br>$\alpha = \gamma = 90^\circ$<br>$\beta = 90^\circ$ | (d) $a \neq b = c$<br>$\alpha = \gamma = 90^\circ$<br>$\beta = 90^\circ$ |
|--|--|---|--|
10. Triclinic crystal system is represented by ( )
- |  |   |   |  |
|--|---|---|--|
| (a) $a \neq b \neq c$<br>$\alpha \neq \beta \neq \gamma \neq 90^\circ$ | (b) $a \neq b = c$<br>$\alpha \neq \beta \neq \gamma \neq 90^\circ$ | (c) $a = b \neq c$<br>$\alpha \neq \beta \neq \gamma \neq 90^\circ$ | (d) $a \neq b \neq c$<br>$\alpha = \beta = \gamma \neq 90^\circ$ |
|--|---|---|--|
11. Rhombohedral [Trigonal] system is represented by ( )
- |  |  |  |   |
|--|--|--|---|
| (a) $a = b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$ | (b) $a = b = c$<br>$\alpha = \beta = \gamma \neq 90^\circ$ | (c) $a = b = c$<br>$\alpha = \beta \neq \gamma = 90^\circ$ | (d) $a \neq b = c$<br>$\alpha = \beta = \gamma \neq 90^\circ$ |
|--|--|--|---|
12. Hexagonal crystal system is represented by ( )
- |  |  |   |   |
|--|--|---|---|
| (a) $a = b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$ | (b) $a = b = c$<br>$\alpha = \beta = 90^\circ$<br>$\gamma = 120^\circ$ | (c) $a = b \neq c$<br>$\alpha = \beta = 90^\circ$<br>$\gamma = 120^\circ$ | (d) $a = b \neq c$<br>$\alpha = \beta = 120^\circ$<br>$\gamma = 90^\circ$ |
|--|--|---|---|
13. The number of atoms per unit cell of BCC structure is: \_\_\_\_\_ ( )
- |       |       |       |       |
|-------|-------|-------|-------|
| (a) 1 | (b) 2 | (c) 3 | (d) 4 |
|-------|-------|-------|-------|
14. In body-centred cubic structure, the length of unit cell edge interms of radius of atom ( $r$ ) is: ( )
- |                    |                           |                           |                           |
|--------------------|---------------------------|---------------------------|---------------------------|
| (a) $\frac{4}{3}r$ | (b) $\frac{4}{\sqrt{3}}r$ | (c) $\frac{\sqrt{4}}{3}r$ | (d) $\frac{4}{3}\sqrt{r}$ |
|--------------------|---------------------------|---------------------------|---------------------------|
15. The packing factor of BCC structure is: \_\_\_\_\_ % ( )
- |        |        |        |        |
|--------|--------|--------|--------|
| (a) 68 | (b) 52 | (c) 74 | (d) 46 |
|--------|--------|--------|--------|
16. The packing factor of face-centred cubic structure is: \_\_\_\_\_ % ( )
- |        |        |        |        |
|--------|--------|--------|--------|
| (a) 68 | (b) 52 | (c) 74 | (d) 46 |
|--------|--------|--------|--------|
17. The total number of atoms per unit cell of diamond is: ( )
- |       |       |       |       |
|-------|-------|-------|-------|
| (a) 2 | (b) 4 | (c) 6 | (d) 8 |
|-------|-------|-------|-------|
18. The unit cell of NaCl contains \_\_\_\_\_ number of NaCl molecules ( )
- |       |       |       |       |
|-------|-------|-------|-------|
| (a) 2 | (b) 4 | (c) 6 | (d) 8 |
|-------|-------|-------|-------|
19. The Bravais lattice of ZnS is: ( )
- |                        |                        |
|------------------------|------------------------|
| (a) simple cubic       | (b) body-centred cubic |
| (c) face-centred cubic | (d) none               |
20. When the periodicity of atoms or molecules is extended throughout the solid, then it is known as \_\_\_\_\_ solid. ( )
- |                        |                     |
|------------------------|---------------------|
| (a) single crystalline | (b) polycrystalline |
| (c) amorphous          | (d) none            |

21. If the periodicity of atoms or molecules is extended in large number of small regions of different sizes in the solid, then it is known as: ( )
- (a) single crystalline solid
  - (b) polycrystalline solid
  - (c) amorphous solid
  - (d) none
22. The study of geometric form and other physical properties of crystalline solids by using X-rays, electron beam and neutron beam constitute: ( )
- (a) spectroscopy
  - (b) physiotherapy
  - (c) crystallography
  - (d) none
23. If an atom or a unit of atoms in a crystal is replaced by a point in space, then it results points in space is called: ( )
- (a) space lattice
  - (b) crystal symmetry
  - (c) spectrum
  - (d) diffraction
24. If the surroundings of each lattice point is the same or the lattice points are identical, then such a lattice is called: ( )
- (a) Bravais lattice
  - (b) space lattice
  - (c) Braggs lattice
  - (d) none
25. The arrangement of atoms in a crystal is called: ( )
- (a) lattice
  - (b) crystal structure
  - (c) crystal symmetry
  - (d) none
26. The number of Bravais lattices in cubic crystal system is: ( )
- (a) one
  - (b) two
  - (c) three
  - (d) four
27. The number of Bravais lattices in orthorhombic crystal system is ( )
- (a) one
  - (b) two
  - (c) three
  - (d) four
28. The number of Bravais lattices in tetragonal and monoclinic systems is ( )
- (a) equal
  - (b) unequal
  - (c) both a and b
  - (d) none
29. The packing factor of simple cubic structure is ( )
- (a) 68%
  - (b) 74%
  - (c) 52%
  - (d) 34%
30. If the number of lattice points per unit cell is one, then it is called \_\_\_\_\_ unit cell ( )
- (a) primitive
  - (b) non-primitive
  - (c) both a and b
  - (d) none
31. The number of atoms per unit cell of face-centred cubic structure is: ( )
- (a) one
  - (b) two
  - (c) three
  - (d) four
32. The structure of diamond crystal unit cell is considered as the interpenetration of \_\_\_\_\_ carbon unit cells along their body diagonal. ( )
- (a) two FCC
  - (b) two SC
  - (c) two BCC
  - (d) none
33. The diamond unit cell is a \_\_\_\_\_ structure. ( )
- (a) BCC
  - (b) FCC
  - (c) SC
  - (d) none
34. The packing factor of diamond is \_\_\_\_\_ %, so this is a loosely packed structure. ( )
- (a) 32
  - (b) 24
  - (c) 34
  - (d) 52

35. The Bravais lattice of NaCl crystal is a: ( )  
 (a) FCC                    (b) BCC                    (c) SC                    (d) none
36. The Bravais lattice of CsCl is a: ( )  
 (a) BCC                    (b) SC                    (c) FCC                    (d) none

## Answers

1. a	2. c	3. a	4. b	5. c	6. c	7. b	8. a	9. b	10. a
11. b	12. c	13. b	14. b	15. a	16. c	17. d	18. b	19. c	20. a
21. b	22. c	23. a	24. a	25. b	26. c	27. d	28. a	29. c	30. a
31. d	32. a	33. b	34. c	35. a	36. b				

## Review Questions

1. Show that FCC is the most closely packed of the three cubic structures by working out the packing factors.  
 (Set-1, Set-3–May 2007), (Set-3–Sept. 2007), (Set-2–June 2005), (Set-3–Nov. 2004), (Set-4–May 2004)
2. Describe the structure of NaCl.  
 (Set-1, Set-3–May 2007), (Set-3–Sept. 2007), (Set-2–June 2005),  
 (Set-3–Nov. 2004), (Set-4–May 2004), (Set-4–May 2003)
3. Explain the terms: (i) basis (ii) space lattice and (iii) unit cell.  
 (Set-4–May 2006), (Set-1–Sept. 2007), (Set-1, Set-2–June. 2005), (Set-1–Nov. 2004), (Set-3–May 2003)
4. Describe seven crystal systems with diagrams.  
 (Set-1–Sept. 2007), (Set-4–May 2007), (Set-4–May 2006), (Set-4–Sept. 2006),  
 (Set-1, Set-2–June 2005), (Set-1–Nov. 2004), (Set-3–May 2003)
5. Obtain the relations between the edge of the unit cell and atomic radius for the BCC and FCC lattices.  
 (Set-4–Nov. 2003)
6. What are Bravais lattices? (Set-3–Sept. 2006), (Set-1–Nov. 2003)
7. Deduce packing factors for simple cubic and BCC structures. (Set-3–Sept. 2006), (Set-1–Nov. 2003)
8. Define co-ordination number and packing factor of a crystal.  
 (Set-1–Sept. 2008), (Set-1, Set-3–May 2007), (Set-2–Sept. 2006), (Set-2–Nov. 2003)
9. Describe FCC crystal structure.  
 (Set-2–Sept. 2006), (Set-1, Set-3–May 2006), (Set-2–Nov. 2003)
10. Obtain an expression for the packing factor of FCC structure.  
 (Set-1–Sept. 2008), (Set-2–Sept. 2006), (Set-1, Set-3–May 2006), (Set-2–Nov. 2003)
11. Explain the crystal structure of diamond with a two-dimensional diagram. (Set-3–Nov. 2003)
12. What is packing fraction? Calculate the packing fraction for a BCC lattice. (Set-3–Nov. 2003)
13. Describe the crystal structure of ZnS. (Set-4–Nov. 2003)
14. Define crystal lattice, unit cell, lattice parameter and coordination number.  
 (Set-1–May 2007), (Set-1–Sept. 2006)
15. Explain the unit cell and lattice parameters. What is a primitive cell and how does it differ from unit cell.  
 (Set-4–May 2007), (Set-4–Sept. 2006)

16. Describe the crystal structure of CsCl. (Set-4–May 2007), (Set-4–Sept. 2006)
17. Consider a body centred cubic lattice of identical atoms having radius ‘R’ compute (i) the number of atoms per unit cell (ii) The coordination number and (iii) the packing fraction (Set-1–Sept. 2006), (Set-1–May 2007)
18. Explain the terms: (i) basis, (ii) space lattice, (iii) lattice parameters and (iv) unit cell. (Set-3–Sept. 2008)
19. Describe BCC structure, with suitable example. (Set-1–Sept. 2008)
20. Describe in detail, the seven crystal systems with diagrams. (Set-4–Sept. 2008)
21. Prove that which type of the cubic crystal structure has closest packing of atoms. Describe the relation between the atomic radius and the unit cell dimension of the crystal, mentioned above. (Set-2–Sept. 2007)
22. Tabulate the characteristics of the unit cells of different crystal systems.
23. Illustrate Bravais lattices.
24. Describe the crystal structures of diamond and sodium chloride.
25. Illustrate simple cubic, FCC and BCC crystal structures.
26. What is space lattice? Find the packing fraction for BCC and FCC crystals.
27. Describe in detail the structure of diamond.
28. Explain various types of bondings in solids with suitable examples.
29. Show that FCC crystals are closely packed than BCC crystals.
30. Classify various lattice types in the crystal system.
31. Describe in detail the structure of ZnS.
32. What is a Bravais lattice? What are the different space lattices in the cubic system?



## C H A P T E R

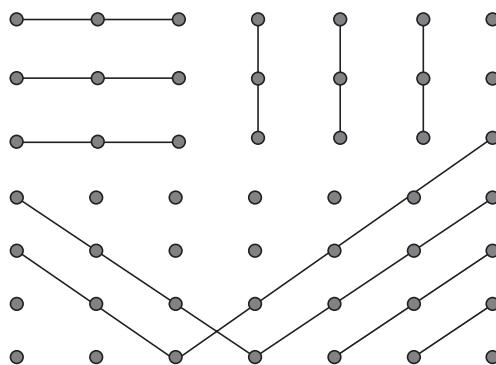
# 3

## Crystal Planes, X-ray Diffraction and Defects in Solids

### 3.1 Crystal planes, directions and Miller indices

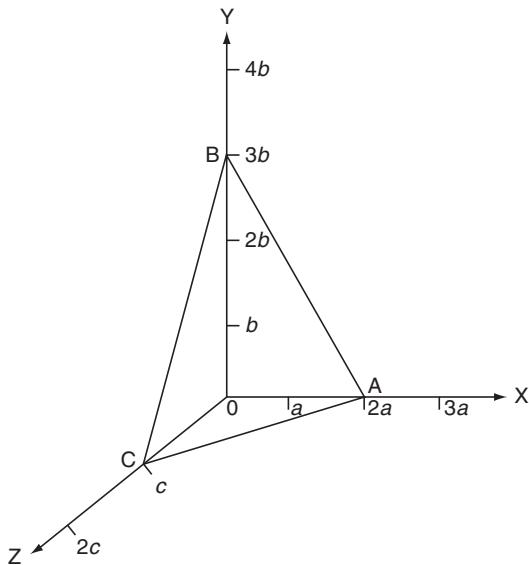
Crystal planes are defined as some imaginary planes inside a crystal in which large concentration of atoms are present. Inside the crystal, there exists certain directions along which large concentration of atoms exists. These directions are called crystal directions. Figure 3.1 shows a two-dimensional lattice with different orientations of crystal planes.

**Figure 3.1** A two-dimensional lattice with crystal planes



Crystal planes and directions can be represented by a set of three small integers called Miller indices [because Miller derived a method of representing crystal planes]. These integers are represented in general as  $b$ ,  $k$  and  $l$ . If these integers are enclosed in round brackets as  $(bkl)$ , then it represents a plane. On the other hand, if they are enclosed in square brackets as  $[bkl]$ , then it represents crystal direction perpendicular to the above-said plane. Next, we will see the way of obtaining Miller indices for a plane.

Figure 3.2 Miller indices for a plane ABC



- (i) As shown in Fig. 3.2, take a lattice point as origin '0' of crystallographic axes X, Y and Z in a space lattice. The unit cell translational distances or lattice constants along X, Y and Z directions are  $a$ ,  $b$  and  $c$ , respectively. Let a crystal plane ABC intersect these three axes at  $2a$ ,  $3b$  and  $c$ . In general, the intercepts can be represented as  $pa$ ,  $qb$ , and  $rc$ .
- (ii) Divide these intercepts with lattice points translational distances along the axes to obtain intercepts of the plane in terms of multiples of unit cell translational lengths.

$$\text{i.e., } \frac{2a}{a}, \frac{3b}{b}, \frac{c}{c}$$

2, 3, 1

$$\text{in general } \frac{pa}{a}, \frac{qb}{b}, \frac{rc}{c}$$

$p, q, r$

(iii) Take the reciprocals of these multiples, they are  $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$ ; in general  $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$

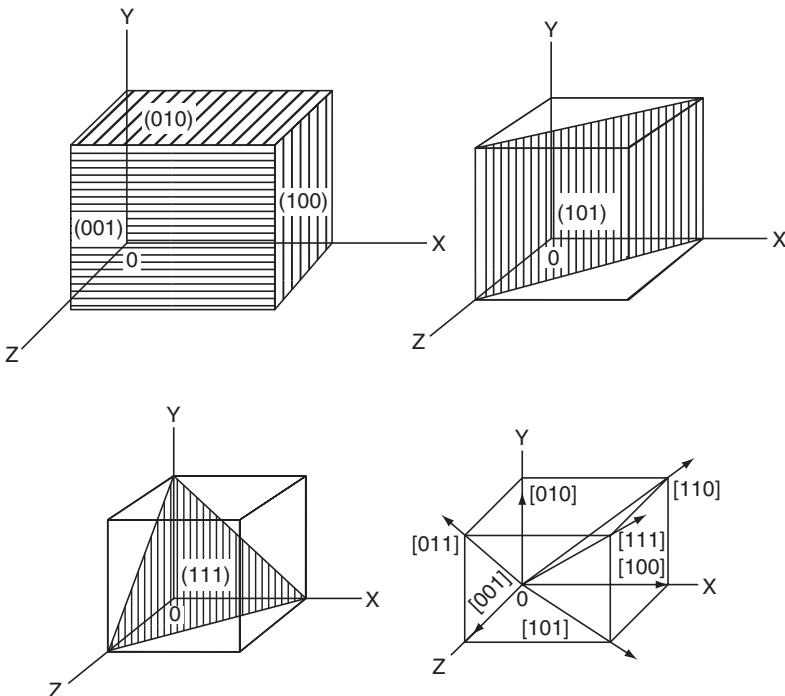
(iv) Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.

$$\frac{1}{2} \times 6, \frac{1}{3} \times 6, \frac{1}{1} \times 6$$

3 2 6

Figure 3.3

Represent some important crystal planes and directions in a cubic crystal



$$\text{in general } \frac{pqr}{p}, \frac{pqr}{q}, \frac{pqr}{r}$$

$$qr \quad pr \quad pq$$

Miller indices of the plane ABC is (326). In general, indices of a plane are represented as  $(hkl) = (qr pr pq)$

$$\text{or } \frac{1}{p} : \frac{1}{q} : \frac{1}{r} = h : k : l$$

Miller indices may be defined as a set of three small integers obtained by clearing the reciprocals of the three intercepts [in terms of multiples of unit cell edges] made by a plane on crystallographic axes.

#### Now, we will see the important features of Miller indices:

- Miller indices represent a set of equidistant parallel planes.
- If the Miller indices of a plane represent some multiples of Miller indices of another plane, then these planes are parallel. For example (844) and (422) or (211) are parallel planes.
- If  $(hkl)$  are the Miller indices of a plane, then the plane divides the lattice constant ' $a$ ' along X-axis into ' $h$ ' equal parts, ' $b$ ' along Y-axis into ' $k$ ' equal parts and ' $c$ ' along Z-axis into ' $l$ ' equal parts.

- (iv) If a plane is parallel to one of the crystallographic axes, then the plane intersects that axis at infinity and the Miller indices along that direction is zero.
- (v) If a plane cuts an axis on the negative side of the origin, then the corresponding index is negative and is indicated by placing a minus sign above the index. For example, if the plane cuts on negative Y-axis, then Miller indices of the plane is  $(h\bar{k}\ell)$ .
- (vi) When Miller indices are enclosed in curly brackets,  $\{hkl\}$ , they refer to planes which in the crystal are equivalent even though their Miller indices may differ. For example in a cubic lattice, all cube faces are equivalent, they are  $(100)$ ,  $(010)$ ,  $(001)$ ,  $(\bar{1}00)$ ,  $(0\bar{1}0)$ ,  $(00\bar{1})$ ; these planes are represented as  $\{100\}$ . Similarly, a full set of equivalent directions in a crystal is represented by a symbol  $\langle hkl \rangle$ . For example, the eight body diagonals of a cube  $[111]$ ,  $[\bar{1}\bar{1}\bar{1}]$ ,  $[\bar{1}\bar{1}1]$ ,  $[1\bar{1}\bar{1}]$ ,  $[1\bar{1}1]$ ,  $[\bar{1}\bar{1}\bar{1}]$ ,  $[11\bar{1}]$ ,  $[\bar{1}\bar{1}\bar{1}]$  are designated as  $\langle 111 \rangle$ .

## 3.2 Distance of separation between successive $hkl$ planes

The separation between successive parallel planes in rectangular axes crystal system can be extracted easily. Let us consider a rectangular [cartesian] coordinate system with origin 'O' at one of the lattice points. Let  $(hkl)$  be the Miller indices of a plane ABC, which makes intercepts OA, OB and OC on X, Y and Z axes, respectively as shown Fig 3.4. A normal to this plane from the origin passes through a point N in the plane ABC, such that  $ON = d_1$ . This normal makes  $\alpha'$ ,  $\beta'$ , and  $\gamma'$  angles with X, Y and Z-axes, respectively. Since the plane segments 'a' into 'b' equal parts, 'b' into 'k' equal parts and 'c' into 'l' equal parts, then the intercepts OA, OB and OC are such that:

$$OA = \frac{a}{b}, \quad OB = \frac{b}{k} \quad \text{and} \quad OC = \frac{c}{l} \quad (3.1)$$

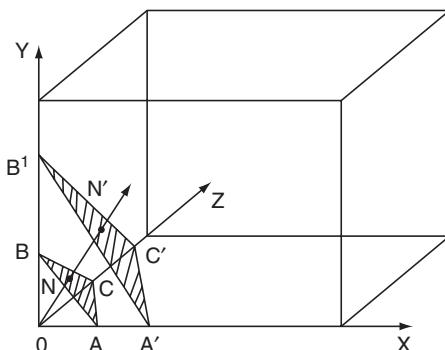
where  $a$ ,  $b$ ,  $c$  are the unit cell edge lengths along X, Y and Z-axes, respectively.

From Fig. 3.4

$$\cos \alpha' = \frac{d_1}{OA}, \quad \cos \beta' = \frac{d_1}{OB} \quad \text{and} \quad \cos \gamma' = \frac{d_1}{OC} \quad (3.2)$$

Let the coordinates of  $N$  be  $x$ ,  $y$  and  $z$  along X, Y and Z axes, then:

**Figure 3.4 Orthorhombic crystal**



$$(\text{ON})^2 = d_1^2 = x^2 + y^2 + z^2 \quad \dots \quad (3.3)$$

Also from Fig. 3.4:

$$\cos \alpha' = \frac{x}{d_1}, \cos \beta' = \frac{y}{d_1}, \cos \gamma' = \frac{z}{d_1} \quad \dots \quad (3.4)$$

Substitute Equation (3.4) in (3.3) gives:

$$\begin{aligned} d_1^2 &= d_1^2 \cos^2 \alpha' + d_1^2 \cos^2 \beta' + d_1^2 \cos^2 \gamma' \\ &= d_1^2 [\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma'] \end{aligned}$$

$$(\text{or}) \quad \cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1 \quad \dots \quad (3.5)$$

Substitute Equation (3.2) in (3.5) gives:

$$\frac{d_1^2}{(\text{OA})^2} + \frac{d_1^2}{(\text{OB})^2} + \frac{d_1^2}{(\text{OC})^2} = 1 \quad \dots \quad (3.6)$$

Again substitute Equation (3.1) in (3.6)

$$\frac{d_1^2 b^2}{a^2} + \frac{d_1^2 k^2}{b^2} + \frac{d_1^2 l^2}{c^2} = 1 \quad (\text{or}) \quad d_1^2 \left[ \frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

$$d_1 = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad \dots \quad (3.7)$$

Let  $\left( \frac{b}{2} \frac{k}{2} \frac{l}{2} \right)$  be the Miller indices of the next plane A' B' C', this plane makes intercepts OA', OB' and OC'

on X, Y and Z axes, respectively. A normal from the origin to this plane passes through a point N', so that  $\text{ON}' = d_2$ . As the extension of  $d_1$  is  $d_2$ , it makes same angles  $\alpha'$ ,  $\beta'$  and  $\gamma'$  with X, Y and Z-axes, respectively. Since the plane segments 'a' into  $b/2$  equal parts,  $b$  into  $k/2$  equal parts and  $c$  into  $l/2$  equal parts, then the intercepts OA', OB' and OC' are such that:

$$\text{OA}' = \frac{a}{\left( \frac{b}{2} \right)} = \frac{2a}{b}, \quad \text{OB}' = \frac{b}{\left( \frac{k}{2} \right)} = \frac{2b}{k} \quad \text{and} \quad \text{OC}' = \frac{c}{\left( \frac{l}{2} \right)} = \frac{2c}{l} \quad \dots \quad (3.1')$$

From Fig. 3.4,

$$\cos \alpha' = \frac{d_2}{(\text{OA}')}, \cos \beta' = \frac{d_2}{(\text{OB}')}, \quad \text{and} \quad \cos \gamma' = \frac{d_2}{(\text{OC}')} \quad \dots \quad (3.2')$$

Let the coordinates of N' are  $x'$ ,  $y'$  and  $z'$  along X, Y and Z-axes, respectively.

$$(\text{ON}')^2 = d_2^2 = x'^2 + y'^2 + z'^2 \quad \dots \quad (3.3')$$

## 3-6 | Applied Physics

Also from Fig 3.4:

$$\cos \alpha' = \frac{x'}{d_2}, \cos \beta' = \frac{y'}{d_2} \quad \text{and} \quad \cos \gamma' = \frac{z'}{d_2} \quad (3.4')$$

Substitute Equation (3.4') in (3.3') gives:

$$d_2^2 = d_2^2 \cos^2 \alpha' + d_2^2 \cos^2 \beta' + d_2^2 \cos^2 \gamma'$$

$$= d_2^2 [\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma']$$

$$(or) \quad \cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1 \quad (3.5')$$

Substitute Equation (3.2') in (3.5') gives:

$$\frac{d_2^2}{(OA')^2} + \frac{d_2^2}{(OB')^2} + \frac{d_2^2}{(OC')^2} = 1 \quad (3.6')$$

Again substitute Equation (3.1') in (3.6') gives:

$$\frac{d_2^2 b^2}{(2a)^2} + \frac{d_2^2 k^2}{(2b)^2} + \frac{d_2^2 l^2}{(2c)^2} = 1 \quad (or) \quad d_2^2 \left[ \frac{b^2}{(2a)^2} + \frac{k^2}{(2b)^2} + \frac{l^2}{(2c)^2} \right] = 1$$

$$(or) \quad d_2 = \frac{1}{\sqrt{\frac{b^2}{(2a)^2} + \frac{k^2}{(2b)^2} + \frac{l^2}{(2c)^2}}} \quad (or) \quad d_2 = \frac{2}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad (3.7')$$

Let the separation between the planes ABC and A'B'C' is 'd'.

$$\therefore d = d_2 - d_1 = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad (3.8)$$

Using Equation (3.8), we can determine the interplanar separation in orthorhombic crystals. For tetragonal crystal  $a = b \neq c$ , substitute these values in Equation (3.8), we have:

$$d = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{c^2}}} = \frac{1}{\sqrt{\frac{b^2 + k^2 + l^2}{a^2}}} \quad (3.9)$$

For cubic crystals:  $a = b = c$ , substitute these values in Equation (3.8), we have:

$$d = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{a^2}}} \quad (or) \quad d = \frac{a}{\sqrt{b^2 + k^2 + l^2}} \quad (3.10)$$

The calculation of interplanar spacing for other crystal systems is complicated, so we will not discuss them.

### 3.3 Imperfections in crystals

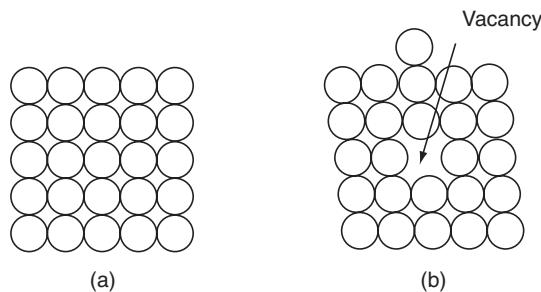
In a sound crystal (or in an ideal crystal), the atoms are arranged regularly and periodically in three dimensions. But the grown crystals [or real crystals] may contain imperfections or defects. These defects are mainly divided into point, line, surface and volume defects. Point and line defects are discussed here, while surface defects are dealt with in Appendix B.

**(1) Point defects:** As the name indicates, these defects are at some points in the crystal. So, these are also called zero-dimensional defects. The point defects are divided into three categories: (a) lattice site defects; this includes vacancies [Schottky defect] and interstitials [Frenkel defect], (b) compositional defects; this includes substitutional impurity and interstitial impurity and (c) electronic defects. These defects are discussed below.

**(a) Lattice site defects:** In this type of defects, some atoms may not be present in their regular atomic sites. They are:

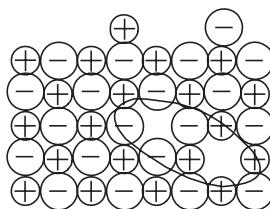
**(i) Vacancies:** As shown in Fig. 3.5, at a lattice point, one or two or three atoms are missed, and this is referred to as single or double or triple vacancies, respectively. The vacancies are formed due to the imperfect packing during crystallization or due to thermal vibrations at high temperatures.

**Figure 3.5** (a) Perfect crystal; (b) Vacancy defect

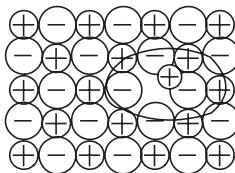


**Schottky defect:** In ionic crystals, if a cation vacancy exists, then in the very nearby place an anion vacancy also exists. i.e., usually an anion and cation pair is moved to the surface of the crystal, so that charge neutrality is maintained in the vacancy region as shown in Fig. 3.6. This is known as Schottky defect. Crystals such as NaCl, KCl, KBr, etc. show Schottky defect.

**Figure 3.6** Schottky defect



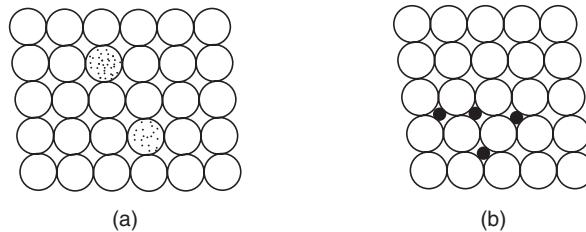
**(ii) Interstitial defect:** If an atom is moved to an interstitial space in the crystal, then the defect is known as interstitial defect.

**Figure 3.7 Frenkel defect**

**Frenkel defect:** In ionic crystals, if a cation [positive ion] moves to an interstitial space, then a vacancy is formed in its atomic position. Here, charge neutrality is maintained in the defective region as shown in Fig. 3.7. This type of defect is known as Frenkel defect. Crystals such as CaF<sub>2</sub>, AgBr, AgI, etc. show Frenkel defect.

**(b) Compositional defect:** The presence of impurity atoms in the crystal leads to compositional defects. Impurity atoms are present at the sites of regular parent atoms or in the interstitial spaces. These defects are described below.

**(i) Substitutional defect:** As shown in Fig. 3.8(a), during crystallization few foreign atoms occupy the regular parental atoms sites. For example, in extrinsic semiconductors either third or fifth group atoms occupy the sites of silicon or germanium atoms.

**Figure 3.8 (a) Substitutional defect; (b) Interstitial defect**

**(ii) Interstitial impurity defect:** The spaces between the parental atoms in a crystal are known as interstitial spaces. Small-sized [lower atomic number] atoms, such as hydrogen, etc. may fit into these interstitial spaces. These atoms are known as interstitial atoms and the defect formed due to the presence of interstitial atoms is known as interstitial defect. This is shown in Fig. 3.8(b). If 'r' is the radius of a parent atom, then a octahedral and a tetrahedral space can accommodate an interstitial atom of radius  $0.414r$  and  $0.225r$ , respectively.

**(c) Electronic defects:** Non-uniformity of charge or energy distribution in the crystal is referred to as electronic defect. The presence of impurity atoms such as substitutional and interstitial atoms and vacancies can vary the uniform distribution of electronic charge in the crystal. So, the presence of these defects also leads to electronic defects. In semiconductors, temperature variation changes charge concentration, so the variation of temperature [i.e., thermal energy] leads to electronic defects.

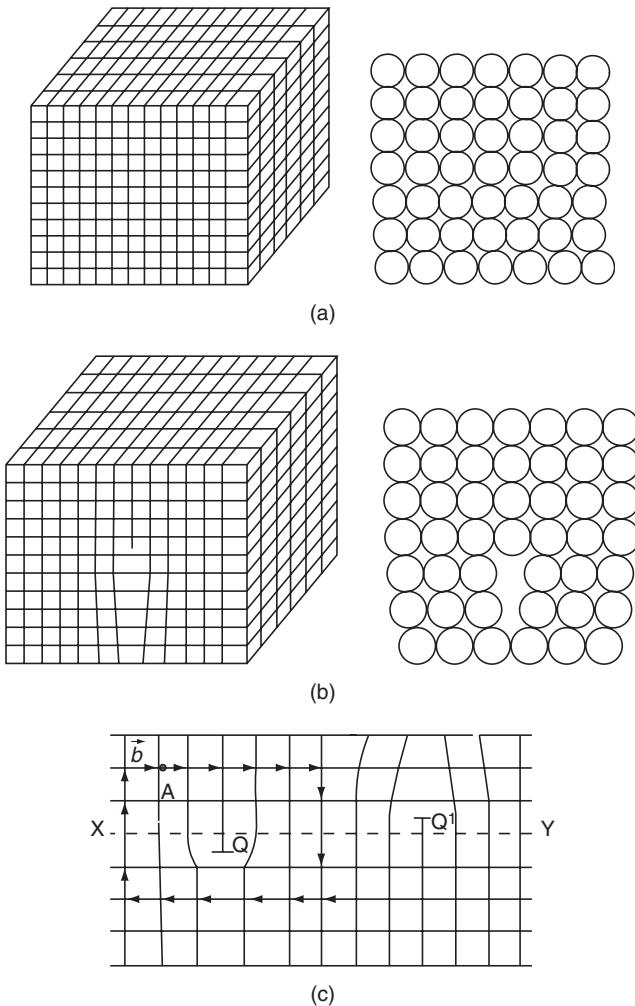
Point defects are formed by thermal fluctuations, by severe deformation [i.e., by hammering or rolling] and by bombarding with high energetic particles.

**(2) Line defects:** If a crystal plane ends somewhere in the crystal, then along the edge of that incomplete plane produces defect in the crystal called line defect. The line defect is of two types: they are (i) edge dislocation and (ii) screw dislocation. These are described below.

**(i) Edge dislocation:** Figure 3.9(a) shows three-dimensional view and front face of a perfect crystal. The vertical crystal planes are parallel to side faces of a crystal is shown in the figure. One of the crystal planes does

Figure 3.9

(a) Three-dimensional view of perfect crystal; Front view of perfect crystal; (b) Three-dimensional view of edge dislocation crystal; Front view of edge dislocation crystal; (c) Positive and negative edge dislocations

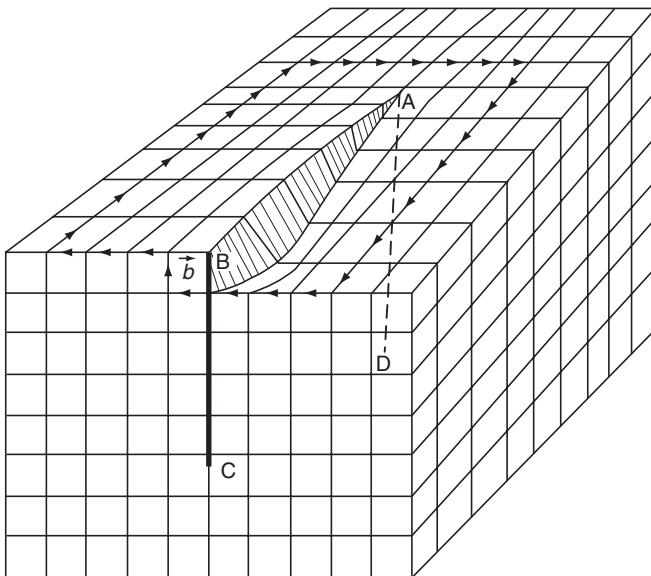


not pass from top to bottom face of the crystal, but ends some where in the crystal as shown in Fig. 3.9(b). In this crystal, just above the edge of incomplete plane, the atoms are in a state of compression so that the bond distances are less than normal values and below the edge of incomplete plane, the atoms are far apart, so the bond distances are larger than normal values. This situation extends all along the edge of this incomplete plane producing edge dislocation. The extra plane indicated in Fig. 3.9(b) can be either above or below the slip plane shown as dotted line X, Y in Fig. 3.9(c). If the incomplete extra plane is above the slip plane, then the edge dislocation is positive and is represented by the symbol  $\perp$ ; on the other hand if it is below the slip plane, then the edge dislocation is negative and is represented by the symbol  $\top$ . If one plane of atoms glides over another separated by an integral multiple of interatomic distance is called slip, and the slip plane is the plane in which slip has taken place. Thus, the crystal consists of slipped and normal regions.

The magnitude and direction of the displacement of crystal planes due to edge dislocation can be represented by a vector called Burger's vector, which is perpendicular to the dislocation line. This indicates how much and in what direction the lattice above the slip plane is shifted with respect to the lattice below the slip plane. Figure 3.9(c) shows a method of determining Burger's vector for edge dislocation. To find the magnitude and direction of Burger's vector, one starts arbitrarily from a lattice point A, drawing atom-to-atom vectors round the dislocation in clockwise direction to form a closed circuit. Here, the number of vectors in horizontal direction at the top and bottom and vertical vectors at the left and right are equal, but the circuit is not closed unless we put the vector  $\vec{b}$ , as shown in the circuit. This is the Burger's vector for the above-said edge dislocation.

**(ii) Screw dislocation:** The crystal planes spiral about a line in the crystal, called dislocation line. The screw dislocation is shown in Fig. 3.10. Due to the spiralling of crystal planes, the atoms at one end of the plane are displaced by one atomic distance with respect to the other end of the plane in perpendicular direction to the plane. As shown in Fig. 3.10, the plane ABCD is the slipped area. The upper portion of the crystal has been sheared by one atomic distance compared to the right side region of the crystal. Slip has not taken place to the right side of AD, so AD is the dislocation line. Burger's circuit is completed around the dislocation. The Burger's vector is parallel to the dislocation line. By knowing the Burger's vector and dislocation line, the dislocation is completely described.

**Figure 3.10** Screw dislocation and Burger's vector



### 3.4 Energy for the formation of a vacancy and number of vacancies – at equilibrium concentration

Energy supply to a crystal moves some of the atoms present at regular atomic sites in the interior of the crystal to the surface, so that vacancies are formed inside the crystal. If we supply energy to an ionic crystal, then

either cation-anion pairs are moved to the surface [Schottky defect] or cations are moved to interstitial spaces [Frenkel defect], so that vacancies are formed inside the ionic crystal. We shall find the relation between number of vacancies and energy of formation of a vacancy in all the above cases.

**(i) In metallic crystals:** Let a crystal contains  $N$  number of atoms. The energy required to move an atom at a regular atomic site in the interior of the crystal to the surface is  $E_v$  i.e., the energy required to create a vacancy. To create ' $n$ ' number of isolated vacant sites, the energy required is  $nE_v$ . At some thermal equilibrium temperature ' $T$ ', let ' $n$ ' number of vacancies present in the crystal. The number of ways these ' $n$ ' vacancies are created is given by ( $P$ ).

$$P = \frac{N!}{(N-n)! n!} \quad (3.11)$$

The vacancies created inside the crystal produces disorder in the crystal. The disorder can be measured in terms of entropy. The increase in entropy ( $S$ ) due to the increase of vacancies is:

$$S = K_B \log P \quad (3.12)$$

where  $K_B$  is Boltzmann constant, substituting Equation (3.11) in (3.2), we have:

$$S = K_B \log \frac{N!}{(N-n)! n!} \quad (3.13)$$

The creation of vacancies produces not only the change in entropy but also change in free energy ( $F$ ) of the crystal.

$$F = U - TS \quad (3.14)$$

where  $U = nE_v$  = internal energy of crystal at temperature  $TK$ . Equations (3.12) and (3.14) are taken from thermodynamics. Substituting Equation (3.13) in (3.14) gives:

$$F = nE_v - K_B T \log \left[ \frac{N!}{(N-n)! n!} \right]$$

$$= nE_v - K_B T [\log N! - \log (N-n)! - \log n!] \quad (3.15)$$

The logarithmic term in the above equation can be simplified using Stirling's approximation,

$$\log x! = x \log x - x$$

Equation (3.15) becomes:

$$F = nE_v - K_B T [N \log N - (N-n) \log (N-n) - n \log n] \quad (3.16)$$

In thermal equilibrium at constant volume, the free energy is minimum with respect to changes in ' $n$ '.

$$\therefore \left[ \frac{\partial F}{\partial n} \right]_T = 0 = E_v - K_B T \log \left( \frac{N-n}{n} \right) \quad (\text{or}) \quad \frac{E_v}{K_B T} = \log \left[ \frac{N-n}{n} \right] \quad (3.17)$$

Taking exponential on both sides of Equation (3.17), we have:

$$\exp\left(\frac{E_V}{K_B T}\right) = \frac{N-n}{n} \quad (\text{or}) \quad n = (N-n) \exp\left[\frac{-E_V}{K_B T}\right] \quad \text{if } n \ll N \text{ then}$$

$$n \approx N \exp\left[\frac{-E_V}{K_B T}\right] \quad \text{_____ (3.18)}$$

The above equation indicates that by decreasing equilibrium temperature, the concentration of vacancies decreases.

**(b) In Ionic crystals:** Here, we see Schottky and Frenkel defects separately.

**(i) Schottky defect:** In ionic crystals, equal number of cations [positive ions] and anions [negative ions] vacancies are formed i.e., usually cation-anion-paired vacancies are formed, so that charge neutrality is maintained in the crystal. The energy required to move a cation and an anion from interior of the crystal to the surface is  $E_p$ . At some thermal equilibrium temperature ( $T$ ), let ' $n$ ' pairs of cation-anion vacancies present in a crystal containing ' $N$ ' pairs of ions. The number of ways these  $n$ -pairs of vacancies are created is given by ( $P$ ).

$$P = \left[ \frac{N!}{(N-n)! n!} \right]^2 \quad \text{_____ (3.19)}$$

The vacancies created inside the crystal produce a disorder in the crystal. The disorder can be measured in terms of entropy. The increase in entropy ( $S$ ), due to the creation of  $n$  pairs of vacancies is

$$S = K_B \log P \quad \text{_____ (3.20)}$$

where  $K_B$  is Boltzmann constant, substituting Equation (3.19) in (3.20) we have:

$$S = K_B \log \left[ \frac{N!}{(N-n)! n!} \right]^2 \quad \text{_____ (3.21)}$$

The vacancies produce not only change in entropy but also change in free energy ( $F$ ) of the crystal.

$$\therefore F = U - TS \quad \text{_____ (3.22)}$$

where  $U = n E_p$  = internal energy of the crystal at temperature  $T$ . Equations (3.20) and (3.22) are taken from thermodynamics; substituting Equation (3.21) in (3.22) gives:

$$F = nE_p - K_B T \log \left[ \frac{N!}{(N-n)! n!} \right]^2$$

$$= nE_p - 2 K_B T [\log N! - \log (N-n)! - \log n!] \quad \text{_____ (3.23)}$$

The logarithmic term in the above equation can be simplified using Stirling's approximation:

$$\log x! = x \log x - x.$$

∴ Equation (3.23) becomes:

$$F = nE_p - 2K_B T [ N \log N - (N - n) \log (N - n) - n \log n ] \quad (3.24)$$

In thermal equilibrium at constant volume, the free energy is minimum with respect to the changes in 'n'.

$$\therefore \left( \frac{\partial F}{\partial n} \right)_T = 0 = E_p - 2K_B T \log \left( \frac{N - n}{n} \right) \quad (\text{or}) \quad \frac{E_p}{2K_B T} = \log \left( \frac{N - n}{n} \right) \quad (3.25)$$

Taking exponential on both sides of Equation (3.25), we get:

$$\exp \left( \frac{E_p}{2K_B T} \right) = \left( \frac{N - n}{n} \right) \quad (\text{or}) \quad n = (N - n) \exp \left( \frac{-E_p}{2K_B T} \right) \quad \text{if } n \ll N \text{ then:}$$

$$n \approx N \exp \left( \frac{-E_p}{2K_B T} \right) \quad (3.26)$$

**(ii) Frenkel defects:** Let the ionic crystal contains  $N$  number of atoms and the number of interstitial spaces are slightly less than the number of atoms. Let  $N_i$  be the number of interstitial spaces in a perfect crystal. The amount of energy required to displace an atom from regular atomic site to an interstitial position is  $E_i$ . At some thermal equilibrium temperature, let there be 'n' number of cation site vacancies and same number of interstitial atoms. The number of ways the 'n' Frenkel defects can be formed is:

$$P = \frac{N!}{(N - n)! n!} \times \frac{N_i!}{(N_i - n)! n!} \quad (3.27)$$

The increase in entropy ( $S$ ) due to the creation of Frenkel defects is given by:

$$S = K_B \log P \quad (3.28)$$

Substituting Equation (3.27) in (3.28), we get:

$$S = K_B \log \left[ \frac{N!}{(N - n)! n!} \times \frac{N_i!}{(N_i - n)! n!} \right] \quad (3.29)$$

These defects produce not only change in entropy but also change in free energy ( $F$ ) given by:

$$F = U - TS \quad (3.30)$$

Equations (3.28) and (3.30) are taken from thermodynamics. Substituting Equation (3.29) in (3.30), we have:

$$F = nE_i - K_B T \log \left[ \frac{N!}{(N - n)! n!} \times \frac{N_i!}{(N_i - n)! n!} \right] \quad (3.31)$$

The logarithmic term in the above equation can be simplified by applying Stirling's approximation  $\log x! = x \log x - x$ .

$$\begin{aligned} \therefore \log \left[ \frac{N!}{(N-n)! n!} \times \frac{N_i!}{(N_i-n)! n!} \right] &= \log \frac{N!}{(N-n)! n!} + \log \frac{N_i!}{(N_i-n)! n!} \\ &\cong N \log N + N_i \log N_i - (N-n) \log (N-n) - (N_i-n) \log (N_i-n) - 2n \log n \quad (3.32) \end{aligned}$$

Substituting Equation (3.32) in (3.31), we have:

$$F = nE_i - K_B T [N \log N + N_i \log N_i - (N-n) \log (N-n) - (N_i-n) \log (N_i-n) - 2n \log n] \quad (3.33)$$

At thermal equilibrium, the change in free energy is minimum w.r.t 'n', so we have:

$$\left[ \frac{\partial F}{\partial n} \right]_T = 0 = E_i - K_B T \log \frac{(N-n)(N_i-n)}{n^2} \quad (3.34)$$

$$\therefore E_i = K_B T \log \frac{(N-n)(N_i-n)}{n^2} \quad (\text{or}) \quad \frac{E_i}{K_B T} = \log \frac{(N-n)(N_i-n)}{n^2}$$

Taking exponential on both sides, we get:

$$\begin{aligned} \exp \left( \frac{E_i}{K_B T} \right) &= \frac{(N-n)(N_i-n)}{n^2} \\ n^2 &= (N-n)(N_i-n) \exp \left( \frac{-E_i}{K_B T} \right) \quad \text{if } n \ll N_i \\ n^2 &\approx N N_i \exp \left( \frac{-E_i}{K_B T} \right) \quad (\text{or}) \quad n = (N N_i)^{1/2} \exp \left( \frac{-E_i}{2K_B T} \right) \quad (3.35) \end{aligned}$$

The above equation shows that  $n$  is proportional to  $(NN_i)^{1/2}$

### 3.5 Diffraction of X-rays by crystal planes and Bragg's law

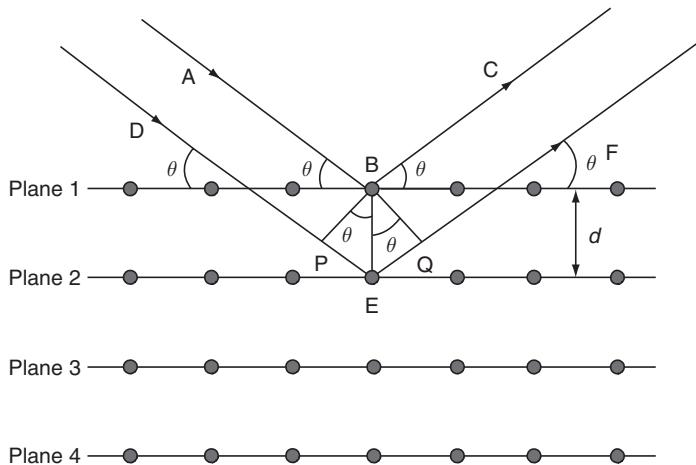
The visible light rays when pass through a sharp edge of an object can form some bright regions inside the geometrical shadow of the object. This is due to the bending nature of light, called diffraction. Diffraction of visible light rays can also be produced using plane-ruled grating. This grating consists of about 6000 lines/cm; so that the spacing between any two consecutive lines in the grating is of the order of the wavelength of visible light used to produce diffraction. The wavelength of X-rays is of the order of

an angstrom, so X-rays are unable to produce diffraction with plane optical grating. To produce diffraction with X-rays, the spacing between the consecutive lines of grating should be of the order of few angstroms. Practically, it is not possible to construct such a grating. In the year 1912, a German physicist Laue suggested that the three-dimensional arrangement of atoms in a crystal can serve as a three-dimensional grating. Inside the crystal, the spacing between the crystal planes can work as the transparent regions as between lines in a ruled grating. Laue's associates Friedrich and Knipping succeeded in diffracting X-rays by passing through a thin crystal.

In 1913, W.L. Bragg and his son W.H. Bragg gave a simple interpretation of the diffraction pattern. According to Bragg, the diffraction spots produced are due to the reflection of some of the incident X-rays by various sets of parallel crystal planes. These planes are called Bragg's planes. The Bragg's interpretation is explained in the following topic.

**Bragg's law:** W.L. Bragg and W.H. Bragg considered the X-ray diffraction as the process of reflection of X-rays by crystal planes as shown in Fig. 3.11. A monochromatic X-ray beam of wavelength  $\lambda$  is incident

**Figure 3.11** Bragg's law



at an angle  $\theta$  to a family of Bragg planes. Let the interplanar spacing of crystal planes is ' $d$ '. The dots in the planes represent positions of atoms in the crystal. Every atom in the crystal is a source of scatterer of X-rays incident on it. A part of the incident X-ray beam AB, incident on an atom at B in plane 1, is scattered along the direction BC. Similarly, a part of incident X-ray DE [in parallel to AB] falls on atom at E in plane 2 and is scattered in the direction EF and it is parallel to BC. Let the beams AB and DE make an angle  $\theta$  with the Bragg's planes. This angle  $\theta$  is called the angle of diffraction or glancing angle.

If the path difference between the rays ABC and DEF is equal to  $\lambda, 2\lambda, 3\lambda \dots$  etc. or  $n\lambda$ , i.e., integral multiples of wavelength, where  $n = 1, 2, 3, \dots$  etc. are called first-order, second-order, third-order ... etc. maxima, respectively. As path difference is equal to  $n\lambda$ , then the rays reflected from consecutive planes are in phase; so, constructive interference takes place among the reflected rays BC and EF, hence the resulting diffracted ray is intense. On the other hand, if the path difference between the rays ABC and DEF is  $\frac{\lambda}{2}, \frac{3\lambda}{2}, \frac{5\lambda}{2}, \dots$  etc.,

then the scattered rays BC and EF are out of phase so that destructive interference takes place and hence the

resulting ray intensity is minimum. To find the path difference between these rays, drop perpendiculars from B on DE and EF. The intersecting points of perpendiculars are P and Q as shown in Fig. 3.11. The path difference between the rays is PE + QE. From the figure, we know that BE is perpendicular to plane 1 and BP is perpendicular to AB. So, as the angle between ray AB and plane 1 is  $\theta$ , then  $\angle PBE = \angle QBE = \theta$ .

In the triangle PBE,  $\sin \theta = \frac{PE}{BE} = \frac{PE}{d}$  or  $PE = d \sin \theta$ . Similarly,  $EQ = d \sin \theta$ .

$\therefore$  For constructive interference,  $PE + EQ = n\lambda$  or  $d \sin \theta + d \sin \theta = n\lambda$

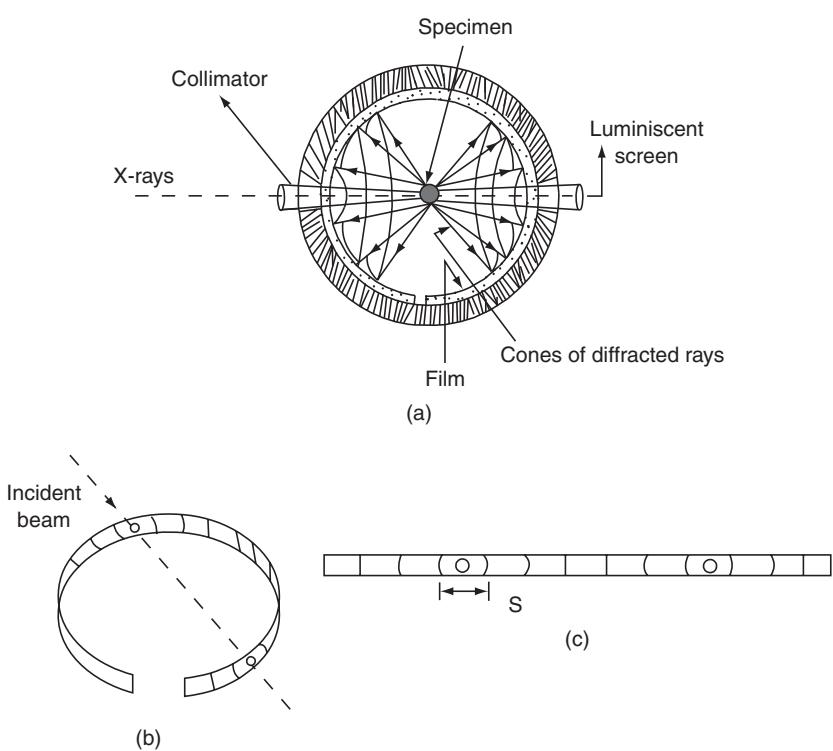
$$\text{i.e., } 2d \sin \theta = n\lambda$$

The above equation is called Bragg's law.

## 3.6 Powder method

X-ray powder method is usually carried for polycrystalline materials. The powder photograph is obtained in the following way. The given polycrystalline material is ground to fine powder and this powder can be taken either in a capillary tube made up of non-diffracting material or is just struck on a hair with small quantity of binding material and fixed at the centre of cylindrical Debye-Scherrer camera as shown in Fig. 3.12(a).

**Figure 3.12** (a) Debye-Scherrer cylindrical camera; (b) Film mounted in camera; (c) Film on stretchout



A stripe of X-ray photographic film is arranged along the inner periphery of the camera. A beam of monochromatic X-rays is passed through the collimator to obtain a narrow fine beam of X-rays. This beam falls on the polycrystalline specimen and gets diffracted. The specimen contains very large number of small crystallites oriented in random directions. So, all possible diffraction planes will be available for Bragg reflection to take place. Such reflections will take place from many sets of parallel planes lying at different angles to the incident X-ray beam. Also, each set of planes gives not only first-order reflections but also of higher orders as well. Since all orientations are equally likely, the reflected rays will form a cone whose axis lies along the direction of the incident beam and whose semi-vertical angle is equal to twice the glancing angle ( $\theta$ ), for that particular set of planes. For each set of planes and for each order, there will be such a cone of reflected X-rays. Their intersections with a photographic film sets with its plane normal to the incident beam, form a series of concentric circular rings. In this case, a part of the reflected cone is recorded on the film and it is a pair of arcs, the resulting pattern is shown in Fig. 3.12(c). Diameter of these rings or corresponding arcs is recorded on the film, and using this the glancing angle and interplanar spacing of the crystalline substance can be determined. Figure 3.12(b) shows the film mounted in the camera and the X-ray powder pattern obtained. The film on spread-out is shown in Fig 3.12(c). The distance between any two corresponding arcs on the film is indicated by the symbol  $S$ .

In case of cylindrical camera, the diffraction angle  $\theta$  is proportional to  $S$ . Then,

$$\theta = \frac{S}{4R} \quad \text{where } R \text{ represents the radius of the camera.}$$

If  $S_1, S_2, S_3 \dots$  etc. are the distances between symmetrical lines on the stretched film, then,

$$\theta_1 = \frac{S_1}{4R}, \theta_2 = \frac{S_2}{4R}, \theta_3 = \frac{S_3}{4R} \dots$$

Using these values of  $\theta_n$  in Bragg's equation  $n\lambda = 2 d_{hkl} \sin \theta_n$

where  $n = 1, 2, 3, \dots$  etc = order of diffraction

$d_{hkl}$  = interplanar spacing

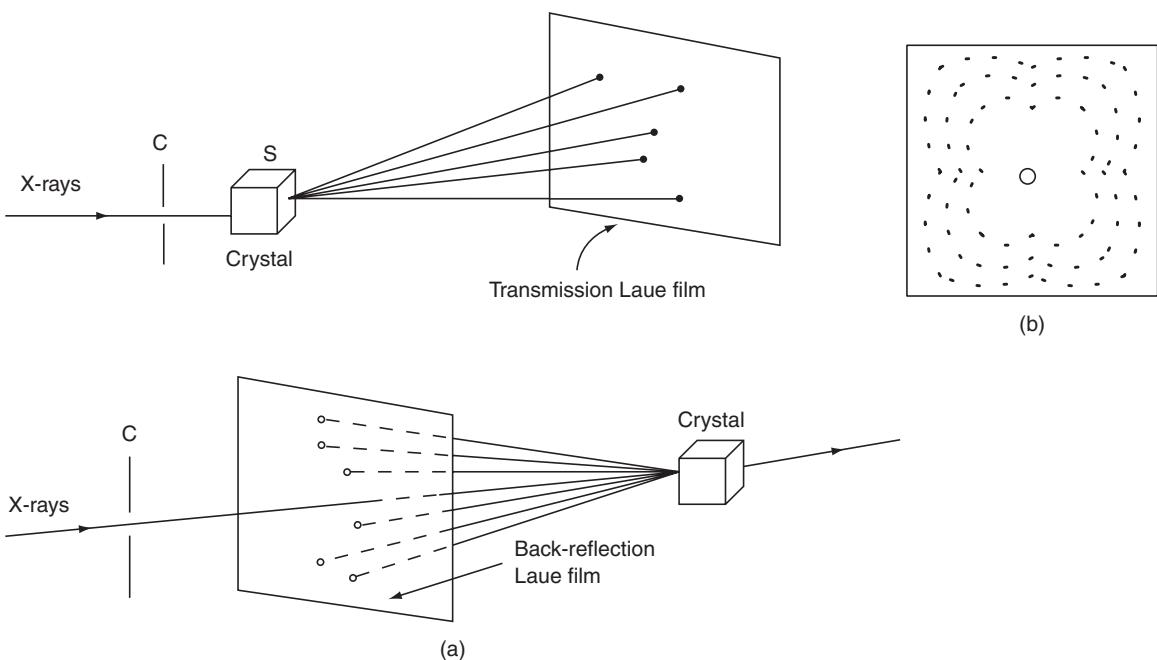
$\theta_n$  = angle of diffraction for  $n$ th order

The interplanar spacing  $d_{hkl}$  can be calculated.

## 3.7 Laue method

In Laue method, a narrow beam of white X-rays [usually in the wavelength range, 0.2 to 2.0 Å] is obtained by passing X-rays through a collimator 'C'. This beam is allowed to fall on a stationary single crystal 'S' as shown in Fig. 3.13(a). The crystal act as a 3-dimensional diffraction grating to the incident beam. The processes of reflection of X-rays by crystal planes is considered as X-ray diffraction. The diffraction phenomenon satisfies Bragg's law,  $n\lambda = 2d \sin \theta$ . where  $n = 1, 2, 3, \dots$  represent the order of diffraction,  $\lambda$  = wavelength of diffracted X-rays from a system of crystal planes with interplanar spacing ' $d$ ' and  $\theta$  = glancing angle i.e., the angle made by X-rays with a crystal plane. As the crystal is not rotated, so, the angle ' $\theta$ ' is fixed for a set of planes having separation ' $d$ '. Different sets of crystal planes satisfy Bragg's law with different wavelengths of X-rays and produce diffraction. The diffracted X-rays from a set of planes produce constructive interference, if they are in phase and form an intense beam, and this produces dark spots on photographic film. If the diffracted rays are out of phase, they produce destructive interference so that photographic film is unaffected.

**Figure 3.13 (a) X-ray diffraction by crystal plane; (b) Lane pattern for NaCl crystal**



Laue photograph is obtained either by allowing the transmitted diffracted rays or by back-reflected diffracted rays on photographic film as shown in Fig. 3.13(b).

As we observe the diffracted film, the diffracted spots lie on certain curves. These curves are either ellipses or hyperbolas on transmission Laue photograph and hyperbolas on back-reflection Laue photograph. The way of arrangement of spots on a film is a characteristic property of the crystal. Laue method is useful to decide the crystal symmetry and orientation of the internal arrangement of atoms/molecules in the crystal. Cell parameters of a crystal cannot be determined using Laue method. For transmission Laue method, the crystal should be thin.

Laue method can be used to study imperfections or strains in the crystal. The presence of above defects forms streaks instead of spots in the Laue photograph.

## Formulae

$$1. \quad d = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

$$2. \quad d = \frac{a}{\sqrt{b^2 + k^2 + l^2}}$$

$$3. \quad n \approx N \exp \left[ \frac{-E_V}{K_B T} \right] \leftarrow \text{Metallic crystal}$$

$$4. \quad n \approx N \exp \left[ \frac{-E_p}{2K_B T} \right] \leftarrow \text{Schottky defect}$$

$$5. \quad n \approx (NN_i)^{1/2} \exp \left[ \frac{-E_i}{2K_B T} \right] \leftarrow \text{Frenkel defect}$$

$$6. \quad 2d \sin \theta = n\lambda$$

## Solved Problems

1. A beam of X-rays of wavelength 0.071 nm is diffracted by (110) plane of rock salt with lattice constant of 0.28 nm. Find the glancing angle for the second-order diffraction.

(Set-1–Sept. 2007), (Set-2, Set-3–Sept. 2006), (Set-2–May 2006), (Set-3–May 2004), (Set-4–May 2003)

**Sol:** Given data are:

Wavelength ( $\lambda$ ) of X-rays = 0.071 nm

Lattice constant ( $a$ ) = 0.28 nm

Plane ( $bkl$ ) = (110)

Order of diffraction = 2

Glancing angle  $\theta$  = ?

Bragg's law is  $2d \sin \theta = n\lambda$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}, \text{ because rock salt is FCC}$$

$$= \frac{0.28 \times 10^{-9}}{\sqrt{1^2 + 1^2 + 0^2}} \text{ m} = \frac{0.28 \times 10^{-9}}{\sqrt{2}} \text{ m}$$

Substitute in Bragg's equation

$$2 \times \frac{0.28 \times 10^{-9}}{\sqrt{2}} \sin \theta = 2 \times 0.071 \times 10^{-9}$$

$$\sin \theta = \sqrt{2} \times \frac{0.071}{0.28} = 0.3586$$

$$\theta = \sin^{-1}(0.3586) = 21.01^\circ \approx 21^\circ$$

2. A beam of X-rays is incident on a NaCl crystal with lattice plane spacing 0.282 nm. Calculate the wavelength of X-rays if the first-order Bragg reflection takes place at a glancing angle of  $8^\circ 35'$ . Also calculate the maximum order of diffraction possible.

(Set-4–Sept. 2007), (Set-3–May 2007), (Set-2–May 2004), (Set-3–May 2003)

**Sol:** Given data are:

NaCl crystal is FCC

Lattice plane spacing ( $d$ ) = 0.282 nm

Wavelength of rays ( $\lambda$ ) = ?

Order of diffraction ( $n$ ) = 1

Glancing angle  $\theta = 8^\circ 35'$

Bragg's equation is  $n\lambda = 2d \sin \theta$

$$\begin{aligned} 1\lambda &= 2 \times 0.282 \times 10^{-9} \sin(8^\circ 35') \\ &= 0.0842 \text{ nm} \end{aligned}$$

Maximum order of diffraction ( $n_{\max}$ ) = ?

$$2d \sin \theta = n\lambda$$

if  $\theta = 90^\circ$  then  $n = n_{\max}$

$$\therefore 2d = n_{\max} \lambda$$

$$n_{\max} = \frac{2d}{\lambda} = \frac{2 \times 0.282 \text{ nm}}{0.0842 \text{ nm}} = 6.7 \approx 7$$

3. The fraction of vacant sites in a metal is  $1 \times 10^{-10}$  at  $500^\circ \text{C}$ . What will be the fraction of vacancy sites at  $1000^\circ \text{C}$ ?  
 (Set-4–Sept. 2006), (Set-1–May 2004), (Set-2–May 2003)

**Sol:** The number of vacancies at temperature ( $T$  K) in a metal is represented by:

$$n \approx N \exp\left(\frac{-E_V}{K_B T}\right) \quad (\text{or}) \quad \frac{n}{N} = \exp\left(\frac{-E_V}{K_B T}\right)$$

The given data are:

$$\frac{n}{N} = 1 \times 10^{-10} \text{ at } 500^\circ \text{C} \quad \text{or} \quad 773 \text{ K} \quad \frac{n'}{N} = ? \text{ at } 1000^\circ \text{C} \quad \text{or} \quad 1273 \text{ K}$$

$$1 \times 10^{-10} = \exp\left(\frac{-E_V}{K_B 773}\right) \quad \text{--- (1)}$$

$$\frac{n'}{N} = \exp\left(\frac{-E_V}{K_B 1273}\right) \quad \text{--- (2)}$$

Taking logarithms on both sides of the above Equations (1) and (2), we get:

$$\ln 10^{-10} = \frac{-E_V}{773 K_B} \quad \text{--- (3)}$$

$$\ln\left(\frac{n'}{N}\right) = \frac{-E_V}{1273 K_B} \quad \text{--- (4)}$$

Dividing Equation (4) by (3),

$$\frac{\ln\left(\frac{n'}{N}\right)}{\ln 10^{-10}} = \frac{\left(\frac{-E_V}{1273 K_B}\right)}{\left(\frac{-E_V}{773 K_B}\right)} = \frac{773}{1273} = 0.60723$$

$$= \ln\left(\frac{n'}{N}\right) = \ln 10^{-10} \times 0.60723$$

$$= -23.026 \times 0.60723 = -13.982$$

Take exponential on both sides,

$$\frac{n'}{N} = \exp[-13.982] \times 10^{-7} = 8.466 \times 10^{-7}$$

The fraction of vacancy sites at 1000°C is  $8.466 \times 10^{-7}$ .

4. Calculate the ratios  $d_{100} : d_{110} : d_{111}$  for a simple cubic structure.

(Set-2–Nov. 2004), (Set-2–Nov. 2003)

**Sol:** Let 'a' be the lattice constant of cubic structure, then,

$$d_{100} = \frac{a}{\sqrt{1^2 + 0^2 + 0^2}} = a$$

$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$$

$$\begin{aligned} \text{The ratios } d_{100} : d_{110} : d_{111} &= a : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}} \\ &= 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} = \sqrt{6} : \sqrt{3} : \sqrt{2} \end{aligned}$$

5. The Bragg's angle in the first order for (220) reflection from nickel (FCC) is  $38.2^\circ$ . When X-rays of wavelength  $1.54 \text{ \AA}$  are employed in a diffraction experiment. Determine the lattice parameter of nickel.

(Set-2–May 2008)

**Sol:** Order of diffraction,  $n = 1$

Diffraction angle,  $\theta = 38.2^\circ$

Wavelength of light,  $\lambda = 1.54 \text{ \AA}$

Plane of reflection = (220)

Lattice parameter,  $a = ?$

Bragg's law is  $2d \sin \theta = n\lambda$

$$d = \frac{n\lambda}{2 \sin \theta} = \frac{1 \times 1.54}{2 \times \sin 38.2} \text{ \AA}$$

$$\text{Also } d = \frac{a}{\sqrt{b^2 + k^2 + l^2}}$$

$$a = d \times \sqrt{b^2 + k^2 + l^2}$$

$$= \frac{1 \times 1.54}{2 \times \sin 38.2} \times \sqrt{2^2 + 2^2 + 0^2}$$

$$= \frac{4.35578}{1.23682} = 3.522 \text{ \AA}$$

6. Monochromatic X-rays of  $\lambda = 1.5 \text{ Å.U}$  are incident on a crystal face having an interplanar spacing of  $1.6 \text{ Å.U}$ . Find the highest order for which Bragg's reflection maximum can be seen.

(Set-4–May 2006)

**Sol:** Given data are

$$\text{Wavelength of light } (\lambda) = 1.5 \text{ Å}$$

$$\text{Interplanar spacing } (d) = 1.6 \text{ Å}$$

$$\text{Glancing angle } (\theta_m) = 90^\circ$$

$$\text{Order of diffraction } (n) = ?$$

Bragg's law

$$n\lambda = 2d \sin \theta$$

$$n = \frac{2d \sin \theta}{\lambda} = \frac{2 \times 1.6 \times \sin 90^\circ}{1.5} = \frac{3.2}{1.5}$$

$$= 2.13 \approx 2$$

$\therefore$  The maximum order of diffraction is 2

7. The distance between (110) planes in a body centred cubic structure is  $0.203 \text{ nm}$ . What is the size of the unit cell? What is the radius of the atom?

(Set-3–Sept. 2007), (Set-3–May 2006)

**Sol:** The given data are

$$\text{The distance between (110) planes of BCC structure } (d_{110}) = 0.203 \text{ nm} = 0.203 \times 10^{-9} \text{ m}$$

$$\text{Length of unit cell } (a) = ?$$

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

$$\text{Radius of the atom } (r) = ?$$

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

$$0.203 \times 10^{-9} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

$$a = 0.203 \times \sqrt{2} = 0.287 \times 10^{-9} \text{ m}$$

$$\text{Volume of unit cell } a^3 = 0.02364 \times 10^{-27} \text{ m}^3$$

$$\text{Radius of atom } (r) = \frac{\sqrt{3}a}{4} = \frac{1.732 \times 0.287 \times 10^{-9}}{4}$$

$$= 0.1243 \times 10^{-9} \text{ m}$$

8. Monochromatic X-rays of  $\lambda = 1.5 \text{ Å.U}$  are incident on a crystal face having an interplaner spacing of  $1.6 \text{ Å.U}$ . Find the highest order for which Bragg's reflection maximum can be seen.

(Set-1–Sept. 2006)

**Sol:** Given data are wavelength of X-rays,  $\lambda = 1.5 \text{ Å}$

$$\text{Interplanar spacing, } d = 1.6 \text{ Å}$$

$$\text{For highest order of diffraction, } \theta = 90^\circ$$

$$\text{Highest order of diffraction, } n = ?$$

Formula  $2d \sin \theta = n \lambda$

$$2 \times 1.6 \times \sin 90^\circ = n \times 1.5$$

$$n = \frac{2 \times 1.6}{1.5} = 2.13 \approx 2$$

$\therefore$  Highest order of diffraction is 2.

9. Calculate the glancing angle at (110) plane of a cubic crystal having axial length 0.26 nm corresponding to the second order diffraction maximum for the X-rays of wavelength 0.065 nm.

(Set-1–May 2007)

**Sol:** The given data are

Edge length of cubic system,  $a = 0.26$  nm

Wavelength of X-rays  $\lambda = 0.065$  nm

Glancing angle, for plane (110),  $\theta = ?$

Order of diffraction,  $n = 2$

$$\begin{aligned} \text{Separation between (110) planes of a cube, } d &= \frac{a}{\sqrt{b^2 + k^2 + l^2}} = \frac{0.26}{\sqrt{1^2 + 1^2 + 0^2}} \text{ nm} \\ &= \frac{0.26}{\sqrt{2}} = 0.184 \text{ nm} \end{aligned}$$

Bragg's law

$$2d \sin \theta = n\lambda$$

$$2 \times 0.184 \text{ nm} \times \sin \theta = 2 \times 0.065 \text{ nm}$$

$$\sin \theta = \frac{0.065}{0.184} = 0.353$$

$$\begin{aligned} \therefore \theta &= \sin^{-1}(0.353) \\ &= 20^\circ 41' 13'' \end{aligned}$$

10. The Bragg's angle for reflection from the (111) plane in a FCC crystal is  $19.2^\circ$  for an X-ray wavelength of 1.54 Å.U. Compute the cube edge of the unit cell.

(Set-2, Set-4–May 2007)

**Sol:** The given data are

Bragg's angle,  $\theta = 19.2^\circ$

Wavelength of X-rays,  $\lambda = 1.54$  Å

Order of diffraction,  $n = 1$

Cube edge,  $a = ?$

Bragg's law

$$2d \sin \theta = n\lambda$$

$$2d \sin 19.2^\circ = 1 \times 1.54$$

$$\begin{aligned} d &= \frac{1.54}{2 \times \sin 19.2^\circ} = \frac{1.54}{2 \times 0.3289} \\ &= 2.3411 \text{ Å} \end{aligned}$$

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

$$\text{or } a = d\sqrt{b^2 + k^2 + l^2} \\ = 2.3411 \times \sqrt{1^2 + 1^2 + 1^2} \\ = 2.3411 \times \sqrt{3} = 4.05 \text{ \AA}$$

11. The Bragg's angle in the first order for (220) reflection from nickel (FCC) is  $38.2^\circ$ . When X-rays of wavelength  $1.54 \text{ \AA}$  are employed in a diffraction experiment. Determine the lattice parameter of nickel.

(Set-2–May 2008)

**Sol:** Order of diffraction,  $n = 1$

Diffraction angle,  $\theta = 38.2^\circ$

Wavelength of light,  $\lambda = 1.54 \text{ \AA}$

Plane of reflection = (220)

Lattice parameter,  $a = ?$

Bragg's law is  $2d \sin\theta = n\lambda$

$$d = \frac{n \lambda}{2 \sin\theta} = \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \text{ \AA}$$

$$\text{Also } d = \frac{a}{\sqrt{b^2 + k^2 + l^2}}$$

$$a = d \times \sqrt{b^2 + k^2 + l^2} \\ = \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \times \sqrt{2^2 + 2^2 + 0^2} \\ = \frac{4.35578}{1.23682} = 3.522 \text{ \AA}$$

12. Copper has FCC structure with lattice constant  $0.36 \text{ nm}$ . Calculate the interplanar spacing for (111) and (321) planes.

**Sol:** Given data is:

Lattice constant ( $a$ ) =  $0.36 \text{ nm} = 0.36 \times 10^{-9} \text{ m}$

Interplanar spacing ( $d$ ) for (111) plane is:

$$d = \frac{a}{\sqrt{b^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3}} \text{ m} \\ = 0.208 \times 10^{-9} \text{ m} = 0.208 \text{ nm}$$

Interplanar spacing for (321) plane

$$d = \frac{a}{\sqrt{b^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3^2 + 2^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{9+4+1}} = \frac{0.36 \times 10^{-9}}{\sqrt{14}} \text{ m} \\ = 0.096 \times 10^{-9} \text{ m} \\ = 0.096 \text{ nm.}$$

13. The first-order diffraction occurs when a X-ray beam of wavelength  $0.675 \text{ \AA}$  incident at a glancing angle of  $5^\circ 25'$  on a crystal. What is the glancing angle for third-order diffraction to occur?

**Sol:** Wavelength of X-rays ( $\lambda$ ) =  $0.675 \text{ \AA}$

Glancing angle for first order ( $n = 1$ ) diffraction ( $\theta_1$ ) =  $5^\circ 25'$

Find the glancing angle for third order ( $n = 3$ ) diffraction ( $\theta_3$ ) = ?

Bragg's equation is  $2d \sin \theta = n\lambda$

For first order,  $2d \sin \theta_1 = 1\lambda$

$$2d \sin 5^\circ 25' = 0.675 \times 10^{-10} \text{ m}$$

$$d = \frac{0.675 \times 10^{-10}}{2 \sin 5^\circ 25'} \text{ m} = \frac{0.675 \times 10^{-10}}{0.1888} = 3.575 \times 10^{-10} \text{ m} = 3.575 \text{ \AA}$$

For third-order diffraction,

$$2d \sin \theta_3 = 3\lambda$$

$$\sin \theta_3 = \frac{3\lambda}{2d} = \frac{3 \times 0.675 \times 10^{-10}}{2 \times 3.575 \times 10^{-10}} = 0.283$$

$$\theta_3 = \sin^{-1}(0.283) = 16.45^\circ = 16^\circ 28'.$$

14. What is the angle at which the third-order reflection of X-rays of  $0.79 \text{ \AA}$  wavelength can occur in a calcite crystal of  $3.04 \times 10^{-8} \text{ cm}$  spacing.

**Sol:** Wavelength of X-rays,  $\lambda = 0.79 \text{ \AA} = 0.79 \times 10^{-8} \text{ cm}$

Interplanar spacing,  $d = 3.04 \times 10^{-8} \text{ cm}$

Order of diffraction,  $n = 3$

Angle of diffraction,  $\theta = ?$

$$2d \sin \theta = n\lambda$$

$$\sin \theta = \frac{n\lambda}{2d} = \frac{3 \times 0.79 \times 10^{-8}}{2 \times 3.04 \times 10^{-8}} = 0.3898$$

$$\theta = \sin^{-1}(0.3898)$$

$$= 25^\circ 29' 28''$$

### Multiple Choice Questions

- Crystal directions are defined as: ( )
  - certain directions inside the crystal along which large concentration of atoms exists
  - certain directions inside the crystal along which low concentration of atoms exists
  - certain directions inside the crystal along which no atoms are present
  - none

2. Crystal planes and directions can be represented by a set of \_\_\_\_\_ small integers. ( )
  - (a) 2
  - (b) 3
  - (c) 4
  - (d) 6
3. To represent crystal direction, the Miller indices should be enclosed in \_\_\_\_\_ ( )
  - (a) square brackets
  - (b) round brackets
  - (c) curly brackets
  - (d) none
4. If the Miller indices of two planes are (211) and (422), then they are: ( )
  - (a) parallel
  - (b) perpendicular
  - (c) they are at an angle of  $45^\circ$
  - (d) none
5. If the Miller indices of a plane along Y and Z-direction is zero, then: ( )
  - (a) the plane is perpendicular to X-axis
  - (b) the plane is parallel to Y-axis
  - (c) the plane is parallel to X-axis
  - (d) the plane is parallel to Z-axis
6. If the Miller indices of a plane is  $(b\bar{k}l)$ , then the plane: ( )
  - (a) intersects negative X-axis
  - (b) intersects negative Z-axis
  - (c) intersects negative Y-axis
  - (d) intersects positive Y-axis
7. If  $\{bkl\}$  are the Miller indices in cubic system, they represent: ( )
  - (a) (100) and  $(\bar{1}00)$  planes
  - (b) (010) and  $(0\bar{1}0)$  planes
  - (c) (001) and  $(00\bar{1})$  planes
  - (d) all
8. The Miller indices  $\langle bkl \rangle$  in cubic system represent the following directions: ( )
  - (a)  $[\bar{1}\bar{1}1]$ ,  $[\bar{1}\bar{1}\bar{1}]$  and  $[1\bar{1}\bar{1}]$
  - (b)  $[\bar{1}\bar{1}\bar{1}]$ ,  $[\bar{1}\bar{1}\bar{1}]$  and  $[\bar{1}\bar{1}\bar{1}]$
  - (c)  $[1\bar{1}1]$  and  $[\bar{1}\bar{1}\bar{1}]$
  - (d) all
9. If  $(bkl)$  represents the Miller indices of planes in cubic crystal of lattice constant ' $a$ ', the separation between the parallel planes is: ( )
  - (a)  $\frac{a}{b^2 + k^2 + l^2}$
  - (b)  $\frac{a}{b + k + l}$
  - (c)  $\frac{a}{\sqrt{b^2 + k^2 + l^2}}$
  - (d)  $\frac{a}{\sqrt{b + k + l}}$
10. Crystal defects are: ( )
  - (a) point and line defects
  - (b) surface defects
  - (c) volume defects
  - (d) all
11. Point defects are: ( )
  - (a) lattice site defects
  - (b) compositional defects
  - (c) electronic defects
  - (d) all
12. Electrical charge neutrality is maintained in: ( )
  - (a) Schottky defect
  - (b) Frenkel defect
  - (c) both a and b
  - (d) none

13. Schottky defect may exist in: ( )  
 (a) NaCl crystal (b) KCl crystal  
 (c) KBr crystal (d) all

14. Substitutional defect and interstitial impurity defect belong to: ( )  
 (a) compositional defect (b) Schottky defect  
 (c) Frenkel defect (d) lattice site defects

15. Non-uniformity of charge or energy distribution in the crystal is referred to as: ( )  
 (a) point defect (b) electronic defect  
 (c) Schottky defect (d) Frenkel defect

16. Point defects in crystals are formed by: ( )  
 (a) thermal fluctuations (b) Large deformation  
 (c) bombarding with high energetic particles (d) all

17. Edge dislocation and screw dislocation belong to: ( )  
 (a) electronic defects (b) compositional defects  
 (c) line defects (d) point defects

18. Just above the edge of an incomplete crystal plane in a crystal, the bond distances are \_\_\_\_\_. ( )  
 (a) equal to normal values (b) lesser than normal values  
 (c) greater than normal values (d) none

19. If the incomplete plane is below the slip plane, then the edge dislocation is: ( )  
 (a) positive (b) negative  
 (c) both a and b (d) none

20. In edge dislocation, the Burger's vector is \_\_\_\_\_ to the dislocation line. ( )  
 (a) parallel (b) at an angle of  $45^\circ$   
 (c) perpendicular (d) at an angle of  $60^\circ$

21. If  $E_v$  is the energy required to form a vacancy in the crystal containing ' $N$ ' atoms at temperature ' $T$ ', the number of vacancies in the crystal is [ $K_B$  = Boltzmann constant] ( )

(a)  $N \exp\left[\frac{-E_v}{K_B T}\right]$  (b)  $N \exp\left[\frac{-K_B T}{E_v}\right]$   
 (c)  $N \exp\left[\frac{E_v}{K_B T}\right]$  (d)  $N \exp\left[\frac{-E_v}{2K_B T}\right]$

22. If  $E_p$  is the energy required to move an anion-cation pair from interior to the surface of an ionic crystal containing  $N$  pairs of ions, the formation of  $n$  pairs of vacancies at temperature ' $T$ ' is given by [ $K_B$  = Boltzmann constant] ( )

(a)  $N \exp\left[\frac{-E_p}{K_B T}\right]$  (b)  $N \exp\left[\frac{E_p}{2K_B T}\right]$   
 (c)  $N \exp\left[\frac{-E_p}{2K_B T}\right]$  (d)  $N \exp\left[\frac{E_p}{K_B T}\right]$

23. Let  $E_i$  is the energy required to move a cation [positive ion] to the interstitial space of an ionic crystal containing ' $N$ ' number of atoms and  $N_i$  be the number of interstitial spaces. The number of ways  $n$  cations are moved to interstitial spaces, at temperature  $T$  is given by [ $K_B$  = Boltzmann constant] ( )
- (a)  $(NN_i)^{1/2} \exp\left(\frac{-E_i}{2K_B T}\right)$       (b)  $(NN_i)^{1/2} \exp\left(\frac{E_i}{2K_B T}\right)$   
 (c)  $(NN_i)^{1/2} \exp\left(\frac{-E_i}{K_B T}\right)$       (d)  $(NN_i) \exp\left(\frac{-E_i}{2K_B T}\right)$
24. If a monochromatic X-ray of wavelength ' $\lambda$ ' incident at an angle ' $\theta$ ' on a parallel set of crystal planes of separation ' $d$ ', then the Bragg's law for constructive interference is [ $n = 1, 2, 3, \dots$  = order of diffraction] ( )
- (a)  $2d \sin \theta = n\lambda$       (b)  $d \sin \theta = n\lambda$   
 (c)  $2\lambda \sin \theta = nd$       (d)  $\lambda \sin \theta = nd$
25. Miller indices of the plane parallel to X and Y axes are: ( )
- (a) (001)      (b) (010)      (c) (100)      (d) (111)
26. The crystal planes are defined as some imaginary planes inside a crystal in which \_\_\_\_\_ of atoms are present. ( )
- (a) large concentration      (b) low concentration  
 (c) medium concentration      (d) none
27. Crystal planes and directions can be represented by a set of three small integers called: ( )
- (a) plane indices      (b) Miller indices      (c) direction indices      (d) none
28. If the Miller indices are enclosed in round brackets, then it represents a crystal ( )
- (a) plane      (b) direction      (c) set of directions      (d) system of planes
29. Miller indices may be defined as a set of three integers obtained by clearing the reciprocals of the \_\_\_\_\_ made by a plane on crystallographic axes. ( )
- (a) intercepts      (b) relations      (c) both a and b      (d) none
30. Miller indices represent a set of equidistant \_\_\_\_\_ planes. ( )
- (a) perpendicular      (b) intersecting  
 (c) parallel      (d) none
31. If  $(hkl)$  is the Miller indices of a plane, then the plane divides the lattice constant ' $a$ ' along 'X' axis into \_\_\_\_\_. ( )
- (a)  $h$  equal parts      (b)  $k$  equal parts      (c)  $l$  equal parts      (d) all
32. Point defects in crystals are also called as \_\_\_\_\_ defects. ( )
- (a) three-dimensional      (b) two-dimensional  
 (c) one-dimensional      (d) zero-dimensional
33. By moving an anion and a cation from interior of an ionic crystal to the surface of the crystal leads to \_\_\_\_\_ defect. ( )
- (a) Frenkel      (b) Schottky      (c) both a and b      (d) none

34. Vacancies and interstitial defects belong to \_\_\_\_\_ defects. ( )  
(a) lattice site      (b) Schottky      (c) Frenkel      (d) none
35. The crystal defect formed by moving a cation to interstitial spaces in an ionic crystal is known as \_\_\_\_\_ defect. ( )  
(a) Schottky      (b) point defect      (c) Frenkel      (d) none
36. Examples for Frenkel defect ( )  
(a)  $\text{CaF}_2$       (b)  $\text{AgBr}$       (c)  $\text{AgI}$       (d) all
37. Presence of impure atoms in the crystal leads to \_\_\_\_\_ defects. ( )  
(a) Schottky      (b) Frenkel      (c) compositional      (d) none
38. If ' $r$ ' is the radius of a parent atom of a crystal, then octahedral and tetrahedral spaces can accommodate an interstitial atom of radius \_\_\_\_\_ and \_\_\_\_\_, respectively. ( )  
(a)  $0.414r, 0.225r$       (b)  $0.225r, 0.414r$   
(c)  $0.0225r, 0.0414r$       (d)  $0.0414r, 0.0225r$
39. Extrinsic semiconductors contain \_\_\_\_\_ crystal defect. ( )  
(a) interstitial      (b) substitutional      (c) Frenkel      (d) Schottky
40. Just below the edge of an incomplete crystal plane in a crystal, the bond distances are \_\_\_\_\_ normal values. ( )  
(a) same as      (b) more than      (c) less than      (d) none
41. If a crystal plane ends some where inside the crystal, then the defect along the edge of the incomplete plane is called \_\_\_\_\_. ( )  
(a) edge dislocation      (b) screw dislocation  
(c) Schottky defect      (d) interstitial defect
42. If the incomplete plane is above the slip plane in the crystal, then the edge dislocation is: ( )  
(a) Schottky      (b) Frenkel      (c) negative      (d) positive
43. The magnitude and direction of the displacement of crystal planes due to edge dislocation can be represented by a vector called: ( )  
(a) Burger's vector      (b) Laue's vector      (c) both a and b      (d) none
44. In screw dislocation, the atoms at one end of a plane are displaced by \_\_\_\_\_ distance with respect to the other end of the plane, perpendicular to plane. ( )  
(a) 3 atomic      (b) 2 atomic      (c) 1 atomic      (d) none
45. In screw dislocation, Burger's vector is \_\_\_\_\_ to dislocation line. ( )  
(a) perpendicular      (b) parallel      (c) both a and b      (d) none
46. By decreasing the equilibrium temperature of a crystal, the concentration of vacancies \_\_\_\_\_. ( )  
(a) decreases      (b) increases      (c) remains the same      (d) none
47. To produce diffraction with X-rays, the spacing between the consecutive lines of grating should be of the order of \_\_\_\_\_ angstroms. ( )  
(a) thousands of      (b) hundreds of      (c) few      (d) none

48. In 1912, Laue suggested that a crystal can serve as a \_\_\_\_\_ for X-ray diffraction. ( )

  - (a) three-dimensional grating
  - (b) two-dimensional grating
  - (c) one-dimensional grating
  - (d) none of the above

49. \_\_\_\_\_ and \_\_\_\_\_ succeeded in diffracting X-rays by passing through a thin crystal. ( )

  - (a) Friedrich and Knipping
  - (b) Bragg and Knipping
  - (c) Friedrich and Laue
  - (d) none of the above

50. If the path difference between the X-rays reflected by successive crystal planes is  $\frac{\lambda}{2}, \frac{3\lambda}{2}, \frac{5\lambda}{2}, \dots$ , then the intensity of diffracted ray: ( )

  - (a) will not change
  - (b) is minimum
  - (c) is maximum
  - (d) none

51. If the path difference between the X-rays reflected by successive crystal planes is  $n\lambda$ , where  $n = 1, 2, 3, \dots$ , then the intensity of diffracted ray: ( )

  - (a) is minimum
  - (b) is maximum
  - (c) remains the same
  - (d) none

52. X-ray powder method is usually carried for \_\_\_\_\_ materials. ( )

  - (a) polycrystalline
  - (b) powder
  - (c) single crystal
  - (d) amorphous

53. Using powder diffraction, \_\_\_\_\_ of a crystal can be determined. ( )

  - (a) the interatomic spacing
  - (b) the interplanar spacing
  - (c) both a and b
  - (d) none

54. In powder method, \_\_\_\_\_ chromatic X-rays are used. ( )

  - (a) mono
  - (b) poly
  - (c) both a and b
  - (d) none

55. In Laue method, \_\_\_\_\_ X-rays are used. ( )

  - (a) monochromatic
  - (b) white
  - (c) both a and b
  - (d) none

56. In transmission Laue method, the diffracted spots lie on the curves of: ( )

  - (a) ellipses
  - (b) hyperbolas
  - (c) a or b
  - (d) none

57. In back reflection Laue method, the diffracted spots lie on curves of: ( )

  - (a) hyperbola
  - (b) parabolas
  - (c) ellipses
  - (d) none

58. Laue method is useful to decide the \_\_\_\_\_ and orientation of the internal arrangement of atoms/molecules in the crystal. ( )

  - (a) cell parameters
  - (b) crystal symmetry
  - (c) both a and b
  - (d) none

59. The diffracted spots will be in the form of \_\_\_\_\_, if the crystal contains imperfections or strains. ( )

  - (a) streaks
  - (b) spots
  - (c) both a and b
  - (d) none

## Answers

- |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1. a  | 2. b  | 3. a  | 4. a  | 5. a  | 6. c  | 7. d  | 8. d  | 9. c  | 10. d | 11. d |
| 12. c | 13. d | 14. a | 15. b | 16. d | 17. c | 18. b | 19. b | 20. c | 21. a | 22. c |
| 23. a | 24. a | 25. a | 26. a | 27. b | 28. a | 29. a | 30. c | 31. a | 32. d | 33. b |
| 34. a | 35. c | 36. d | 37. c | 38. a | 39. b | 40. b | 41. a | 42. d | 43. a | 44. c |
| 45. b | 46. a | 47. c | 48. a | 49. a | 50. b | 51. b | 52. a | 53. b | 54. a | 55. b |
| 56. c | 57. a | 58. b | 59. a |       |       |       |       |       |       |       |

## Review Questions

1. Derive Bragg's law of X-ray diffraction.  
(Set-1–Sept. 2006), (Set-4–May 2006), (Set-3–May 2003), (Set-3–Nov. 2003)
2. What are Miller indices? How are they obtained?  
(Set-1–May 2006), (Set-1, Set-2, Set-3, Set-4–June 2005), (Set-4–Nov. 2004),  
(Set-1–May 2003), (Set-4–Nov. 2003)
3. Explain Schottky and Frenkel defects with the help of suitable figures.  
(Set-2–Sept. 2007), (Set-2–May 2007), (Set-4–Sept. 2006), (Set-1, Set-2, Set-3, Set-4–June 2005),  
(Set-4–Nov. 2004), (Set-1–May 2003), (Set-4–Nov. 2003)
4. State and explain Bragg's law.  
(Set-1–Sept. 2007), (Set-2, Set-3–Sept. 2006), (Set-2–May 2006), (Set-3–May 2004), (Set-4–May 2003)
5. Describe with a suitable diagram, the powder method for the determination of crystal structure.  
(Set-1–Sept. 2007), (Set-2–Sept. 2006), (Set-2, Set-3–May 2006), (Set-3–May 2004), (Set-4–May 2003)
6. Explain Bragg's law of X-ray diffraction.  
(Set-2, Set-4–Sept. 2007), (Set-2, Set-3, Set-4–May 2007), (Set-1–May 2006),  
(Set-4–Sept. 2006), (Set-3–Nov. 2004), (Set-2–May 2004)
7. Describe Laue's method for determination of crystal structure.  
(Set-2–May 2008), (Set-2, Set-4–Sept. 2007), (Set-3–May 2007),  
(Set-4–Sept. 2006), (Set-2–May 2004), (Set-3–May 2003)
8. Explain the significance of Miller indices.  
(Set-1–May 2004), (Set-2–May 2003)
9. Derive an expression for the number of Schottky defects in equilibrium at a temperature  $T$ .  
(Set-4–Sept. 2006), (Set-1–May 2004), (Set-2–May 2003)
10. Explain the various point defects in a crystal.  
(Set-1–Sept. 2007), (Set-1–Nov. 2004), (Set-1–Nov. 2003)
11. Obtain the expression for the equilibrium concentration of vacancies in a solid at a given temperature.  
(Set-1–Sept. 2007), (Set-1–Nov. 2004), (Set-1–Nov. 2003)
12. Deduce the expression for the interplanar distance in terms of Miller indices for a cubic structure.  
(Set-3–Sept. 2008), (Set-2–Nov. 2004), (Set-2–Nov. 2003)
13. Sketch the following planes of a cubic unit cell: (001), (120) and  $(\bar{2}11)$ .  
(Set-2–Sept. 2007), (Set-2–Nov. 2004), (Set-2–Nov. 2003)
14. Define Miller indices. Sketch the following atomic planes in a simple cubic structure (010), (110) and (111).  
(Set-4–May 2004)
15. How can the interplanar spacing of a set of Miller planes be calculated in terms of Lattice parameters?  
(Set-4–May 2004)
16. What is Bragg's law? Explain.  
(Set-2–May 2008)
17. What are Miller Indices? Draw (111) and (110) planes in a cubic lattice.  
(Set-2, Set-4–May 2007)
18. Draw the (112) and (120) planes and the [112] and [120] directions of a simple cubic crystal.  
(Set-1–May 2007)
19. Sketch the following planes of a cubic unit cell: (001), (120) and  $(\bar{2}11)$ .  
(Set-4–Sept. 2006)
20. What is Frenkel defect? Explain.  
(Set-1, Set-3–May 2007)

21. Describe edge and screw dislocations. Draw Burger's circuit and slip planes for them.  
(Set-4–Sept. 2007), (Set-4–May 2006)
22. Explain the significance to Burger's vector.  
(Set-2, Set-4–Sept. 2007), (Set-2–May 2007), (Set-3–Sept. 2006), (Set-4–May 2006)
23. Describe Bragg's X-ray spectrometer and explain how Bragg's law can be verified.  
(Set-1–Sept. 2006), (Set-4–May 2006)
24. Explain the influence of point defects in crystals and how do they affect the properties of materials.  
(Set-3–Sept. 2007)
25. Obtain an expression for the energy required to create a vacancy in the crystal.  
(Set-3–Sept. 2007)
26. Derive an expression for the interplanar spacing in the case of a cubic structure?  
(Set-1–May 2007)
27. Derive an expression for the energy change due to creation of vacancies inside a solid.  
(Set-2–May 2006)
28. Derive an expression for the concentration of Frenkel defects present in a crystal at any temperature.  
(Set-1, Set-3–May 2007)
29. Sketch the planes  $(120)$ ,  $(2\bar{1}3)$  and directions  $[100]$  and  $[211]$ .  
(Set-4–Sept. 2008)
30. Explain how the X-ray diffraction can be employed to determine the crystal structure. Give the ratio of interplanar distances of  $(100)$ ,  $(110)$  and  $(111)$  planes for a simple cubic structure.  
(Set-3–Sept. 2007), (Set-3–May 2006)
31. Distinguish between Frenkel defects and Schottky defects.  
(Set-2–May 2006)
32. Explain edge dislocation, screw dislocation and significance of Burger's vector.  
(Set-3–Sept. 2006)
33. Write short notes on Burger's vector in dislocations.
34. What are Miller indices? Derive an expression for the interplanar spacing between two adjacent planes of Miller indices  $(hkl)$  in a cubic lattice of edge length ' $a$ '.
35. Explain and illustrate, with neat sketches, the edge and screw dislocations; show the Burger's vector in them.
36. Write short notes on interstitial defects of crystals.
37. What are point defects in crystals? Derive an expression for the concentration of Schottky defect in a crystal.
38. Explain the principle, procedure and advantage of Debye–Scherrer method of X-ray diffraction.
39. Mention the different kinds of crystal imperfections.
40. Compare and contrast Frenkel and Schottky defects.
41. Write short notes on screw dislocation.
42. What are crystal imperfections? Explain.
43. Distinguish between edge and screw dislocations. What is Burger's vector?
44. Discuss the Schottky defect in the case of ionic crystals.
45. Explain the powder method of crystal structure analysis.
46. What are Miller indices? How they are determined?
47. Show that the number of Frenkel defects in equilibrium at a given temperature is proportional to  $(NN_i)^{1/2}$ , where  $N$  be the number of atoms and  $N_i$  be the number of interstitial atoms.
48. Obtain the Miller indices of a plane which intercepts at  $a$ ,  $b/2$  and  $3c$  in simple cubic unit cell. Draw a neat diagram showing the plane.

49. What do you understand by Miller indices of a crystal plane? Show that in a cubic crystal the spacing between consecutive parallel planes of Miller indices  $(hkl)$  is given by:

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

50. Define Schottky defect and derive an expression for the density of Schottky defects at a specified temperature.
51. Calculate the first nearest neighbour atom distance in ZnS (i.e., from Zn to S atoms) system.
52. Derive an expression for the interplanar distance in the case of cubic systems following Miller indices concept.
53. Define a Frenkel defect and derive an expression for the density of such defects as a function of temperature.
54. Write short notes on the Burger's vector in dislocation with appropriate diagrams.
55. Derive the Bragg's law of X-ray diffraction and obtain the relation that connects the interplanar distance ' $d$ ' in orthogonal systems with lattice parameters  $a$ ,  $b$  and  $c$ .

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## C H A P T E R

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# 4

# Elements of Statistical Mechanics and Principles of Quantum Mechanics

## 4.1 Introduction

Statistical mechanics mainly deals with the distribution of identical, distinguishable and indistinguishable particles of a system in different states of the system. The number of ways, in which the particles can be arranged in different energy states depends on the distinguishability of the particles. Here we are going to see three different types of distributions: (i) Maxwell–Boltzmann distribution, (ii) Fermi–Dirac distribution and (iii) Bose–Einstein distribution.

## 4.2 Phase space

Let us consider a system consisting of a large number of particles. The state of a particle at an instant can be represented with three position and three momentum coordinates. To specify the position and momentum of a particle in a system, a six-dimensional space called phase space or  $\mu$ -space is used. Any point in this space can be represented with three position coordinates  $x, y, z$  and with three momentum coordinates  $P_x, P_y, P_z$ . The points in this space are called phase points or representative points. The phase space is considered to be divided into large number of small elements called cells or groups. The volume of each element is  $dx, dy, dz, dP_x, dP_y, dP_z$  and this is equal to  $\hbar^3$ . Each group possesses as a large number of phase points.

## 4.3 Maxwell–Boltzmann distribution

This distribution is applied to a macroscopic system consisting of a large number  $n$  of identical but distinguishable particles, such as gas molecules in a container. This distribution tells us the way of distribution of total energy  $E$  of the system among the various identical particles. Let us consider that the entire system is divided into groups of particles, such that in every group the particles have nearly the same energy.

## 4-2 | Applied Physics

Let the number of particles in the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, ... i<sup>th</sup>, ... groups be  $n_1, n_2, n_3, \dots, n_i, \dots$  respectively. Also assume that the energies of each particle in the 1<sup>st</sup> group is  $E_1$ , in the second group is  $E_2$  and so on. Let the degeneracy parameter be denoted by 'g' [or the number of electron states] in the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, ... i<sup>th</sup>, ... groups be  $g_1, g_2, g_3, \dots, g_i, \dots$  and so on respectively. In a given system the total number of particles is constant.

$$\text{i.e., } n = n_1 + n_2 + n_3 + \dots + n_i + \dots = \sum_i n_i = \text{constant}$$

Hence its derivative  $\sum_i \delta n_i = 0$  \_\_\_\_\_ (4.1)

The total energy of all particles present in different groups is equal to the energy of the system (E).

$$\text{i.e., } E = E_1 n_1 + E_2 n_2 + E_3 n_3 + \dots + E_i n_i + \dots = \sum_i E_i n_i = \text{constant}$$

$$\text{Hence its derivative } \sum_i \delta E_i n_i = 0 \quad \text{_____} \quad (4.2)$$

The probability of given distribution  $W$  is given by the product of two factors. The first factor is, the number of ways in which the groups of  $n_1, n_2, n_3, \dots, n_i, \dots$  particles can be chosen. To obtain this, first we choose  $n_1$  particles which are to be placed in the first group. This is done in  $n C_{n_1}$  ways.

$$\text{i.e., } \frac{n!}{n_1!(n-n_1)!}$$

The remaining total number of particles is  $(n - n_1)$ . Now, we rearrange  $n_2$  particles in the second group. This is done in  $(n - n_1) C_{n_2}$  ways

$$\text{i.e., } \frac{(n - n_1)!}{n_2!(n - n_1 - n_2)!}$$

$\therefore$  The number of ways in which the particles in all groups are chosen is

$$W_1 = \frac{n!}{n_1!(n-n_1)!} \times \frac{(n-n_1)!}{n_2!(n-n_1-n_2)!} \times \dots \\ = \frac{n!}{n_1! n_2! \dots n_i! \dots} = \frac{n!}{\prod_i n_i!} \quad \text{_____} \quad (4.3)$$

where  $\prod_i$  is the multiplication parameter

The second factor is the distribution of particles over the different states and is independent of each other.

Of the  $n_i$  particles in the  $i^{\text{th}}$  group the first particle can occupy any one of the  $g_i$  states. So there are  $g_i$  ways, and each of the subsequent particles can also occupy the remaining states in  $g_i$  ways. So, the total number of ways the  $n_i$  particles are distributed among the  $g_i$  states is  $g_i^{n_i}$  ways.

$\therefore$  The probability distribution or the total number of ways in which  $n$  particles can be distributed among the various energy states is  $W_2$

$$W_2 = (g_1)^{n_1} (g_2)^{n_2} (g_3)^{n_3} \dots (g_i)^{n_i} \dots = \prod_i (g_i)^{n_i} \quad \text{_____} \quad (4.4)$$

The number of different ways by which  $n$  particles of the system are to be distributed among the available electron states is

$$W = W_1 W_2 = \frac{n!}{n_1! n_2! n_3! \dots n_i! \dots} (g_1)^{n_1} (g_2)^{n_2} (g_3)^{n_3} \dots (g_i)^{n_i} \dots \quad \text{_____} \quad (4.5)$$

$$= \frac{n!}{\prod_i n_i!} \prod_i (g_i)^{n_i} = n! \prod_i \left[ \frac{g_i^{n_i}}{n_i!} \right] \quad \text{_____} \quad (4.6)$$

where  $\Pi_i$  represents the multiplication parameter

Taking natural logarithms on both sides of equation (4.5) we have,

$$\ln W = \ln n! - \sum_i \ln n_i! + \sum_i n_i \ln g_i \quad (4.7)$$

Applying Stirling's theorem,  $\ln x! = x \ln x - x$ , on equation (4.7)

$$\begin{aligned} \ln W &= n \ln n - n - \sum_i n_i \ln n_i + \sum_i n_i + \sum_i n_i \ln g_i \\ &= n \ln n - \sum_i n_i \ln n_i + \sum_i n_i \ln g_i \end{aligned} \quad (4.8)$$

For the most probable distribution,  $W$  is maximum provided  $n$  and  $E$  are constants. Differentiate equation (4.8) and equate to zero for maximum value of  $W$ .

$$\begin{aligned} \delta \ln W_{\max} = 0 &= -\sum_i n_i \frac{1}{n_i} \delta n_i - \sum_i (\ln n_i) \delta n_i + \sum_i (\ln g_i) \delta n_i \\ &= -\sum_i (\ln n_i) \delta n_i + \sum_i (\ln g_i) \delta n_i = 0 \quad (\because \sum_i \delta n_i = 0) \end{aligned} \quad (4.9)$$

Multiplying equation (4.1) by  $-\alpha$  and equation (4.2) by  $-\beta$  and adding to equation (4.9), we get

$$\sum_i [-\ln n_i + \ln g_i - \alpha - \beta E_i] \delta n_i = 0 \quad (4.10)$$

$$\text{or } -\ln n_i + \ln g_i - \alpha - \beta E_i = 0$$

$$\text{or } \ln \left( \frac{n_i}{g_i} \right) = -\alpha - \beta E_i$$

Taking exponential on both sides,

$$\frac{n_i}{g_i} = e^{-\alpha} e^{-\beta E_i} \quad (4.11)$$

Equation (4.11) is called Maxwell–Boltzmann (M-B) law. The value of  $\beta$  has been extracted separately and is equal to  $\frac{1}{k_B T}$ , where  $k_B$  = Boltzmann constant and

$T$  = absolute temperature

Equation (4.11) becomes

$$f_{MB}(E_i) = \frac{n_i}{g_i} = \frac{1}{e^{\alpha} e^{\frac{E_i}{k_B T}}}$$

## 4.4 Fermi–Dirac distribution

The Fermi–Dirac distribution is applicable to indistinguishable particles like electrons. They have a spin in the order of half-integral multiples of  $n$ . They obey Pauli exclusion principle (no two electrons in an atom have the same quantum state).

Hence occupation number is 0 or 1. Let the system contains ' $n$ ' number of indistinguishable particles possessing different energies  $E_1, E_2, \dots, E_i, \dots$ . Let the system be divided into groups. The  $i^{\text{th}}$  group contains  $n_i$  number of particles, distributed in  $g_i$  quantum states, all these particles have nearly the same energy  $E_i$ . First

## 4-4 | Applied Physics

we find out the number of ways in which these  $n_i$  particles can be distributed in  $g_i$  states with not more than one particle in a state, as follows.

First, the particles can be arranged in  $g_i$  ways. Secondly, the remaining particles are arranged in the  $(g_i - 1)$  states in  $(g_i - 1)$  ways. Thirdly, in the  $(g_i - 2)$  states in  $(g_i - 2)$  ways and so on. Therefore the total number of ways of arranging  $n_i$  particles is

$$g_i(g_i - 1)(g_i - 2) \cdots (g_i - n_i + 1) \cdots = \frac{g_i!}{(g_i - n_i)!} \quad (4.12)$$

Of these arrangements, the permutation  $n_i!$  of the  $n_i$  particles is not relevant, because of exclusion principle. Hence we have

$$= \frac{g_i!}{n_i!(g_i - n_i)!} \quad (4.13)$$

Here, the number of possible ways in which  $n_1$  particles may have energy  $E_1$  and  $n_2$  particles may have the energy  $E_2$  and so on for the other groups of the system. Therefore the total distribution for the complete system is given as

$$W = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!} \quad (4.14)$$

Taking logarithms on both sides of equation (4.14) we have

$$\ln W = \sum_i [\ln g_i! - \ln n_i! - \ln(g_i - n_i)!] \quad (4.15)$$

Applying Stirling's formula,  $\ln x! = x \ln x - x$ , on equation (4.15) we have

$$\begin{aligned} \ln W &= \sum_i [g_i \ln g_i - g_i - n_i \ln n_i + n_i - (g_i - n_i) \ln(g_i - n_i) + (g_i - n_i)] \\ &= \sum_i [g_i \ln g_i - n_i \ln n_i - (g_i - n_i) \ln(g_i - n_i)] \end{aligned} \quad (4.16)$$

For most probable distribution, the derivative of equation (4.16) is zero. We have

$$\begin{aligned} \delta \ln W &= 0 = \sum_i \left[ \frac{n_i}{n_i} \delta n_i - \ln n_i \delta n_i - \frac{(g_i - n_i)}{(g_i - n_i)} (-\delta n_i) + \ln(g_i - n_i) \delta n_i \right] \\ &= \sum_i [\ln(g_i - n_i) - \ln n_i] \delta n_i = 0 \end{aligned} \quad (4.17)$$

At equilibrium, the total number of particles in the system  $n$ , and the total energy of the system,  $E$  are constant, hence we have

$$\delta n = \sum_i \delta n_i = 0 \quad (4.18)$$

and

$$\delta E = \sum_i E_i \delta n_i = 0 \quad (4.19)$$

Applying the Lagrange method of undetermined multipliers, multiply equation (4.18) by  $-\alpha$  and equation (4.19) by  $-\beta$  and add to equation (4.17), we obtain

$$\sum_i [-\ln n_i + \ln(g_i - n_i) - \alpha - \beta E_i] \delta n_i = 0 \quad (4.20)$$

Since  $\delta_{ni}$  is arbitrarily chosen, the term in the bracket must be zero for each value of  $i$ .

$$\text{So, } -\ln n_i + \ln(g_i - n_i) - \alpha - \beta E_i = 0$$

$$\text{or } \ln \frac{(g_i - n_i)}{n_i} - \alpha - \beta E_i = 0$$

$$\text{or } \ln \left( \frac{g_i - n_i}{n_i} \right) = \alpha + \beta E_i$$

Taking exponential on both sides,

$$\frac{g_i - n_i}{n_i} = e^{\alpha + \beta E_i}$$

$$\text{or } \frac{g_i}{n_i} - 1 = e^{\alpha + \beta E_i}$$

$$\text{or } \frac{g_i}{n_i} = 1 + e^{\alpha + \beta E_i}$$

$$\text{or } \frac{n_i}{g_i} = \frac{1}{1 + e^{\alpha + \beta E_i}}$$

The Fermi-Dirac distribution function is

$$f_{F-D}(E_i) = \frac{n_i}{g_i} = \frac{1}{1 + e^{\alpha e^{\beta E_i}}} \quad (4.21)$$

Here  $\frac{n_i}{g_i}$  represents the average number of particles in each of the quantum states of that energy.

Dropping the subscript 'i' and substituting the values of  $\alpha = \frac{-E_F}{k_B T}$  and  $\beta = \frac{1}{k_B T}$  equation (4.21) becomes

$$f_{F-D}(E) = \frac{1}{e^{-\frac{E_F}{k_B T}} e^{\frac{E}{k_B T}} + 1} = \frac{1}{1 + e^{\frac{(E-E_F)}{k_B T}}} \quad (4.22)$$

## 4.5 Bose-Einstein distribution

The Bose-Einstein distribution deals with the distribution of identical indistinguishable particles like photons or phonons called bosons. They possess spin of integral multiple of  $n$ . Let the system contains  $n$  number of particles. The system is divided into groups. Let  $n_1$  number of particles have each of energy  $E_1$  are present in 1<sup>st</sup> group has  $g_1$  states and  $n_2$  number of particles have each of energy  $E_2$  present in the 2<sup>nd</sup> group which has  $g_2$  states and so on.

The number of ways of distributing  $n_i$  particles among the  $g_i$  states is as follows. The  $g_i$  states will have  $(g_i - 1)$  partitions. The  $(g_i - 1)$  partitions and  $n_i$  particles constitute  $(g_i + n_i - 1)$  objects. They can be arranged in  $(g_i + n_i - 1)!$  ways among themselves. Whereas  $n_i$  particles can be arranged in  $n_i!$  ways among themselves and  $(g_i - 1)$  partitions in  $(g_i - 1)!$  ways among themselves. The effective number of ways of arranging them is

$$W_i = \frac{(g_i + n_i - 1)!}{n_i! (g_i - 1)!} \quad (4.23)$$

Similar expressions can be written for other quantum states. Therefore, the total number of ways of distinct arrangement of all the 'n' particles of the system in various available states is  $W$

$$W = \frac{(n_1 + g_1 - 1)!}{n_1! (g_1 - 1)!} \dots \frac{(n_2 + g_2 - 1)!}{n_2! (g_2 - 1)!} \dots \frac{(n_i + g_i - 1)!}{n_i! (g_i - 1)!} \dots$$

## 4-6 | Applied Physics

$$= \prod_i \frac{(n_i + g_i - 1)!}{(n_i)!(g_i - 1)!} \quad (4.24)$$

Taking logarithms of equation (4.24), we have

$$\ln W = \sum_i [\ln(n_i + g_i - 1)! - \ln n_i! - \ln(g_i - 1)!] \quad (4.25)$$

Using Stirling's approximation,  $\ln x! = x \ln x - x$ , equation (4.25) becomes

$$\begin{aligned} \ln W &= \sum_i [(n_i + g_i - 1) \ln(n_i + g_i - 1) - n_i \ln n_i - (g_i - 1) \ln(g_i - 1)] \\ &= \sum_i [(n_i + g_i) \ln(n_i + g_i) - n_i \ln n_i - g_i \ln g_i] \end{aligned} \quad (4.26)$$

Here, we neglected 1 in comparison to  $n_i$  and  $g_i$  as they are very large numbers.

Differentiating equation (4.26)

$$\begin{aligned} \delta \ln W &= \sum_i \left[ \delta n_i \ln(n_i + g_i) + \frac{(n_i + g_i)}{(n_i + g_i)} \delta n_i - \delta n_i \ln n_i - \frac{n_i}{n_i} \delta n_i \right] \\ &= \sum_i [\delta n_i \ln(n_i + g_i) - \delta n_i \ln n_i] = -\sum_i \left[ \ln \left( \frac{n_i}{n_i + g_i} \right) \right] \delta n_i \end{aligned} \quad (4.27)$$

For maximum probability the condition is  $\delta \ln W = 0$

$$\therefore \sum_i \left[ -\ln \left( \frac{n_i}{n_i + g_i} \right) \right] \delta n_i = 0 \quad (4.28)$$

As the total number of particles in the system  $n$  and the total energy of the system  $E$  are constant, hence their derivatives are equal to zero.

$$\text{i.e., } \delta_n = \sum_i \delta n_i = 0 \quad (4.29)$$

and

$$\delta E = \sum_i E_i \delta n_i = 0 \quad (4.30)$$

Applying the Lagrange method of undetermined multipliers i.e., multiplying equation (4.29) by  $-\alpha$  and equation (4.30) by  $-\beta$  and adding to equation (4.28), we get

$$\begin{aligned} \sum_i \left[ -\ln \left( \frac{n_i}{n_i + g_i} \right) - \alpha - \beta E_i \right] \delta n_i &= 0 \\ \text{or } \ln \left( \frac{n_i + g_i}{n_i} \right) &= \alpha + \beta E_i \end{aligned} \quad (4.31)$$

Taking exponential on both sides of equation (4.31), we have

$$\frac{n_i + g_i}{n_i} = e^{\alpha + \beta E_i}$$

$$\text{or } 1 + \frac{g_i}{n_i} = e^{\alpha + \beta E_i}$$

$$\begin{aligned} \text{or } \frac{g_i}{n_i} &= e^{\alpha + \beta E_i} - 1 \\ &= e^\alpha e^{\beta E_i} - 1 \end{aligned}$$

Hence, the Bose–Einstein's distribution function is

$$f_{B-E}^{(E_i)} = \frac{n_i}{g_i} = \frac{1}{e^{\alpha} e^{\beta E_i} - 1} = \frac{1}{e^{\alpha} e^{\frac{E_i}{k_B T}} - 1} \quad (4.32)$$

When  $k_B$  = Boltzmann constant Since  $\beta = \frac{1}{k_B T}$

## 4.6 Comparison of Maxwell–Boltzmann, Fermi–Dirac and Bose–Einstein distributions

Parameter	Maxwell – Boltzmann distribution	Fermi – Dirac distribution	Bose – Einstein distribution
1. System of particles	Applies to identical, distinguishable particles	Applies to identical indistinguishable particles which obey Pauli exclusion principle	Applies to identical indistinguishable particles, which will not obey Pauli exclusion principle.
2. Distribution of particles	Any number of particles can occupy a state	Not more than one particle per state	No limit to number of particles per state
3. Spin properties of particles	Any spin	Half-integral multiples of $\hbar$	Integral multiples of $\hbar$
4. Examples	Gas molecules	Free electrons in a metal	Photons and phonons
5. Distribution function $f(E_i)$	$\frac{1}{e^{\alpha - \frac{E_i}{k_B T}}}$	$\frac{1}{1 + \exp\left(\frac{E_i - E_t}{k_B T}\right)}$	$\frac{1}{e^{\alpha - \frac{E_i}{k_B T}} - 1}$

## 4.7 Photon gas

Einstein proposed the concept of localized small packets of light energy. This is similar to Planck's idea of quanta and named such packets as photons. The energy of a photon is given by  $E = h\gamma$ , where  $h$  = Planck's constant.

According to Einstein, light is transmitted in terms of particles like photons. As the intensity of light beam increases, the photon density increases. Photons have particle character as well as wave character. Light contains a very large number of photons and when the particle character of light is considered, photons may be visualized as moving similar to gas molecules in a container, or free electrons in a metal (i.e., electron gas). Hence light photons is considered as photon gas.

## 4.8 Concept of electron gas and Fermi energy

### (a) Electron gas

A metal consists of immobile positive ions and free electrons. These free electrons are very large in metals. They move in random directions inside a metal as we see the gas molecules in a container. Hence they are referred to as the free electron gas or electron gas in short.

When an electric field is applied on metals, the free electrons drift in a direction opposite to the applied field. Free electrons participate in thermal and electrical conductivity. They obey gas laws.

### (b) Fermi energy

The electron gas obey Fermi-Dirac distribution. Let  $g(E)$  be the density of electron states. i.e., the number of available electron states per unit volume of metal in unit range of energies  $E$ . Let the number of electron-filled states be  $N(E)$  in  $g(E)$ . Then the Fermi-Dirac distribution function  $f(E)$  is

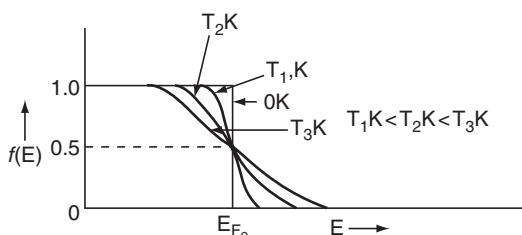
$$f(E) = \frac{N(E)}{g(E)} = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \quad (4.33)$$

The distribution function  $f(E)$  is defined as the probability that an energy level  $E$  is occupied by an electron. Suppose, if the level is empty then  $f(E) = 0$  or if the level is filled, then  $f(E) = 1$ . In general the value of  $f(E)$  lies in between 0 and 1.

$$\begin{aligned} \text{At } 0\text{K} \quad f(E) &= 1 \quad \text{for } E < E_F \\ &= 0 \quad \text{for } E > E_F \end{aligned} \quad (4.34)$$

This shows that all states below  $E_F$  are completely filled and all states above  $E_F$  are completely empty. This function is plotted in Fig. 4.1 for  $T = 0\text{K}$  and for higher temperatures. As temperature increases, the  $f(E)$  decreases below  $E_F$ . At higher temperatures the curves pass through a point at which the probability of the electron being in the conduction or valence band is 0.5. The energy at which the probability of occupation is 0.5 at all temperatures is called Fermi energy. Alternatively, the highest energy possessed by an electron at absolute zero of temperature (0K) in a metal is called Fermi energy.

**Figure 4.1** Fermi-Dirac distribution function for electrons



## 4.9 Density of electron states

The number of available electron states present per unit volume of a material in unit energy range at energy  $E$  is the density of electron states. To obtain an expression for the density of electron states, let us consider all possible energies of electrons in a material. The electrons are distributed in various electron states in three dimensional space. The electron states are considered in a quantum space. Let the coordinate axes of this space be represented by  $n_x, n_y, n_z$  with origin at 'O' as shown in Fig. 4.2. In this space, every point with integral values of coordinates represent an energy state or the unit volume of the space contains one electron state.

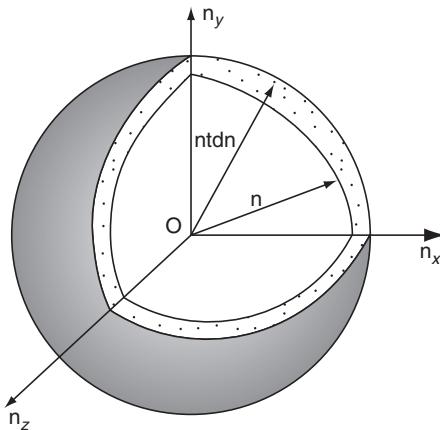
To find the density of states at energy,  $E$ , let us consider a sphere of radius  $n$  such that the origin of the sphere coincides with the origin of the coordinate system. The energy of a state on the surface of the sphere is  $E$ . A point on the surface of the sphere can be represented with  $n_x, n_y, n_z$  such that

$$n^2 = n_x^2 + n_y^2 + n_z^2 \quad (4.35)$$

The numbers of electron states inside a sphere is equal to the volume of the sphere in the positive quadrant.  
 $\therefore$  The number of available electron states within a sphere of radius  $n$  is

$$g_1(E) = \frac{1}{8} \left( \frac{4}{3} \pi n^3 \right) = \frac{\pi}{6} n^3 \quad (4.36)$$

**Figure 4.2 Density of electron states sphere**



Similarly, the number of available electron states in a sphere of radius  $(n + dn)$  is

$$g_2(E + dE) = \frac{1}{8} \left[ \frac{4}{3} \pi (n + dn)^3 \right] = \frac{\pi}{6} (n + dn)^3 \quad (4.37)$$

The number of electron states whose energies lie between  $E$  and  $E + dE$  is obtained by subtracting equation (4.36) from equation (4.37).

$$\begin{aligned} g'(E)dE &= g_2(E + dE) - g_1(E) = \frac{\pi}{6} (n + dn)^3 - \frac{\pi}{6} n^3 \\ &= \frac{\pi}{6} [n^3 + 3n^2dn + 3ndn^2 + dn^3 - n^3] \\ &\approx \frac{\pi}{6} 3n^2dn = \frac{\pi}{2} n^2dn = \frac{\pi}{2} n(ndn) \end{aligned} \quad (4.38)$$

(neglecting higher power terms, because they are very small)

The expression for energies of electrons in a cubical box of side  $a$  is given by

$$E = \frac{n^2 h^2}{8ma^2} \quad \text{or} \quad n^2 = \frac{8ma^2 E}{h^2} \quad (4.39)$$

$$\therefore n = \left[ \frac{8ma^2 E}{h^2} \right]^{\frac{1}{2}} \quad (4.40)$$

Differentiate equation (4.39) with respect to  $n$ . We get,

$$\begin{aligned} 2ndn &= \frac{8ma^2}{h^2} dE \\ \text{or} \quad ndn &= \frac{1}{2} \left( \frac{8ma^2}{h^2} \right) dE \end{aligned} \quad (4.41)$$

Substituting equation (4.40) and equation (4.41) in equation (4.38) gives

$$\begin{aligned} g'(E)dt &= \frac{\pi}{2} \left( \frac{8ma^2 E}{b^2} \right)^{\frac{1}{2}} \times \frac{1}{2} \left( \frac{8ma^2}{b^2} \right) dE \\ &= \frac{\pi}{2} \left( \frac{8ma^2}{b^2} \right)^{\frac{1}{2}} E^{\frac{1}{2}} \times \frac{1}{2} \left( \frac{8ma^2}{b^2} \right) dE \\ &= \frac{\pi}{4} \left( \frac{8ma^2}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \quad (4.42) \end{aligned}$$

According to Pauli's exclusion principle, each state can accommodate two electrons of opposite spin, hence the number of electron energy states available for electron occupancy is

$$\begin{aligned} g''(E)dE &= 2 \times \frac{\pi}{4} \left( \frac{8ma^2}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \\ &= \frac{\pi}{4} \left( \frac{8ma^2}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \\ &= \frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} a^3 E^{\frac{1}{2}} dE \quad (4.43) \end{aligned}$$

Density of states is given as the number of energy states per unit volume.

$\therefore$  Density of states between  $E$  and  $E + dE$  is

$$g(E)dE = \frac{g''(E)dE}{a^3} = \frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \quad (4.44)$$

This is a parabolic function.

## 4.10 Black body radiation

A body that completely absorbs all wave lengths of radiation incident on it at low temperatures or emits different wave lengths of radiation at higher temperatures is known as a black body. A black body may be idealized by a small hole drilled in a cavity. A graph has been plotted between intensity (or energy density spectral) versus wave length of radiation from a black body. The temperature of the body is raised to different values and distribution curves are plotted for different temperatures as shown in Fig. 4.3. From the graph it has been observed that:

- (i) the intensity of radiation increases for each wave length as the temperature of the body increases.
- (ii) At any given temperature, the intensity of radiation from the body is maximum for a particular wave length represented as  $\lambda_{1m}, \lambda_{2m}, \lambda_{3m}, \dots$ . This wave length shifts towards shorter wave length region with increase of temperature.
- (iii) The area under the curve is proportional to the total radiation energy emitted by the body in unit time.

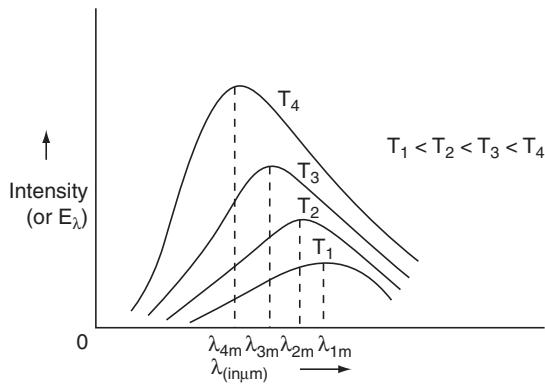
The spectral energy distribution of black body has been explained by many scientists as given below.

**(a) Wien's law:** Wien showed that the maximum energy,  $E_m$  of the emitted radiation from black body is proportional to fifth power of absolute temperature ( $T^5$ )

$$\text{i.e } E_m \propto T^5 \quad \text{or} \quad E_m = \text{constant} \times T^5.$$

Figure 4.3

Graphs drawn between intensity versus wavelength of radiation from black body at different temperatures



Wien deduced the relation between the wave length of emission and the temperature of the body as

$$U_\lambda d\lambda = \frac{C_1}{\lambda^5} e^{-\left[\frac{C_2}{\lambda T}\right]} d\lambda = 8 \frac{\pi c b}{\lambda^5} \left[ \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} \right] d\lambda$$

where  $U_\lambda d\lambda$  is the energy per unit volume in the wave length range  $\lambda$  and  $\lambda + d\lambda$ . Here  $C_1$  and  $C_2$  are constants.

Wien's law is valid at lower wave length region, where as it deviates from experimental values at higher wave length regions. This is shown in Fig. 4.4.

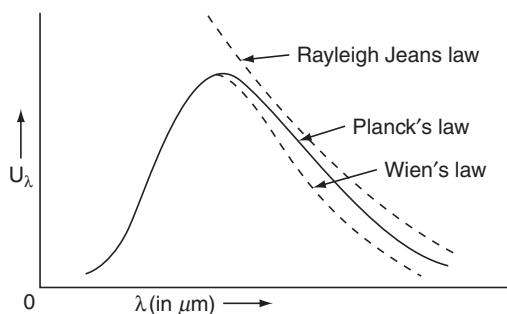
**(b) Rayleigh-Jeans law:** Rayleigh deduced an equation for the black body radiation based on the principle of equipartition of energy. According to equipartition of energy, each mode of vibration has assigned an average energy of  $k_B T$ . The number of vibrations per unit volume in the wave length range  $\lambda$  and  $\lambda + d\lambda$  is given by  $8\pi\lambda^{-4}d\lambda$ . The vibration energy per unit volume in the range of  $\lambda$  and  $\lambda + d\lambda$  is

$$U_\lambda d\lambda = 8\pi k_B T \lambda^{-4} d\lambda$$

This is the Rayleigh-Jeans equation. This law correctly predicts the fall of intensity in the longer wave length side. However, it fails to explain the lower wave length side of the spectrum.

Figure 4.4

The three laws of black body radiation



**(c) Planck's law:** Planck assumed that the walls of the black body consists of a large number of electrical oscillators, vibrating with their own natural frequencies. An oscillator possesses an energy equal to  $h\gamma$ . Where  $h$  is Planck's constant and  $\gamma$  is the frequency of the oscillator.

An oscillator may lose or gain energy by emitting or by absorbing photons respectively. Planck derived an equation for the energy per unit volume of black body in the entire spectrum of black body radiation. It is given by

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \left[ \frac{1}{e^{\frac{h\lambda}{k_B T}}} - 1 \right] d\lambda$$

This is Planck's law.

## 4.11 Waves and particles—de Broglie hypothesis—Matter waves

Classical theory of Newtonian mechanics successfully explains the motion of macroscopic particles, but fails to explain the motion of microscopic particles such as electrons. Whereas, the quantum theory successfully explains the motion of microscopic particles, interference, diffraction and polarization of electromagnetic waves, black body radiation (1901), photoelectric effect (1905), line spectra (1913) and Compton effect (1924), etc. Explanation of the above effects by quantum theory shows the dual nature of waves [wave nature and particle nature]. To explain some of the above facts, we consider packets of energy [photons] and waves. For example, in case of photoelectric effect when photons of sufficient energy or radiation of frequency above a certain value incident on an alkali metal, then electrons are emitted. In this case, absorption of energy does not take place continuously but in the form of packets of energy called quanta (photons). These photons have particle nature. In case of Compton effect, a photon of certain energy makes collision with a stationary electron, after collision the electron and photon get scattered with lesser energy (or longer wavelength). To explain the collision of photon and electron, we consider the particle nature of light wave. With this background, a French scientist de Broglie in the year 1924, proposed the dual nature of matter.

According to him, moving objects and particles possess wave nature. The dual nature of matter was explained by combining Planck's equation for energy of a photon,  $E = h\nu$  and Einstein's mass and energy relation  $E = mc^2$

$$\text{i.e., } h\nu = mc^2 \quad (4.45)$$

where  $h$  = Planck's constant,  $\nu$  = frequency of radiation and  $c$  = velocity of light.

$$\text{We know the velocity of light } c = \nu\lambda \quad (\text{or}) \quad \nu = \frac{c}{\lambda} \quad (4.46)$$

Substituting equation (4.46) in (4.45) gives:

$$\frac{hc}{\lambda} = mc^2 \quad (\text{or}) \quad \frac{h}{\lambda} = mc = p$$

where  $p$  = momentum and  $\lambda$  is the wavelength of photon.

$$\therefore \lambda = \frac{h}{p} \quad (4.47)$$

The above equation indicates that a photon is associated with a momentum  $p$ . From this, de Broglie proposed the concept of matter waves. According to de Broglie, a particle of mass  $m$ , moving with velocity ' $v$ ' is associated with a wave called matter wave or de Broglie wave of wavelength  $\lambda$ , given by:

$$\lambda = \frac{h}{p} = \frac{h}{\text{momentum}} = \frac{h}{mv} \quad (4.48)$$

This is known as de Broglie equation.

According to the theory of relativity, the mass  $m$  used in the above equation is not constant but varies with its velocity, given by:

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (4.49)$$

where  $m_0$  is the rest mass of the particle.

Suppose an electron is accelerated to a velocity ' $v$ ' by passing through a potential difference  $V$ , then work done on the electron,  $eV$  is equal to increase in its K.E.

$$\text{i.e., } \frac{1}{2}mv^2 = eV \quad (\text{or}) \quad v = \left( \frac{2eV}{m} \right)^{1/2}$$

and  $mv = (2meV)^{1/2}$  = momentum of an electron.

Substituting this momentum in de Broglie equation,

$$\text{We have } \lambda = \frac{h}{p} = \frac{h}{(2meV)^{1/2}}$$

taking  $m \approx m_0$ , rest mass of an electron, the above equation becomes:

$$\begin{aligned} \lambda &= \frac{h}{\sqrt{2meV}} = \frac{6.62 \times 10^{-34}}{\sqrt{2 \times 9.11 \times 10^{-31} \times 1.6 \times 10^{-19} V}} \text{ m} \\ &= \frac{12.27}{\sqrt{V}} \times 10^{-10} \text{ m} = \frac{1.227}{\sqrt{V}} \text{ nm} \end{aligned}$$

Suppose an electron is accelerated through a potential difference of 100 V, it is associated with a wave of wavelength equal to 0.1227 nm.

## Matter waves

The de Broglie concept that a moving particle is associated with a wave can be explained by using one of the postulates of Bohr's atomic model.

The angular momentum ( $L$ ) of a moving electron in an atomic orbit of radius ' $r$ ' is quantized in terms of  $\hbar$ . So, we have:

$$L = mvr = n\hbar = \frac{n\hbar}{2\pi} \quad (4.50)$$

where  $v$  = Linear velocity of an electron

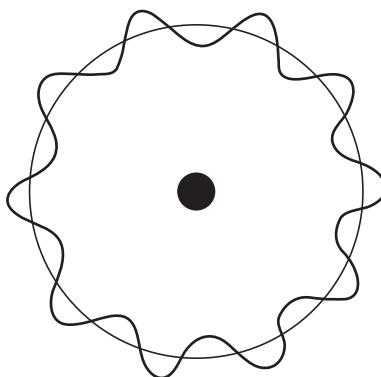
$n$  = an integer

Equation (4.50) can be written as:

$$2\pi r = \frac{n\hbar}{mv} = \frac{n\hbar}{p} = n\lambda \quad (4.51)$$

In the above equation,  $2\pi r$  is the circumference length of the orbit and it is equal to  $n$  times the wavelength of the associated wave of a moving electron in the orbit. This can be diagrammatically represented for  $n = 10$  in Fig. 4.5.

**Figure 4.5 Bohr's orbit and de Broglie waves of an electron in the orbit**



According to de Broglie, a moving particle behaves as a wave and as a particle. The waves associated with a moving material particles are called matter waves or de Broglie waves. They are seen with particles like electrons, protons, neutrons, etc.

### Properties of matter waves

- de Broglie waves are not electromagnetic waves; they are called pilot waves, which means the waves that guide the particle. Matter waves consist of a group of waves or a wave packet associated with a particle. The group has the velocity of particle.
- Each wave of the group travel with a velocity known as phase velocity given as  $V_{ph} = \frac{\omega}{k}$ .
- These waves cannot be observed.
- The wavelength of these waves,  $\lambda = \frac{h}{p}$ .

## 4.12 Relativistic correction

When an electron is accelerated through a high potential difference ( $V$ ), then the mass of electron varies with its velocity. Hence, we have to consider its relativistic mass. Hence, we calculate its relativistic wavelength and total energy in the following way.

### (a) Relativistic wavelength is calculated as follows:

The momentum of an electron is:

$$p = mv = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (4.52)$$

Divide Equation (4.52) by  $m_0 c$ , then:

$$\frac{p}{m_0 c} = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \times \frac{1}{m_0 c} = \left[ \frac{v^2/c^2}{1 - v^2/c^2} \right]^{1/2}$$

Add and subtract 1 to the numerator,

$$\frac{p}{m_0 c} = \left[ \frac{-1 + \frac{v^2}{c^2} + 1}{1 - \frac{v^2}{c^2}} \right]^{1/2} = \left[ \frac{-1 + \frac{v^2}{c^2}}{1 - \frac{v^2}{c^2}} + \frac{1}{1 - \frac{v^2}{c^2}} \right]^{1/2} = \left[ -1 + \frac{1}{1 - \frac{v^2}{c^2}} \right]^{1/2} \quad (4.53)$$

Squaring and rearranging Equation (4.53),

$$1 + \frac{p^2}{m_0^2 c^2} = \frac{1}{1 - \frac{v^2}{c^2}} \quad (4.54)$$

The kinetic energy ( $E$ ) of an electron is given by:

$$\begin{aligned} E = mc^2 - m_0 c^2 &= \frac{m_0 c^2}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}} - m_0 c^2 \\ &= m_0 c^2 \left[ \frac{1}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}} - 1 \right] \quad (\text{or}) \quad \frac{E}{m_0 c^2} = \frac{1}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}} - 1 \end{aligned}$$

$$(\text{or}) \quad 1 + \frac{E}{m_0 c^2} = \frac{1}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}} \quad (4.55)$$

Squaring Equation (4.55) gives:

$$\left(1 + \frac{E}{m_0 c^2}\right)^2 = \frac{1}{1 - \frac{v^2}{c^2}} \quad (4.56)$$

Equating Equations (4.54) and (4.56), we get:

$$1 + \frac{p^2}{m_0^2 c^2} = \left(1 + \frac{E}{m_0 c^2}\right)^2 = 1 + \frac{2E}{m_0 c^2} + \frac{E^2}{m_0^2 c^4} \Rightarrow \frac{p^2}{m_0^2 c^2} = \frac{2E}{m_0^2 c^2} + \frac{E^2}{m_0^2 c^4} \quad (\text{or}) \quad p^2 = 2m_0 E + \frac{E^2}{c^2}$$

$$(\text{or}) \quad p = \sqrt{2m_0 E + \frac{E^2}{c^2}} \quad (4.57)$$

Substituting Equation (4.57) in de Broglie equation,  $\lambda = \frac{h}{p}$

$$\text{We have } \lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_0E + \frac{E^2}{c^2}}}$$

$$= \frac{h}{\left[ 2m_0E \left( 1 + \frac{E}{2m_0c^2} \right) \right]^{1/2}} = \frac{h}{\sqrt{2m_0E}} \times \left[ 1 + \frac{E}{2m_0c^2} \right]^{-1/2}$$

$$\lambda = \frac{h}{\sqrt{2m_0E}} \left[ 1 - \frac{E}{2 \times 2m_0c^2} \right] = \frac{h}{\sqrt{2m_0E}} \times \left[ 1 - \frac{E}{4m_0c^2} \right] \quad (4.58)$$

As the electron is accelerated through a potential  $V$ , then its kinetic energy ( $E$ ) =  $eV$ . So, Equation (4.58) becomes:

$$\lambda = \frac{h}{\sqrt{2m_0eV}} \left[ 1 - \frac{eV}{4m_0c^2} \right] = \frac{1.227}{\sqrt{V}} \left[ 1 - \frac{eV}{4m_0c^2} \right] \text{ nm} \quad (4.59)$$

Equation (4.15) represents, the relativistically corrected wavelength.

### (b) Relativistic formula for total energy is calculated as follows:

The rest mass ( $m_0$ ) equivalent energy of a particle is  $m_0c^2$  i.e.,  $E_0 = m_0c^2$

The mass equivalent energy of a particle when it is in motion is  $mc^2$  and this is equal to its total energy.

$$\text{where } m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

The total energy ( $E$ ) when it is in motion is:

$$E = mc^2 = \frac{m_0c^2}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{m_0c^2}{\sqrt{1 - \beta^2}} = \frac{E_0}{\sqrt{1 - \beta^2}} \quad (4.60)$$

$$\text{where } \beta = \frac{v}{c}$$

Squaring Equation (4.60),

$$E^2 = \frac{E_0^2}{1 - \beta^2} \quad (4.61)$$

Cross-multiplying Equation (4.61),

$$E^2 - \beta^2 E^2 = E_0^2$$

$$\text{(or)} \quad E^2 - E_0^2 = \beta^2 E^2 = (mc^2)^2 \frac{v^2}{c^2} = m^2 v^2 c^2$$

$$E^2 - E_0^2 = p^2 c^2 \quad \text{(or)} \quad E^2 = E_0^2 + (pc)^2$$

$$\therefore E = \sqrt{E_0^2 + (pc)^2} \quad \text{_____ (4.62)}$$

Equation (4.62) represents the relativistic total energy of the particle. Hence, kinetic energy of the electron = total energy – rest mass equivalent energy

$$= \sqrt{E_0^2 + (pc)^2} - m_0 c^2.$$

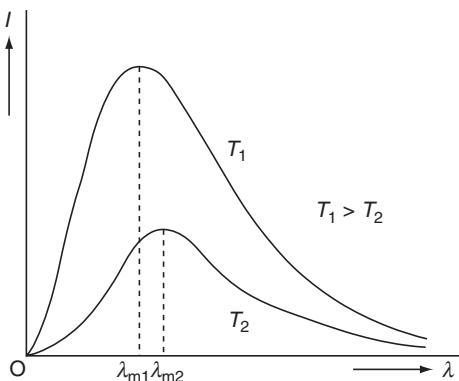
## 4.13 Planck's quantum theory of black body radiation

A body that absorbs all wavelengths of radiation at low temperatures and emits all wavelengths of radiation at high temperatures is known as black body. Figure 4.6 shows the graphs plotted between the intensities of emitted light and wavelengths at different temperatures. The area under the plot indicates total radiation ( $R$ ), the power emitted per unit area. According to Stefan–Boltzmann law, the radiation is proportional to  $T^4$ .

$$R = \sigma T^4 \quad \text{_____ (4.63)}$$

where  $\sigma$  is the Stefan–Boltzmann constant.

**Figure 4.6** Plots of black body radiation



Expression for the radiated energy density per unit wavelength range ( $R_\lambda$ ) was derived by Wien based on thermodynamics is:

$$R_\lambda = C_1 \lambda^{-5} e^{-C_2/\lambda T} \quad (4.64)$$

where  $C_1$  and  $C_2$  are constants. This formula explains the black body radiation in short wavelengths as shown in Fig. 4.3.

Rayleigh–Jean's derived another formula for  $R_\lambda$  based on statistical mechanics as:

$$R_\lambda = 8\pi K_B T \lambda^{-4} \quad (4.65)$$

where  $K_B$  = Boltzmann constant

The above formula could partly explain in the longer wavelength region as shown in Fig. 4.3.

In 1901, Max Planck proposed the particle character of radiation similar to Newton's corpuscular theory known as Planck's quantum theory. According to this theory,

- (1) The black body walls contain large number of oscillators having different frequencies.
- (2) The energy radiated by an oscillator during transition from one quantum state to another is:

$$E = nh\nu \quad (4.66)$$

where  $n$  is an integer and  $h$  = Planck's constant

$h\nu$  is the quantum of energy. This shows that energy is radiated in the form of wave-packets. This energy packet has both wave and particle character. Based on this concept, Planck derived an expression for  $R_\lambda$  known as Planck's radiation law.

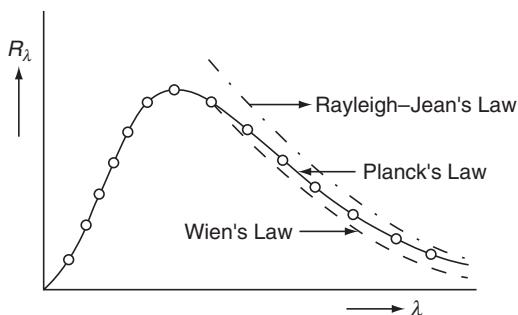
$$R_\lambda = \frac{8\pi}{\lambda^4} \frac{h\nu}{[e^{h\nu/K_B T} - 1]} \quad (4.67)$$

The above equation exactly fits the experimental graph shown in Fig. 4.7. The Planck's law, reduces to Wien's law when  $h\nu \gg K_B T$  and to Rayleigh–Jeans law when  $h\nu \ll K_B T$ .

Based on this Planck's quantum theory, Einstein developed the theory of relativity and successfully explained photoelectric effect. Raman effect of light, Compton effect of X-rays, etc., support Planck's quantum theory.

Figure 4.7

Comparison of the three radiation laws with the experimental curve [shown with dots]



## 4.14 Experimental study of matter waves

de Broglie proposed matter waves but he did not prove it experimentally. Many scientists proved the existence of matter waves individually. In 1927, Davisson and Germer in the United States and in 1928 Thomson proved experimentally the existence of matter waves. Also, Stern and others showed the existence of matter waves in connection with molecular and atomic beams.

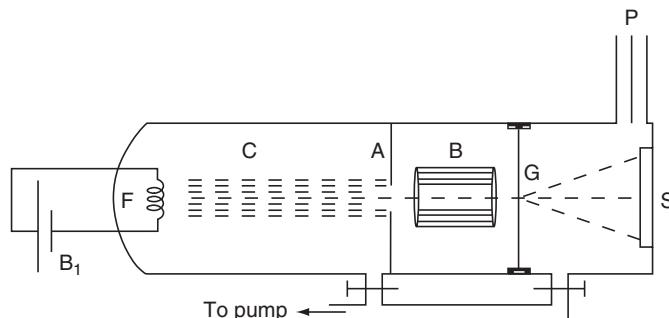
**(a) G.P. Thomson Experiment:** The diffraction of electrons by metal foil in G.P. Thomson experiment showed the wave nature of electrons and hence supports the de Broglie hypothesis. Now, we will study in detail the experimental set-up and theory of G.P. Thomson experiment. From the theory, we can estimate the wavelength of the waves associated with the moving electrons.

**Experimental set-up:** As shown in Fig. 4.8, the apparatus consists of a highly evacuated cylindrical tube 'C'. Inside the tube, electrons are produced by heating the filament 'F' with low-voltage source. The emitted electrons are attracted by the anode 'A' to which high positive voltage has been applied and the beam is allowed to pass through a fine hole in a metallic block 'B'. A fine narrow electron beam, which comes out from 'B' is allowed to fall on a polycrystalline thin gold foil 'G' of thickness  $10^{-8}$  m. The gold foil consists of a large number of micro-sized crystallites, which are oriented in random directions. Hence, the crystal planes of these crystallites are oriented in all possible directions in the gold foil. Some of the electrons incident on the crystal planes, which satisfy Bragg's law ( $2d \sin \theta = n\lambda$ ) gets reflected by the planes (or diffracted). In the Bragg's equation,  $d$  = interplanar spacings of crystal planes,  $\theta$  = diffraction angle,  $\lambda$  = wavelength of the waves associated with electrons and  $n$  = order of diffraction. The diffracted electrons will go in the form of concentric cones and fall on fluorescent screen (S) present at the end surface of the evacuated tube. So, we can see concentric circles of diffraction pattern on the fluorescent screen. To record the diffraction pattern, a photographic plate (P) can be inserted in front of fluorescent screen in the tube as shown in Fig. 4.8. We can see the diffraction pattern on the photographic plate after processing it. The diffraction pattern consists of a series of concentric diffracted rings corresponding to different diffraction orders. The diameter of these rings are measured.

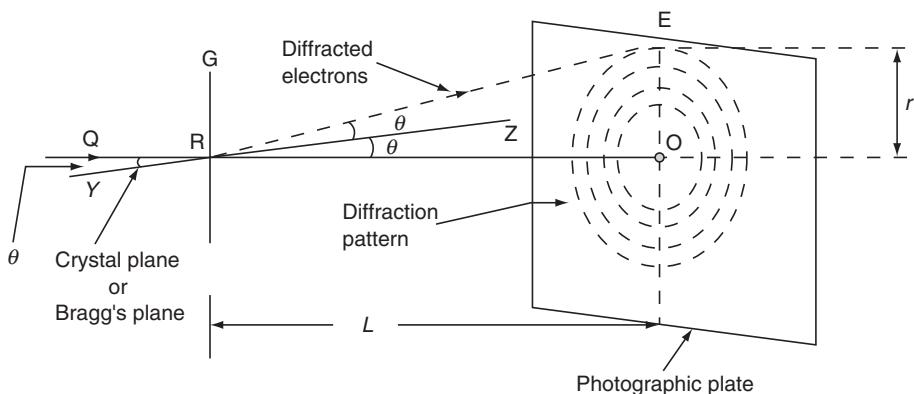
**Theory:** Figure 4.9 shows the diffraction of an electron beam by a crystal plane and the diffracted rings on photographic plate. In the theory of this experiment, we derive expressions for interplanar spacing and the de Broglie wavelength of waves associated with electrons.

**Expression for interplanar spacing:** As shown in Fig. 4.9, Let QR be an electron beam, which undergoes diffraction in the gold foil 'G' and falls on a photographic plate at a point E, at a distance  $r$  from the central

Figure 4.8    G.P. Thomson experimental set-up



**Figure 4.9 Schematic representation of electron diffraction in gold foil**



point 'O' of the concentric circles. Let the incident and the first-order diffracted electrons make an equal angle ' $\theta$ ' with the crystal plane YZ. Let RO = L, be the distance between gold foil and photographic plate.

Bragg's law is:

$$2d \sin \theta = n\lambda \quad \text{where } n = 1, 2, 3, \dots$$

For first-order diffraction ( $n = 1$ )

$$2d \sin \theta = 1\lambda \quad (\text{or}) \quad d = \frac{\lambda}{2 \sin \theta} \approx \frac{\lambda}{2\theta} \quad \text{_____ (4.68)} \quad [\text{as } \theta \text{ is small}]$$

$$\text{From Fig. 4.5, } \tan 2\theta = \frac{r}{L} \quad \text{also} \quad \tan 2\theta \approx 2\theta \quad [\text{Since } \theta \text{ is small}]$$

$$\text{So} \quad 2\theta = \frac{r}{L} \quad \text{_____ (4.69)}$$

Substituting Equation (4.69) in (4.68) gives:

$$d = \frac{\lambda}{(r/L)} = \frac{L}{r} \lambda \quad \text{_____ (4.70)}$$

**To find the de Broglie wavelength of an electron:** In G.P. Thomson's experiment, the particles [electrons] are accelerated by a potential difference of about 25 to 60 KV. Let an electron be accelerated to a velocity ' $v$ '. Then the moving electron is associated with a wave. The de Broglie wavelength of this electron is given by:

$$\lambda = \frac{h}{mv} = \frac{h}{m_0 \frac{v}{\sqrt{1 - \frac{v^2}{c^2}}}} \quad \text{_____ (4.71)}$$

The quantity  $\frac{v}{\sqrt{1 - \frac{v^2}{c^2}}}$  is obtained by equating the increase in kinetic energy of the electron to workdone on it by the accelerating potential [i.e.,  $eV$ ]

According to the theory of relativity, the increase in kinetic energy of an electron ( $E$ ) is:

$$E = mc^2 - m_0 c^2$$

where  $m_0$  = rest mass of an electron,

$m$  = relativistic mass when it is moving with velocity ' $v$ ' and

$c$  = velocity of light

$$\therefore E = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}} - m_0 c^2 = m_0 c^2 \left[ \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right] \quad (4.72)$$

Since this gain in kinetic energy is equal to  $eV$ .

$$\text{i.e.,} \quad E = eV$$

$$= m_0 c^2 \left[ \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right] = eV$$

$$\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = 1 + \frac{eV}{m_0 c^2} \quad (4.73)$$

Equation (4.73) is a part of Equation (4.71)

Again ' $v$ ' can be evaluated from Equation (4.73) in the following way. In Equation (4.73), put  $\frac{eV}{m_0 c^2} = x$ .

$$\text{Then,} \quad \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = 1 + x \quad (4.74)$$

Squaring and inverting Equation (4.74),

$$1 - \frac{v^2}{c^2} = (1 + x)^{-2} \quad (\text{or}) \quad \frac{v^2}{c^2} = 1 - (1 + x)^{-2}$$

$$(\text{or}) \quad v = c \left[ 1 - (1 + x)^{-2} \right]^{\frac{1}{2}} \quad (4.75)$$

Multiplying Equations (4.74) and (4.75),

$$\begin{aligned}
 \frac{v}{\sqrt{1 - \frac{v^2}{c^2}}} &= c \left[ 1 - (1+x)^{-2} \right]^{1/2} [1+x] \\
 &= c \left[ \left\{ 1 - (1+x)^{-2} \right\} (1+x)^2 \right]^{1/2} = c \left[ (1+x)^2 - 1 \right]^{1/2} \\
 &= c \left[ 2x + x^2 \right]^{1/2} \\
 \frac{v}{\sqrt{1 - \frac{v^2}{c^2}}} &= c \left[ 2x \left( 1 + \frac{x}{2} \right) \right]^{1/2} \quad \text{--- (4.76)}
 \end{aligned}$$

Substituting Equation (4.76) in (4.71), we have:

$$\lambda = \frac{b}{m_0 c \left[ 2x \left( 1 + \frac{x}{2} \right) \right]^{1/2}} = \frac{b \left[ 1 + \frac{x}{2} \right]^{-1/2}}{m_0 c [2x]^{1/2}}$$

Substituting the value of 'x', we have:

$$\lambda = \frac{b}{m_0 c \left[ \frac{2eV}{m_0 c^2} \right]^{1/2} \left[ 1 + \frac{eV}{2m_0 c^2} \right]^{-1/2}} = \frac{b}{\sqrt{2m_0 eV}} \left[ 1 + \frac{eV}{2m_0 c^2} \right]^{-1/2} \quad \text{--- (4.77)}$$

Equation (4.77) represents the relativistic expression for de Broglie wavelength of an electron accelerated through a high potential difference of 'V' volts. If the relativistic effect is ignored, then Equation (4.77) reduces to:

$$\lambda = \frac{b}{\sqrt{2m_0 eV}} \quad \text{--- (4.78)}$$

Substituting Equation (4.77) in (4.70), we get:

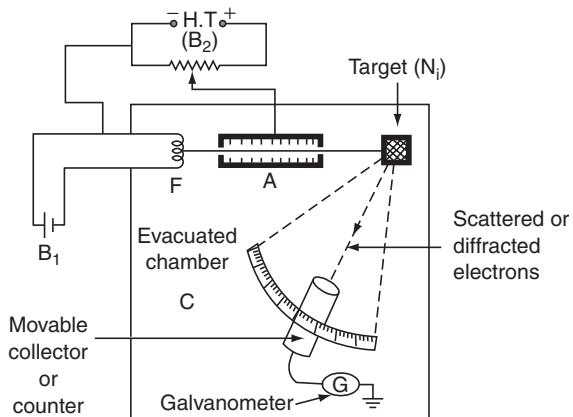
$$d = \frac{L\lambda}{r} = \frac{L}{r} \frac{b}{\sqrt{2m_0 eV}} \left[ 1 + \frac{eV}{2m_0 c^2} \right]^{-1/2} \quad \text{--- (4.79)}$$

The value of 'd' calculated using the above equation agree very well with that of the value obtained using X-ray method. This suggests the validity of this experiment. For example, the values of 'd' obtained by G.P. Thomson and X-ray method are 4.08 Å and 4.06 Å, respectively for gold foil.

**(b) The Davisson and Germer experiment:** This experiment proved the de Broglie hypothesis of matter waves of electrons in 1927. The original aim of this experiment was to find the intensity of scattered

electrons by a metal target in different directions. The experimental arrangement of this experiment is shown in Fig. 4.10. The apparatus consists of an evacuated chamber 'C'; inside this chamber, electrons are produced by heating the filament 'F' with a low-voltage battery  $B_1$ . The emitted electrons are attracted by

**Figure 4.10 Davisson and Germer experimental arrangement**



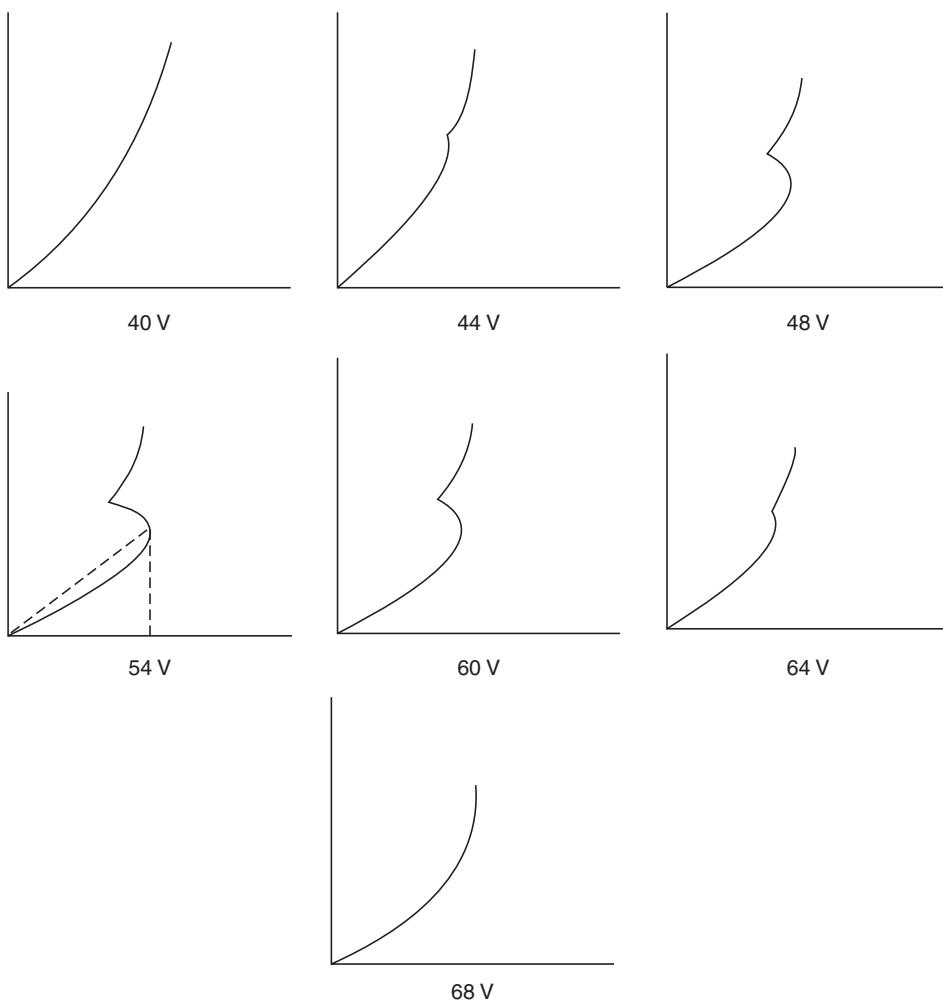
a cylindrical anode 'A' to which high variable positive voltage is applied with battery  $B_2$  and a potential divider. A narrow fine beam of electrons is obtained by passing the electrons through a series of pin hole arrangement present inside the cylindrical anode. This beam of electrons is allowed to incident on a single nickel crystal. This nickel crystal acts as a target material. The target is rotated about an axis perpendicular to the plane of the paper to bring various crystal planes for electron scattering. Nickel crystallizes in cubic system so that the crystal possess three-fold symmetry. The intensities of the scattered electrons are measured with the help of electron collector by moving it along a circular scale. The counter can be rotated about the same axis as the target. The counter receives the scattered electrons ranging from  $20^\circ$  to  $90^\circ$  with respect to the incident beam. The accelerating potential to anode is varied in the range of 30 to 600 V. The electrons received by the counter are allowed to pass through a galvanometer and earthed. The deflection in the galvanometer is proportional to the number of scattered electrons received by the counter in unit time. The galvanometer readings are noted when the counter is at different angles with respect to the incident beam, as the crystal is rotated through  $360^\circ$  in its own plane for different accelerating voltages. There are three variables in the experiment, these being the potential applied to the anode, the position of the collector and number of electrons collected by the counter in unit time or galvanometer reading.

Graphs are plotted between galvanometer readings [or the number of electrons collected per unit time] against the angles of scattered electrons with incident beam [i.e., angle of galvanometer with incident beam] for different accelerating voltages as shown in Fig. 4.11.

The graph remains fairly smooth till the accelerating voltage is less than 44 V. When the accelerating voltage is 44 V, then a spur is observed on the curve. The spur becomes more clear as the voltage reaches 54 V. The spur diminishes afterwards, above 68 V the spur disappears as shown in Fig. 4.11. The voltage and position of the collector are kept fixed at values corresponding to the largest spur and the crystal is rotated. The spur appears thrice in a complete rotation of the crystal corresponding to the three-fold symmetry of the crystal. Subordinate maxima occurs at the intermediate positions. From this, we know that the intensity of scattered [or diffracted] electrons is maximum at an angle of  $50^\circ$  with incident beam, when the accelerating voltage is 54 V in case of nickel crystal. The accelerating voltage sets up the correct wavelength

Figure 4.11

Curve showing the development of diffracted beam in the setting of crystal face



of waves associated with the electrons incident on the nickel crystal for diffraction to take place with  $50^\circ$  scattering angle in this experiment. We know that incident and diffracted electron beam makes an angle  $[\theta]$  of  $65^\circ$  with the family of Bragg's planes [a set of parallel crystal planes] as shown in Fig. 4.12.

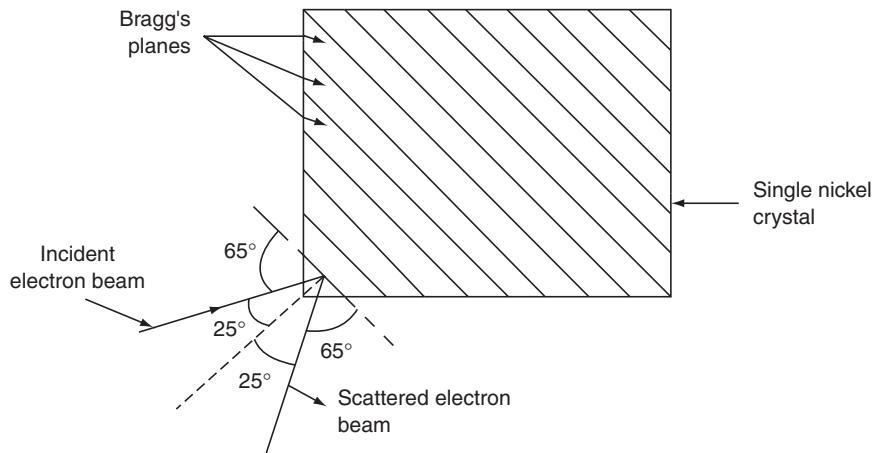
The above diffracted angle ( $\theta$ ) is substituted in Bragg's diffraction formula  $2d \sin \theta = n\lambda$ , where  $d$  = interplanar spacing,  $n$  = order of diffraction and  $\lambda$  is wavelength. The interplanar spacing in nickel crystal can be determined using X-rays, it comes to  $0.091 \text{ nm}$ . Substituting the experimental values for first-order diffraction [ $n = 1$ ] in Bragg's law,

$$\text{we have } 2d \sin \theta = 1\lambda$$

$$2 \times 0.091 \times 10^{-9} \times \sin 65^\circ = \lambda$$

$$\therefore \lambda = 0.165 \text{ nm.}$$

**Figure 4.12** Electron diffraction in nickel crystal



Wavelength of the waves associated with the incident beam of electrons in this experiment can also be obtained by applying de Broglie equation:

$$\lambda = \frac{1.227}{\sqrt{V}} \text{ nm}$$

In the above experiment, the electron diffraction is maximum for an accelerating voltage of 54 V, so the wavelength associated with these electrons is:

$$\lambda = \frac{1.227}{\sqrt{54}} = 0.166 \text{ nm}$$

This value is in very good agreement with the experimental value [0.165 nm]. Thus, this experiment proves the de Broglie hypothesis of the wave nature of moving particles.

## 4.14 Schrödinger's time-independent wave equation

Based on de Broglie's idea of matter waves, Schrödinger derived a mathematical equation known as Schrödinger's wave equation. To derive Schrödinger's wave equation, consider a particle of mass ' $m$ ' moving freely along X-direction [one dimensional] with velocity  $v$ . This moving particle is associated with a de Broglie wave of wavelength ' $\lambda$ ' and has frequency ' $\nu$ '. The expression for the displacement of a de Broglie wave associated with a moving particle is similar to an expression for undamped harmonic waves:

$$\Psi(x, t) = A \exp \left[ -i\omega \left( t - \frac{x}{v} \right) \right] \quad (4.80)$$

where  $\omega = 2\pi\nu$  = angular frequency and  $v = \nu\lambda$  = velocity of the wave.  $\Psi$  is called wave function, it is function of  $x$  and  $t$ . Substituting the values of  $\omega$  and  $v$  in Equation (4.80), we have:

$$\begin{aligned}\Psi &= A \exp \left[ -2\pi i \nu \left( t - \frac{x}{\nu \lambda} \right) \right] \\ &= A \exp \left[ -2\pi i \left( \nu t - \frac{x}{\lambda} \right) \right] \quad (4.81)\end{aligned}$$

The energy of the wave can be represented by Planck's equation  $E = h\nu$  (or)  $\nu = E/h$  and the de Broglie wavelength,  $\lambda = h/p$ . The values of  $\nu$  and  $\lambda$  are substituted in Equation (4.81).

$$\begin{aligned}\text{So, } \Psi(x, t) &= A \exp \left[ -2\pi i \left( \frac{Et}{h} - \frac{px}{h} \right) \right] \\ &= A \exp \left[ \frac{-2\pi i}{h} (Et - px) \right] \\ &= A \exp \left[ \frac{-i}{\hbar} (Et - px) \right] \quad (4.82)\end{aligned}$$

where  $\hbar = \frac{h}{2\pi}$  in quantum mechanics. The above equation represents wave function for a freely moving

particle along X-direction. If the particle is subjected to external fields or forces, then Equation (4.82) is not valid. In such cases, we have to obtain a differential equation and solving that differential equation in specific situations give  $\Psi$ . To obtain the differential equation, differentiate Equation (4.82) twice with respect to 'x' and once with respect to 't' and substitute in the energy equation for the particle.

$$\begin{aligned}\frac{\partial \Psi}{\partial x} &= A \exp \left[ -\frac{i}{\hbar} (Et - px) \right] \left[ \frac{i p}{\hbar} \right] \\ \frac{\partial^2 \Psi}{\partial x^2} &= A \exp \left[ -\frac{i}{\hbar} (Et - px) \right] \left[ \frac{i^2 p^2}{\hbar^2} \right] \\ \frac{\partial^2 \Psi}{\partial x^2} &= \frac{-p^2}{\hbar^2} \Psi \quad (\text{or}) \quad \hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = -P^2 \Psi \quad (4.83)\end{aligned}$$

$$\begin{aligned}\text{And } \frac{\partial \Psi}{\partial t} &= A \exp \left[ -\frac{i}{\hbar} (Et - px) \right] \left[ -\frac{i E}{\hbar} \right] \\ \frac{\partial \Psi}{\partial t} &= -\frac{i E}{\hbar} \Psi \\ (\text{or}) \quad \frac{\hbar}{i} \frac{\partial \Psi}{\partial t} &= -E \Psi \quad (4.84)\end{aligned}$$

The total energy,  $E$  of the particle is the sum of kinetic energy and potential energy,  $V(x)$ .

$$\therefore E = \frac{1}{2} mv^2 + V(x)$$

$$= \frac{1}{2} \left( \frac{m^2 v^2}{m} \right) + V = \frac{p^2}{2m} + V$$

Multiplying both sides of the above equation with  $\Psi$ , we get:

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi \quad \text{_____ (4.85)}$$

Substituting Equations (4.83) and (4.84) in Equation (4.85), we get:

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

$$\text{(or)} \quad \frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - V\Psi \quad \text{_____ (4.86)}$$

The above equation is known as time-dependent, one-dimensional Schrödinger's wave equation. In three dimensions, it can be represented as:

$$\frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = \left( \frac{\hbar^2}{2m} \right) \left[ \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] - V\Psi \quad \text{_____ (4.87)}$$

Here,  $\Psi$  is a function of  $x, y, z$  and  $t$ .

[The differential operator  $\vec{\nabla} = \vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y} + \vec{k} \frac{\partial}{\partial z}$  where  $\vec{i}, \vec{j}$  and  $\vec{k}$  are unit vectors along X, Y and Z directions]

Using Laplacian operator  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  in Equation (4.88)

$$\text{We have} \quad \frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \Psi - V\Psi \quad \text{_____ (4.89)}$$

In many cases, the potential energy depends on the position only and independent of time. To obtain time-independent wave equation, Equation (4.82) can be represented as:

$$\begin{aligned} \Psi &= A \exp \left( -\frac{iEt}{\hbar} \right) \exp \left( \frac{ipx}{\hbar} \right) \\ &= A\varphi(t)\psi(x) \quad \text{_____ (4.90)} \end{aligned}$$

$$\text{where} \quad \varphi(t) = \exp \left( -\frac{iEt}{\hbar} \right) \quad \text{and} \quad \psi(x) = \exp \left( \frac{ipx}{\hbar} \right)$$

Here,  $\Psi$  is a function of  $x$  and  $t$  whereas  $\psi$  is a function of  $x$  alone and  $\varphi$  is a function of ' $t$ ' alone. Equation (4.90) can be represented as:

$$\Psi = A\psi \exp \left( -\frac{iEt}{\hbar} \right) \quad \text{_____ (4.91)}$$

Differentiating Equation (4.91) twice w.r.t. 'x' and once w.r.t. 't' and substituting in Equation (4.86), we have:

$$\frac{\partial \Psi}{\partial x} = A \exp\left(-\frac{iEt}{\hbar}\right) \frac{d\psi}{dx} \quad \text{and} \quad \frac{\partial^2 \Psi}{\partial x^2} = A \exp\left(-\frac{iEt}{\hbar}\right) \frac{d^2\psi}{dx^2} \quad (4.92)$$

$$\text{and} \quad \frac{\partial \Psi}{\partial t} = A \psi \exp\left(-\frac{iEt}{\hbar}\right) \left(\frac{-iE}{\hbar}\right) = \frac{-AiE\psi}{\hbar} \exp\left(-\frac{iEt}{\hbar}\right) \quad (4.93)$$

Substituting Equations (4.92) and (4.93) in Equation (4.87), we get:

$$\begin{aligned} \left(\frac{-\hbar}{i}\right) \left(\frac{AiE\psi}{\hbar}\right) \exp\left(-\frac{iEt}{\hbar}\right) &= \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} A \exp\left(-\frac{iEt}{\hbar}\right) - VA\psi \exp\left(-\frac{iEt}{\hbar}\right) \\ -E\psi &= \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V\psi \quad (\text{or}) \quad \left(\frac{\hbar^2}{2m}\right) \frac{d^2\psi}{dx^2} + E\psi - V\psi = 0 \\ (\text{or}) \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi &= 0 \end{aligned} \quad (4.94)$$

Equation (4.94) is the time-independent one-dimensional Schrödinger's wave equation. In three dimensions, it is represented as:

$$\begin{aligned} \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \psi &= 0 \\ (\text{or}) \quad \nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi &= 0 \end{aligned} \quad (4.95)$$

Here,  $\psi$  is a function of  $x, y$  and  $z$  only and independent of time.

## 4.15 Heisenberg uncertainty principle

Heisenberg proposed the uncertainty principle in connection with the dual nature of waves and particles. The uncertainty principle has been explained in the following way: suppose if a particle is moving along X-direction, then according to uncertainty principle, it is impossible to measure accurately simultaneously its position ( $x$ ) and also its momentum ( $p_x$ ). If  $\Delta x$  is the uncertainty in measuring its position then  $\Delta p_x$  is the uncertainty in measuring its momentum.

Then,

$$\Delta x \Delta p_x \gtrsim h \quad (4.96)$$

where  $h$  is Planck's constant

The above equation is applicable in all directions. Along Y- and Z- directions, it is:

$$\Delta y \Delta p_y \gtrsim h \quad \text{and} \quad \Delta z \Delta p_z \gtrsim h \quad (4.97)$$

The above uncertainty has been already proved using diffraction of electrons by a long narrow slit.

The uncertainties  $\Delta x$  and  $\Delta p_x$  associated with the simultaneous measurement of  $x$  and  $p_x$  can be explained by considering the diffraction of electrons by a narrow slit as follows:

As shown in Fig. 4.13, let us consider a beam of electrons pass through a long narrow slit of width  $d$ , let the momentum of electrons along X-direction is negligible.

As the electrons enter the slit, there will be spreading due to diffraction. Let the diffraction angle is  $\Delta\theta$ , such that:

$$\Delta\theta \approx \frac{\lambda}{d} \quad (\text{For diffraction through a single slit})$$

So, that an electron acquires momentum along X-direction given by:

$$\Delta p_x \approx p\Delta\theta \approx p \frac{\lambda}{d} \quad \text{or} \quad \Delta p_x \approx p \frac{\lambda}{d} \quad [\text{Using above equation; } p = \text{momentum of an electron}]$$

As the electron pass through the slit, the uncertainty in simultaneous measurement of position along X-direction is  $\Delta x \approx d$ , then the above equation becomes:

$$\Delta p_x \approx p \frac{\lambda}{\Delta x} \quad \text{or} \quad \Delta p_x \Delta x \approx p\lambda \quad \text{or} \quad \Delta p_x \Delta x \approx h \quad [\text{using the Broglie equation, } \lambda = \frac{h}{p}]$$

Thus, the uncertainty principle is explained.

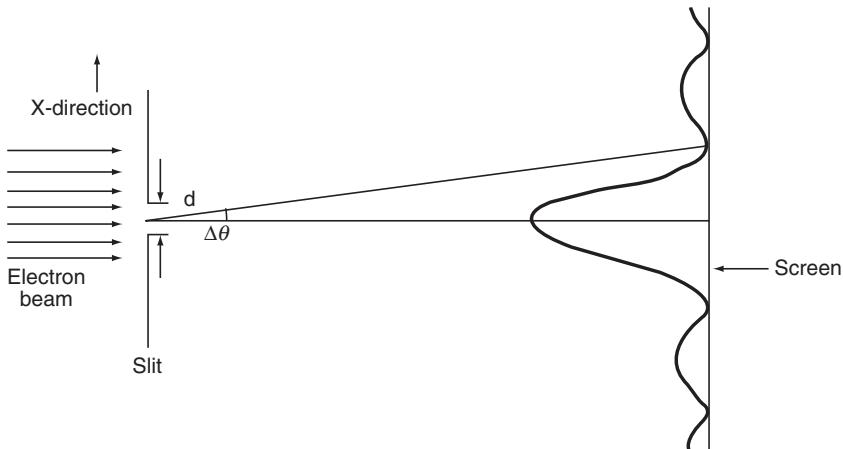
Similar to uncertainty in position and momentum, we have uncertainty in measuring time and energy of a wave packet. The uncertainty relation is:

$$\Delta E \Delta t \gtrsim h \quad (4.98)$$

Suppose the uncertainty in the energy determination of a wave packet is  $\Delta E \approx \frac{h}{\Delta t}$ , then the maximum time available for energy determination is  $\Delta t$ .

The time-energy uncertainty can be explained by considering the wave packet moving with velocity  $v$  along X-direction and let it occupies a region  $\Delta x$ . The uncertainty in passing this particle at a given point is:

**Figure 4.13 Diffraction of electron beam by a narrow slit**



$$\Delta t \approx \frac{\Delta x}{v} \quad \text{_____} \quad (4.99)$$

As the packet is localized to a region  $\Delta x$ , then the spread in the momentum is  $\Delta p$ , so,

$$\Delta p \geq \frac{\hbar}{\Delta x} \quad \text{_____} \quad (4.100)$$

$$\text{or} \quad \Delta x \geq \frac{\hbar}{\Delta p} \quad \text{_____} \quad (4.101)$$

Substitute Equation (4.101) in (4.99). Then,

$$\Delta t \gtrsim \frac{\hbar}{v \Delta p}$$

$$\text{or} \quad \Delta t v \Delta p \gtrsim \hbar \quad \text{_____} \quad (4.102)$$

$$\text{But} \quad \Delta E \approx \frac{\partial E}{\partial p} \Delta p = v \Delta p \quad \text{_____} \quad (4.103)$$

Substitute Equation (4.103) in (4.102)

$$\text{We have} \quad \Delta t \Delta E \gtrsim \hbar \quad \text{_____} \quad (4.104)$$

The above equation shows that the spread in the energy of a particle is  $\Delta E$ , then the uncertainty in passing that particle through a point is  $\Delta t$

$$\text{so that} \quad \Delta t \gtrsim \frac{\hbar}{\Delta E}.$$

## 4.16 Physical significance of the wave function

The wave function  $\Psi$  associated with a moving particle is not an observable quantity and does not have any direct physical meaning. It is a complex quantity. The complex wave function can be represented as  $\Psi(x, y, z, t) = a + ib$  and its complex conjugate as  $\Psi^*(x, y, z, t) = a - ib$ . The product of wave function and its complex conjugate is  $\Psi(x, y, z, t)\Psi^*(x, y, z, t) = (a + ib)(a - ib) = a^2 + b^2$  is a real quantity. However, this can represent the probability density of locating the particle at a place in a given instant of time. The positive square root of  $\Psi(x, y, z, t)\Psi^*(x, y, z, t)$  is represented as  $|\Psi(x, y, z, t)|$ , called the modulus of  $\Psi$ . The quantity  $|\Psi(x, y, z, t)|^2$  is called the probability density, denoted as  $P$ .

If a particle is moving in a volume  $V$ , then the probability of the particle in a volume element  $dV$ , surrounding the point  $x, y, z$  at an instant 't' is  $PdV$ .

$$PdV = \Psi(x, y, z, t) \Psi^*(x, y, z, t) dV = |\Psi(x, y, z, t)|^2 dV$$

Integrating this probability throughout the volume  $V$ , is equal to 1

$$\text{i.e.,} \quad \int |\Psi|^2 dV = 1$$

If the particle is not present in that volume, then  $\int |\Psi|^2 dV = 0$ .

For a particle moving along X-direction [one dimensional] the quantity,  $Pdx = \Psi(x, t) \Psi^*(x, t) dx = |\Psi(x, t)|^2 dx$ , represent the probability of the particle over a small distance 'dx', centred at  $x$ , at time 't'. The probability per unit distance [i.e.,  $dx = 1$ ] is called the probability density represented as  $|\Psi(x, t)|^2$ .

The wave function that satisfies time-independent wave equation has probability independent of time.

## 4.17 Particle in a potential box

A free electron (particle) in a metallic crystal may move freely inside the crystal from one place to another place but will not come out of the crystal because at the surface of the crystal, the electron experiences very large (infinite) potential [called potential barrier]. The potential barrier present at the surface [covering the metal surface] will act as a three-dimensional potential box for the free particle [electron]. This potential box can also be called as potential well because the electron will remain in that region only. For simplicity, first we see one-dimensional potential box [or potential well] and extend it to three-dimensional box.

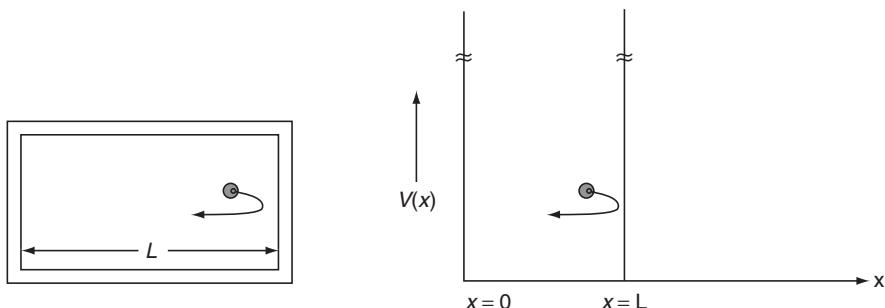
### (a) Particle in a one-dimensional box [or one dimensional potential well]

Suppose an electron (particle) of mass 'm' moves back and forth in a one-dimensional crystal of length 'L' parallel to X-direction. At the ends of the crystal, i.e., at  $x = 0$  and at  $x = L$ , two potential walls of infinite height exist, so that the particle may not penetrate the walls. Due to collisions, the energy of the particle does not change. Throughout the length 'L' of the box, the potential energy  $V$  of the particle is constant and this constant potential energy of the particle inside the box is considered to be equal to zero for all practical purposes. A plot of potential energy of an electron versus distance is shown in Fig. 4.14. As the particle is inside the box, then the probability of the particle inside the crystal,  $P = \psi\psi^*$  is equal to 1 and outside the well probability is equal to zero, hence  $\psi$  must be zero when  $0 \geq x \geq L$ .

Inside the box,  $V = 0$ , by solving one-dimensional Schrödinger's time-independent wave equation gives the motion of the particle inside the box. The study will show quantum numbers, discrete values of energy, zero-point energy and the wave function associated with the particle.

Figure 4.14

One dimensional potential box with potential walls of infinite height at  $x = 0$  and at  $x = L$



One-dimensional Schrödinger's time-independent equation is:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \quad \text{For the above case, } V = 0, \text{ so we have:}$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{_____ (4.105)}$$

$$(or) \quad \frac{d^2\psi}{dx^2} + K^2\psi = 0 \quad \text{_____ (4.106)}$$

$$\text{where} \quad K^2 = \frac{2mE}{\hbar^2} \quad \text{_____ (4.107)}$$

The  $K$  in Equation (4.107) is the wave vector,  $K = \frac{2\pi}{\lambda}$ , this can be shown easily using de Broglie

hypothesis in the total energy of the particles. The total energy  $E$  is equated to K.E because P.E of an electron is considered as zero in this case.

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\text{From de Broglie hypothesis,} \quad p = \frac{\hbar}{\lambda} = \frac{\hbar}{2\pi/K} = \hbar K$$

$$\therefore E = \frac{p^2}{2m} = \frac{\hbar^2 K^2}{2m}$$

$$\text{From this,} \quad K^2 = \frac{2mE}{\hbar^2}$$

A solution for Equation (4.106) is of the form  $\psi = e^{\alpha x}$  \_\_\_\_\_ (4.108)

Differentiating Equation (4.109) twice with respect to  $x$  and substituting in Equation (4.60) gives:

$$\frac{d\psi}{dx} = \alpha e^{\alpha x} \quad \text{and} \quad \frac{d^2\psi}{dx^2} = \alpha^2 e^{\alpha x} = \alpha^2 \psi \quad \text{_____ (4.109)}$$

Substituting in Equation (4.106), we have:

$$\alpha^2 \psi + K^2 \psi = 0$$

$$\alpha^2 + K^2 = 0 \Rightarrow \alpha = \pm iK$$

The two solutions of  $\psi$  are  $\psi_1 = e^{iKx}$  and  $\psi_2 = e^{-iKx}$

$\therefore$  The general solution will be of the form:

$$\psi(x) = ae^{\alpha_1 x} + be^{\alpha_2 x}, \text{ where } a \text{ and } b \text{ arbitrary constants}$$

$$\text{or} \quad \psi(x) = ae^{iKx} + be^{-iKx} \quad \text{_____ (4.110)}$$

On expansion, we get:

$$\psi(x) = a \cos Kx + ia \sin Kx + b \cos Kx - ib \sin Kx$$

$$= (a + b) \cos Kx + i(a - b) \sin Kx \\ = A \cos Kx + B \sin Kx \quad \text{_____} \quad (4.111)$$

where  $A = (a + b)$  and  $B = i(a - b)$  are again constants.

Equation (4.111) represents a general solution for Equation (4.106). The values of constants in Equation (4.111) can be obtained by applying boundary conditions at the ends of the crystal.

(i) At  $x = 0$ ,  $\psi(x) = 0$ , applying this on Equation (4.111), we get:

$$0 = A \times 1 + B \times 0 \Rightarrow A = 0$$

Substituting  $A = 0$  in Equation (4.111) gives:

$$\psi(x) = B \sin Kx \quad \text{_____} \quad (4.112)$$

(ii) At  $x = L$   $\psi(x) = 0$

Substituting this in Equation (4.112), we have:

$$0 = B \sin KL, \text{ we cannot take } B = 0, \text{ because for } B = 0, \psi(x) = 0 \text{ (from Equation 4.112)}$$

$$\text{So, } \sin KL = 0 \quad (\text{or}) \quad KL = n\pi$$

$$K = \frac{n\pi}{L} \quad \text{_____} \quad (4.113) \quad \text{where } n = 1, 2, 3, \dots$$

Substituting Equation (4.113) in (4.112) gives:

$$\psi_n(x) = B \sin \frac{n\pi x}{L} \quad \text{for } 0 < x < L \quad \text{_____} \quad (4.114)$$

Here,  $\psi(x)$  is changed to  $\psi_n(x)$  because wave function takes different values as ' $n$ ' changes.

If  $n = 0$ , then  $K = 0$ ,  $E = 0$  and  $\psi(x) = 0$  for all values of  $x$  in the well, so  $n \neq 0$ . This means that a particle with zero energy cannot be present in the box.

Substituting Equation (4.113) in (4.107) gives:

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow E = \frac{n^2\hbar^2\pi^2}{2mL^2} = \frac{n^2\hbar^2\pi^2}{(4\pi^2)2mL^2}$$

For different values of  $n$ ,  $E$  also takes different values and hence  $E$  can be written as  $E_n$

$$\therefore E_n = \frac{n^2\hbar^2}{8mL^2} \quad \text{_____} \quad (4.115)$$

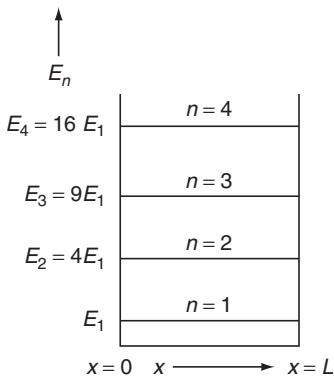
The lowest energy of the particle is obtained by putting  $n = 1$  in Equation (4.115) and it is:

$$E_1 = \frac{\hbar^2}{8mL^2} \quad \text{and} \quad E_n = n^2E_1 \quad \text{_____} \quad (4.116)$$

Equations (4.115) and (4.116) indicates that a particle in the box can take discrete values of energy, for  $n = 1, 2, 3, \dots$  i.e., the energy is quantized. These discrete energy values are called eigen values of energy. The number  $n$  is called the quantum number. Figure 4.11. shows the energy level diagram for a particle in a box. For the same value of quantum number  $n$ , the energy is inversely proportional to the mass of the particle and square of the length of the box. The energy is quantized and so it cannot vary continuously. But according to classical mechanics, there is a continuous range of possible energies. The increase in spacing between  $n$ th energy level and the next higher level is:

$$(n + 1)^2E_1 - n^2E_1 = (2n + 1)E_1 \quad \text{_____} \quad (4.117)$$

Figure 4.15 Eigen values of energy



The wave function  $\psi_n$  corresponding to  $E_n$  is called eigen function of the particle.

#### Determination of B by normalization

The value of  $B$  in Equation (4.114) can be obtained by equating the total probability of finding the particle inside the potential well is equal to unity, and this process is called normalization. Let  $P_n(x)$  is the probability density of the particle at  $x$  along X-direction:

$$\text{Then, } \int_0^L P_n(x) dx = \int_0^L |\psi_n|^2 dx = 1$$

Using Equation (4.114)

$$\int_0^L B^2 \sin^2 \left( \frac{n\pi x}{L} \right) dx = B^2 \int_0^L \frac{1}{2} \left[ 1 - \cos \frac{2\pi nx}{L} \right] dx = 1$$

$$\frac{B^2}{2} \left[ x - \frac{L}{2\pi n} \sin \frac{2\pi nx}{L} \right]_0^L = 1$$

The second term of the above equation becomes zero at both the limits.

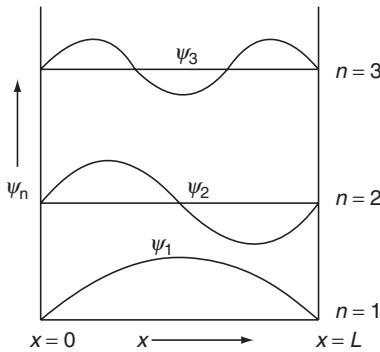
$$\text{Thus, } \frac{B^2 L}{2} = 1 \Rightarrow B = \sqrt{\frac{2}{L}} \quad \text{_____} \quad (4.118)$$

Substituting Equation (4.118) in (4.114) gives the normalized wave function:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \text{_____} \quad (4.119)$$

The first three wave functions for  $n = 1, 2$  and  $3$  are shown in Fig. 4.16. The shapes of wave functions shown in Fig. 4.16 have been obtained by substituting different values for  $x$  for each  $n$  value.

From Fig. 4.16, it is seen that the wave function  $\psi_1$  has two nodes at  $x = 0$  and at  $x = L$ , the wave function  $\psi_2$  has three nodes at  $x = 0, L/2$  and  $L$ . The wave function  $\psi_3$  has four nodes at  $x = 0, L/3, 2L/3$  and  $L$ . Thus, the wave function  $\psi_n$  will have  $(n + 1)$  nodes.

**Figure 4.16 Eigen functions**

### Probability of location of the particle

The probability of finding a particle in a small distance  $dx$  centred at  $x$  is given by:

$$P_n(x) dx = |\psi_n|^2 dx = \frac{2}{L} \sin^2 \left( \frac{n\pi x}{L} \right) dx$$

Probability density is:

$$P_n(x) = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

This is maximum when,

$$\frac{n\pi x}{L} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots \quad (\text{or}) \quad x = \frac{L}{2n}, \frac{3L}{2n}, \frac{5L}{2n}, \dots$$

For  $n = 1$ , the most probable positions of the particle is at  $x = L/2$ .

For  $n = 2$ , the most probable positions are at  $x = L/4$  and  $3L/4$ .

For  $n = 3$ , the most probable positions are at  $x = L/6, 3L/6$  and  $5L/6$ .

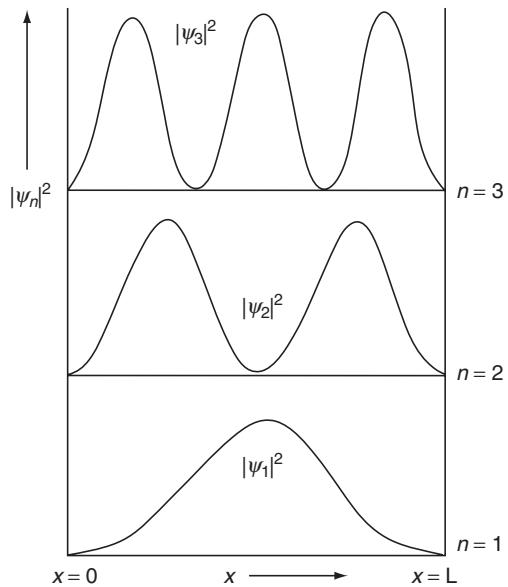
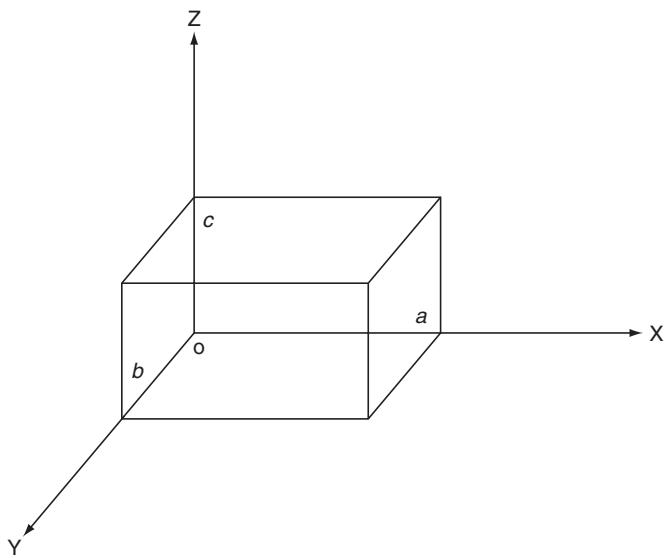
These positions are shown in Fig. 4.17.

The wave mechanical result is quite contradictory to the classical concept. According to classical mechanics, a particle in a potential box would travel with a uniform velocity from one wall to the other and at the walls it would be perfectly reflected. Therefore, the probability of finding the particle within a small distance  $dx$ , anywhere in the box is same and is equal to  $dx/L$ .

### (b) Particle in a rectangular three-dimensional box

Consider a particle [electron] of mass ' $m$ ' constrained to move freely in the space of the rectangular metallic crystal with edges of length  $a, b$  and  $c$  along X, Y and Z-axes as shown in Fig. 4.18. Potential barrier which exists at the surface of the crystal will be in the form of rectangular box for the free electron inside this crystal. We take the origin of coordinate system at one corner of the box. We will solve three-dimensional time-independent Schrödinger's wave equation in the box.

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

**Figure 4.17** Probability density of particle in well**Figure 4.18** Three-dimensional potential box

The potential energy of the particle is considered to be equal to zero inside the box and it is infinity ( $V = \infty$ ) at the boundaries (surface) and in the remaining space.

$$\text{Hence, } \nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0$$

$$(\text{or}) \quad \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad (4.120)$$

$\psi$  is function of the three variables  $x, y$  and  $z$ . One way of solving Equation (4.120) is to write  $\psi$  as the product of three functions as:

$$\psi(x, y, z) = X(x) Y(y) Z(z) \quad (4.121)$$

Here, the wave function is equal to the product of three wave functions  $X, Y$  and  $Z$ . Again,  $X$  is function of  $x$  only,  $Y$  is function of  $y$  only and  $Z$  is a function of  $z$  only. In simple, Equation (4.121) is represented as:

$$\psi = XYZ \quad (4.122)$$

If  $\psi$  is a solution of Equation (4.121), then differentiate Equation (4.122) with respect to  $x, y$  and  $z$  twice and substitute in Equation (4.120), we get:

$$\frac{\partial\psi}{\partial x} = YZ \frac{dX}{dx} \quad \text{and} \quad \frac{\partial^2\psi}{\partial x^2} = YZ \frac{d^2X}{dx^2}$$

$$\text{Similarly, } \frac{\partial^2\psi}{\partial y^2} = XZ \frac{d^2Y}{dy^2} \quad \text{and} \quad \frac{\partial^2\psi}{\partial z^2} = XY \frac{d^2Z}{dz^2}$$

Substituting these in Equation (4.120), we get:

$$YZ \frac{d^2X}{dx^2} + XZ \frac{d^2Y}{dy^2} + XY \frac{d^2Z}{dz^2} = -\left(\frac{2mE}{\hbar^2}\right)XYZ$$

dividing throughout by  $XYZ$ , we have:

$$\frac{1}{X} \frac{d^2X}{dx^2} + \frac{1}{Y} \frac{d^2Y}{dy^2} + \frac{1}{Z} \frac{d^2Z}{dz^2} = -\frac{2mE}{\hbar^2} = -K^2 \quad (4.123)$$

$$\text{where } K^2 = K_x^2 + K_y^2 + K_z^2 = \frac{2mE}{\hbar^2} \quad (4.124)$$

We, therefore, write Equation (4.123) as:

$$\frac{1}{X} \frac{d^2X}{dx^2} = -K_x^2 \quad (4.125)$$

$$\frac{1}{Y} \frac{d^2Y}{dy^2} = -K_y^2 \quad (4.126)$$

$$\text{and } \frac{1}{Z} \frac{d^2Z}{dz^2} = -K_z^2 \quad (4.127)$$

Similar to the solution for one-dimensional Schrödinger's wave equation, the general solution of Equation (4.126) will be of the form:

$$X(x) = A_x \cos K_x x + B_x \sin K_x x \quad \text{_____} \quad (4.128)$$

Applying boundary conditions, we have:

- (i) at  $x = 0$ , the wave function along X-direction is zero i.e.,  $X = 0$  applying this on Equation (4.128) gives  $A_x = 0$ .

So, Equation (4.128) becomes:

$$X(x) = B_x \sin K_x x \quad \text{_____} \quad (4.129) \quad \text{and}$$

- (ii) at  $x = a$ ,  $X = 0 = B_x \sin K_x a$

$B_x$  cannot be zero, since  $B_x = 0$  gives the wave function along X-direction is zero [ $X = 0$ ]. i.e., the wave function does not exist.

$$\text{So } \sin K_x a = 0, \text{ therefore } K_x a = n_x \pi$$

$$(\text{or}) \quad K_x = \frac{n_x \pi}{a} \quad \text{_____} \quad (4.130)$$

where  $n_x = 1, 2, 3, \dots, n_x \neq 0$ , because if  $n_x = 0$  gives,  $X = 0$  for all values of  $x$  in the box.

Substituting Equation (4.130) in (4.129) gives:

$$X = B_x \sin \frac{n_x \pi x}{a} \quad \text{_____} \quad (4.131)$$

Applying the normalization condition on Equation (4.131) between the limits  $x = 0$  and  $x = a$ , we have:

$$\int_0^a |X|^2 dx = B_x^2 \int_0^a \sin^2 \left( \frac{n_x \pi x}{a} \right) dx = 1$$

Solving this, we get:

$$\frac{B_x^2 a}{2} = 1 \quad (\text{or}) \quad B_x = \sqrt{\frac{2}{a}} \quad \text{_____} \quad (4.132)$$

Substituting Equation (4.132) in (4.131) gives:

$$X = \sqrt{\frac{2}{a}} \sin \frac{n_x \pi x}{a} \quad \text{_____} \quad (4.133)$$

With similar treatment on Equation (4.126) and (4.127), we obtain:

$$Y = \sqrt{\frac{2}{b}} \sin \frac{n_y \pi y}{b} \quad \text{_____} \quad (4.134)$$

$$\text{and } Z = \sqrt{\frac{2}{c}} \sin \frac{n_z \pi z}{c} \quad \text{_____} \quad (4.135)$$

Substituting Equations (4.133), (4.134) and (4.135) in Equation (4.122) gives:

$$\psi = \sqrt{\frac{2}{a}} \sin \frac{n_x \pi x}{a} \sqrt{\frac{2}{b}} \sin \frac{n_y \pi y}{b} \sqrt{\frac{2}{c}} \sin \frac{n_z \pi z}{c}$$

$$\psi_n(x, y, z) = \frac{2\sqrt{2}}{\sqrt{abc}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c} \quad \text{_____ (4.136)}$$

Equation (4.124) is:

$$E = \frac{\hbar^2}{2m} (K_x^2 + K_y^2 + K_z^2)$$

$$= \frac{\hbar^2}{2m} \left[ \frac{n_x^2 \pi^2}{a^2} + \frac{n_y^2 \pi^2}{b^2} + \frac{n_z^2 \pi^2}{c^2} \right] = \frac{\hbar^2 \pi^2}{2m} \left[ \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right]$$

As  $n_x$ ,  $n_y$  and  $n_z$  takes different values, so  $E$  takes the form:

$$\text{i.e., } E_{n_x}, E_{n_y}, E_{n_z} = \left( \frac{\hbar^2}{8m} \right) \left[ \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right] \quad \text{_____ (4.137)}$$

where  $n_x = n_y = n_z = 1, 2, 3, \dots$

Equation (4.136) gives the total normalized wave functions inside the rectangular box for the stationary states. Equation (4.137) gives the eigen values of energy of the particle. These values are called the energy levels of the particle.

If the particle is confined in a cubical box i.e.,  $a = b = c$ , the eigen values of energy are given by:

$$E_{n_x}, E_{n_y}, E_{n_z} = \frac{\hbar^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\hbar^2 n^2}{8ma^2} \quad \text{_____ (4.138)}$$

where  $n^2 = n_x^2 + n_y^2 + n_z^2$  and the normalized wave functions are:

$$\psi(x, y, z) = \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \quad \text{_____ (4.139)}$$

From equation (4.138), we know that several combinations of the three integers give different stationary states or different wave functions, in which some energies remain same, then they are said to be degenerate states and energy levels.

## Formulae

$$1. f_{M-B}^{(E_i)} = \frac{1}{e^\alpha e^{\frac{E_i}{k_B T}}}$$

$$2. f_{F-D}^{(E_i)} = \frac{1}{1 + e^{\left( \frac{E_i - E_F}{k_B T} \right)}}$$

$$3. f_{B-E}^{(E_i)} = \frac{1}{e^\alpha e^{\left(\frac{E_i}{k_B T}\right)} - 1}$$

$$5. \text{ Wien's law, } U_\lambda d\lambda = \frac{C_1}{\lambda^5} e^{-\left(\frac{C_2}{\lambda}\right)} d\lambda$$

$$7. \text{ Planck's law, } U_\lambda d\lambda = \frac{8\pi bc}{\lambda^5} \left[ \frac{1}{e^{\left(\frac{h\nu}{k_B T}\right)} - 1} \right] d\lambda$$

$$9. \lambda = \frac{1.227}{\sqrt{V}} \left[ 1 - \frac{eV}{4m_0 c^2} \right] \text{ nm}$$

$$11. \text{ Kinetic energy} = \text{Total energy} - \text{Rest mass equivalent energy} = \sqrt{E_0^2 + (pc)^2} - m_0 c^2$$

$$12. 2d \sin \theta = n\lambda$$

$$14. \lambda = \frac{b}{\sqrt{2m_0 eV}} \left[ 1 + \frac{eV}{2m_0 c^2} \right]^{-1/2} \approx \frac{b}{\sqrt{2m_0 eV}}$$

$$16. \Psi = A \exp \left[ \frac{i}{\hbar} (Et - px) \right]$$

$$18. \frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \Psi - V \Psi$$

$$20. \nabla^2 \psi = \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$22. E_n = \frac{n^2 \hbar^2}{8mL^2} = n^2 E_1$$

$$24. \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$26. \psi(x, y, z) = \frac{2\sqrt{2}}{\sqrt{abc}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c}$$

$$28. \psi(x, y, z) = \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c}$$

$$4. g(E) dE = \frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

$$6. \text{ Rayleigh-Jean's law, } U_\lambda d\lambda = 8 \pi k_B T \lambda^{-4} d\lambda$$

$$8. \lambda = \frac{b}{p} = \frac{b}{(2meV)^{\frac{1}{2}}} = \frac{1.227}{\sqrt{V}} \text{ nm}$$

$$10. E = \sqrt{E_0^2 + (pc)^2}$$

$$13. d = \frac{L\lambda}{r}$$

$$15. d = \frac{L\lambda}{r} = \frac{L}{r} \frac{b}{\sqrt{2m_0 eV}} \left[ 1 + \frac{eV}{2m_0 c^2} \right]^{-1/2}$$

$$17. \frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - V \Psi$$

$$19. \frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$21. \int P dv = \int \Psi(x, y, z, t) \Psi^*(x, y, z, t) dv = \int |\Psi(x, y, z, t)|^2 dv = 1$$

$$23. E_{n+1} - E_n = (2n+1) E_1$$

$$25. P_n(x) = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

$$27. E_{n_x, n_y, n_z} = \left( \frac{b^2}{8m} \right) \left[ \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right]$$

## Solved Problems

1. Calculate the average energy of Planck's oscillator of frequency  $5.6 \times 10^{12}$  Hz at 330K.

**Sol:** The average energy of planck's oscillator =  $\frac{h\gamma}{\left[ e^{\frac{h\gamma}{k_B T}} - 1 \right]}$

$k_B$  = Boltzmann constant =  $1.38 \times 10^{-23}$  J/K

$h$  = Planck's constant =  $6.625 \times 10^{-34}$  JS

$\gamma$  = frequency of oscillator =  $5.6 \times 10^{12}$  Hz

$T$  = Temperature of the oscillator = 330 K

Substituting the above values in the expression

$$\text{Average energy of Planck's oscillator} = \frac{(6.625 \times 10^{-34}) \times (5.6 \times 10^{12})}{\exp \left[ \frac{6.625 \times 10^{-34} \times 5.6 \times 10^{12}}{1.38 \times 10^{-23} \times 330} \right]} \\ = 2.945 \times 10^{-21} \text{ Joules}$$

2. A black body emits radiation at a temperature of 1500K. calculate the energy density per unit wave length at  $6000\text{\AA}$  of black body radiation.

**Sol:** Temperature of the black body = 1500K

The wave length at which energy density is to be determined,  $\lambda = 6000\text{\AA}$

Planck's equation for energy density in the wave length range between  $\lambda$  and  $\lambda + d\lambda$ ,  $U\lambda d\lambda =$

$$\frac{8\pi hc}{\lambda^5} \left[ \frac{1}{e^{\frac{h\gamma}{k_B T}} - 1} \right] d\lambda$$

$$\text{For one unit range of wave lengths, it is } U_\lambda = \frac{8\pi hc}{\lambda^5} \left[ \frac{1}{e^{\frac{h\gamma}{k_B T}} - 1} \right]$$

$$\text{Here } \frac{h\gamma}{k_B T} = \frac{hc}{\lambda k_B T} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{6000 \times 10^{-10} \times 1.38 \times 10^{-23} \times 1500} = 16$$

$$\therefore U_\lambda \frac{8 \times 22 \times 6.63 \times 10^{-34} \times 3 \times 10^8}{7 \times [6000 \times 10^{-10}]^5} \times \frac{1}{e^{16} - 1} 7.23 \text{ Jm}^{-4}$$

3. Calculate the wavelength associated with an electron with energy 2000 eV.

(Set-1–Sept. 2006), (Set-1–May 2004), (Set-1–May 2003), (Set-4–Nov. 2003)

**Sol:**  $E = 2000 \text{ eV} = 2000 \times 1.6 \times 10^{-19} \text{ J}$

$$\text{Kinetic energy (E)} = \frac{1}{2} mv^2 = \frac{p^2}{2m} \quad (\text{or}) \quad p = \sqrt{2mE}$$

$$\begin{aligned}\therefore \lambda &= \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 2000 \times 1.6 \times 10^{-19}}} \text{ m} \\ &= \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 1.6 \times 2000 \times 10^{-50}}} = \frac{6.63 \times 10^{-34}}{241.33 \times 10^{-25}} \text{ m} \\ &= 0.0275 \times 10^{-9} \text{ m} = 0.0275 \text{ nm}\end{aligned}$$

4. Calculate the velocity and kinetic energy of an electron of wavelength  $1.66 \times 10^{-10} \text{ m}$ .

(Set-1, Set-3-May 2006), (Set-2, Set-3-June 2005), (Set-2-May 2004), (Set-4-May 2003)

**Sol:** Wavelength of an electron ( $\lambda$ ) =  $1.66 \times 10^{-10} \text{ m}$

$$\begin{aligned}\lambda &= \frac{h}{mv} \\ v &= \frac{h}{m\lambda} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 1.66 \times 10^{-10}} \text{ m/s} \\ &= \frac{6.63}{9.1 \times 1.66} \times 10^7 \text{ m/s} = 438.9 \times 10^4 \text{ m/s.}\end{aligned}$$

To calculate KE:

We know  $E = P = \sqrt{2mE}$

$$\begin{aligned}\text{and } \lambda &= \frac{h}{p} = \frac{h}{\sqrt{2mE}} \\ \text{or } \lambda^2 &= \frac{h^2}{2mE} \quad \text{or} \quad E = \frac{h^2}{2m\lambda^2} = \frac{[6.626 \times 10^{-34}]^2}{2 \times 9.1 \times 10^{-31} \times (1.66 \times 10^{-10})^2} \\ &= \frac{(6.626)^2 \times 10^{-68}}{2 \times 9.1 \times (1.66)^2 \times 10^{-51}} \text{ J} = 8.754 \times 10^{-18} \text{ J} = \frac{8.754 \times 10^{-18}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 54.71 \text{ eV}\end{aligned}$$

5. An electron is bound in one-dimensional infinite well of width  $1 \times 10^{-10} \text{ m}$ . Find the energy values in the ground state and first two excited states.

(Set-4-June 2005), (Set-2-Nov. 2004), (Set-3-May 2003)

**Sol:** Potential well of width ( $L$ ) =  $1 \times 10^{-10} \text{ m}$

$$E_n = \frac{n^2 h^2}{8mL^2}$$

For ground state  $n = 1$ ,

$$\begin{aligned}E_1 &= \frac{h^2}{8mL^2} = \frac{[6.63 \times 10^{-34}]^2}{8 \times 9.1 \times 10^{-31} \times 10^{-10} \times 10^{-10}} \text{ J} = \frac{(6.63)^2}{8 \times 9.1} \times 10^{-17} \text{ J} \\ &= 0.6038 \times 10^{-17} \text{ J} \\ (\text{or}) \quad &= \frac{0.6038 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV} = 37.737 \text{ eV}\end{aligned}$$

$$E_2 = 4E_1 = 2.415 \times 10^{-17} \text{ J}$$

$$= 150.95 \text{ eV}$$

$$E_3 = 9E_1 = 5.434 \times 10^{-17} \text{ J}$$

$$= 339.639 \text{ eV.}$$

6. An electron is bound in one-dimensional box of size  $4 \times 10^{-10} \text{ m}$ . What will be its minimum energy?

(Set-2–Sept. 2006), (Set-1–Nov. 2004), (Set-2–May 2003)

**Sol:** Potential box of size ( $L$ ) =  $4 \times 10^{-10} \text{ m}$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 4 \times 10^{-10} \times 4 \times 10^{-10}} \text{ J}$$

$$= \frac{6.63 \times 6.63}{8 \times 9.1 \times 16} \times 10^{-17} \text{ J}$$

$$= 0.0377 \times 10^{-17} \text{ J}$$

$$\text{(or)} \quad = \frac{0.0377 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV}$$

$$= 2.3586 \text{ eV}$$

7. An electron is moving under a potential field of 15 kV. Calculate the wavelength of the electron waves.

**Sol:**  $V = 15 \times 10^3 \text{ V}$        $\lambda = ?$

$$\lambda = \frac{1.227}{\sqrt{V}} \text{ nm} = \frac{1.227}{\sqrt{15000}} \text{ nm} = \frac{1.227}{122.47} \text{ nm} = 0.01 \text{ nm}$$

6. Find the least energy of an electron moving in one-dimensional potential box (infinite height) of width 0.05 nm.

**Sol:**  $E_n = \frac{n^2 h^2}{8mL^2}$        $L = 0.05 \text{ nm} = 0.05 \times 10^{-9} \text{ m}$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 0.5 \times 10^{-10} \times 0.5 \times 10^{-10}} \text{ J}$$

$$= \frac{6.63 \times 6.63}{8 \times 9.1 \times 0.25} \times 10^{-17} \text{ J} = 2.4 \times 10^{-17} \text{ J}$$

$$= \frac{2.4 \times 10^{-17}}{1.6 \times 10^{-19}} = 150.95 \text{ eV}$$

8. A quantum particle confined to one-dimensional box of width 'a' is known to be in its first excited state. Determine the probability of the particle in the central half.

(Set-1–Nov. 2003)

**Sol:** Width of the box,  $L = a$

First excited state means,  $n = 2$

Probability at the centre of the well,  $P_2(L/2) = ?$

$$P_n(x) = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

$$P_2(L/2) = \frac{2}{L} \sin^2 \frac{2\pi L/2}{L}$$

$$= \frac{2}{L} \sin^2 \pi = 0$$

The probability of the particle at the centre of the box is zero.

9. An electron is confined in one-dimensional potential well of width  $3 \times 10^{-10}$  m. Find the kinetic energy of electron when it is in the ground state.

(Set-2–Nov. 2004), (Set-1–May 2004), (Set-1–Nov. 2003)

**Sol:** One-dimensional potential well of width,  $L = 3 \times 10^{-10}$  m

Electron is present in ground state, so  $n = 1$

$$E_1 = ?$$

$$E_n = \frac{n^2 h^2}{8mL^2}$$

$$E_1 = \frac{1^2 \times [6.63 \times 10^{-34}]^2}{8 \times 9.1 \times 10^{-31} \times [3 \times 10^{-10}]^2} \text{ J} = 0.067 \times 10^{-17} \text{ J}$$

$$\text{or } E_1 = \frac{0.067 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV}$$

$$= 4.2 \text{ eV}$$

10. Calculate the de Brogile wavelength of neutron whose kinetic energy is two times the rest mass of electron (given  $m_n = 1.676 \times 10^{-27}$  kg,  $m_e = 9.1 \times 10^{-31}$  kg,  $C = 3 \times 10^8$  m/s and  $h = 6.63 \times 10^{-34}$  JS).

**Sol:** Kinetic energy of neutron,  $\frac{1}{2} m_n v^2 = \frac{P_n^2}{2m_n} = 2m_e$

$$P_n = \sqrt{4m_n m_e} \quad \text{where } m_n = \text{mass of neutron}$$

$$m_e = \text{mass of an electron}$$

$$\text{de Brogile wavelength of neutron, } \lambda_n = ?$$

$$\lambda_n = \frac{h}{P_n} = \frac{h}{\sqrt{4m_n m_e}} = \frac{6.63 \times 10^{-34}}{\sqrt{4 \times 9.1 \times 10^{-31} \times 1.676 \times 10^{-27}}}$$

$$= \frac{6.63 \times 10^{-34}}{7.811 \times 10^{-29}} \text{ m} = 0.8488 \times 10^{-5} \text{ m} = 8488 \text{ nm.}$$

11. An electron is confined to a one-dimensional potential box of length 2 Å. Calculate the energies corresponding to the second and fourth quantum states (in eV).

(Set-2–Nov. 2003)

**Sol:** Length of the one-dimensional potential box,  $L = 2\text{\AA} = 2 \times 10^{-10} \text{ m}$

$$\text{Energy of electron in } n\text{th level, } E_n = \frac{n^2 h^2}{8mL^2} = n^2 E_1$$

$$\therefore E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times [2 \times 10^{-10}]^2} \text{ J}$$

$$= 0.150951 \times 10^{-17} \text{ J}$$

$$= \frac{0.150951 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV} = 9.43 \text{ eV}$$

Energy corresponding to second and fourth quantum states is:

$$E_2 = 2^2 E_1 = 4 \times 9.43 \text{ eV} = 37.72 \text{ eV}$$

and

$$E_4 = 4^2 E_1 = 16 \times 9.43 \text{ eV} = 150.88 \text{ eV}$$

12. Electrons are accelerated by 344 V and are reflected from a crystal. The first reflection maximum occurs when the glancing angle is  $60^\circ$ . Determine the spacing of the crystal.

(Set-4–Nov. 2004), (Set-3–Nov. 2003)

**Sol:** Accelerating potential,  $V = 344 \text{ V}$

Order of diffraction,  $n = 1$

Glancing angle,  $\theta = 60^\circ$

Interplanar spacing,  $d = ?$

$$\text{We know that } 2d \sin \theta = n\lambda \text{ and } \lambda = \frac{h}{\sqrt{2meV}}$$

$$\text{So, } 2d \sin \theta = \frac{nh}{\sqrt{2meV}}$$

$$\begin{aligned} d &= \frac{nh}{2 \sin \theta \sqrt{2meV}} = \frac{1 \times 6.63 \times 10^{-34}}{2 \times \sin 60^\circ \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 344}} \text{ m} \\ &= \frac{66.3 \times 10^{-10}}{173.3547} \text{ m} = 0.382 \times 10^{-10} \text{ m} = 0.382 \text{ \AA} \end{aligned}$$

The interplanar spacing is 0.382 \AA.

13. Calculate the energy required to pump an electron from ground state to the 2nd excited state in a metal of length  $10^{-10} \text{ m}$ .

**Sol:** The energy of an electron of mass ' $m$ ' in  $n$ th quantum state in a metal of side ' $L$ ' is:

$$E_n = \frac{n^2 h^2}{8mL^2} = n^2 E_1$$

$n = 1$ , corresponds to ground state

$n = 2$ , corresponds to first excited state and

$n = 3$ , corresponds to second excited state

$$E_1 = \frac{1^2 h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times 10^{-10} \times 10^{-10}} \text{ J}$$

$$= 6.0314 \times 10^{-18} \text{ J} = \frac{6.0314 \times 10^{-18}}{1.6 \times 10^{-19}} \text{ eV} = 37.64 \text{ eV}$$

$$E_3 = \frac{3^2 h^2}{8mL^2} = 9E_1 = 9 \times 37.64 \text{ eV} = 338.76 \text{ eV}$$

$\therefore$  Energy required to pump an electron from ground state to 2nd excited state =  $E_3 - E_1$

$$= 338.76 \text{ eV} - 37.64 \text{ eV}$$

$$= 301.12 \text{ eV}$$

14. Calculate the minimum energy of free electron trapped in a one-dimensional box of width 0.2 nm. (Given,  $h = 6.63 \times 10^{-34}$  J-S and electron mass  $\times 9.1 \times 10^{-31}$  kg)

**Sol:** One-dimensional box of width,  $L = 0.2 \text{ nm} = 2 \times 10^{-10} \text{ m}$

Minimum energy of the electron,  $E_1 = ?$

$$E_n = \frac{n^2 h^2}{8mL^2}$$

$$E_1 = \frac{1^2 \times [6.63 \times 10^{-34}]^2}{8 \times 9.1 \times 10^{-31} \times [2 \times 10^{-10}]^2} \text{ J} = 0.15095 \times 10^{-17} \text{ J}$$

$$= \frac{0.15095 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV} = 9.43 \text{ eV.}$$

15. Calculate the wavelength associated with an electron raised to a potential 1600 V.

(Set-1, Set-4-May 2008), (Set-3-May 2004)

**Sol:** Potential ( $V$ ) = 1600 V

Wavelength ( $\lambda$ ) = ?

$$\lambda = \frac{1.227}{\sqrt{V}} \text{ nm}$$

$$= \frac{1.227}{\sqrt{1600}} \text{ nm}$$

$$= 0.031 \text{ nm} = 0.31 \text{ Å.}$$

### Multiple Choice Questions

- Phase space is a \_\_\_\_\_ dimensional space. (a) 3 (b) 4 (c) 5 (d) 6
- Maxwell-Boltzmann statistics is applicable to
  - identical distinguishable particles
  - identical indistinguishable particles
  - fermions
  - bosons

3. A point in phase space or  $\mu$ -space can be represented with (0)
- (a) Six position coordinates
  - (b) Six momentum coordinates
  - (c) Three position and three momentum coordinates
  - (d) Six position and six momentum coordinates
4. At temperature  $T$ K, if a particle possess energy  $E_i$  then the Maxwell–Boltzmann distribution for it can be represented as [  $\alpha = \text{constant}$ ,  $K_B = \text{Boltzmann constant}$ ] (0)
- (a)  $\frac{1}{e^\alpha e^{\frac{E_i}{k_B T}}}$
  - (b)  $\frac{1}{e^\alpha e^{-\frac{E_i}{k_B T}}}$
  - (c)  $\frac{1}{e^{-\alpha} e^{\frac{E_i}{k_B T}}}$
  - (d)  $\frac{1}{e^{-\alpha} e^{-\frac{E_i}{k_B T}}}$
5. Fermi–Dirac distribution is applicable to (0)
- (a) distinguishable particles
  - (b) indistinguishable particles
  - (c) Both a and b
  - (d) None of the above
6. The Fermions possess a spin of (0)
- (a) integral multiples of  $\hbar$
  - (b) half-integral multiples of  $\hbar$
  - (c) They possess any spin
  - (d) None of the above
7. The Fermi–Dirac distribution function of a particle possessing energy  $E$  at temperature  $T$ k is (0)
- (a)  $\frac{1}{1 - e^{\frac{(E-E_F)}{k_B T}}}$
  - (b)  $\frac{1}{1 + e^{\frac{(E-E_F)}{k_B T}}}$
  - (c)  $\frac{1}{e^{\frac{(E-E_F)}{k_B T}} - 1}$
  - (d)  $\frac{1}{1 + e^{\frac{E-E_F}{k_B T}}}$
8. Bose–Einstein statistics is applicable to (0)
- (a) identical distinguishable particles
  - (b) identical indistinguishable particles
  - (c) Both a and b
  - (d) None of the above
9. Bosons possess a spin of (0)
- (a) integral multiples of  $\hbar$ .
  - (b) half-integral multiples of  $\hbar$ .
  - (c) They can have any spin.
  - (d) They would not possess spin.
10. For a particle of energy  $E$ , the Bose–Einstein distribution can be represented as [  $\alpha, \beta = \text{const.}$ ,  $K_B = \text{Boltzmann constant}$ ] (0)
- (a)  $\frac{\alpha}{e^{\frac{E_i}{k_B T}} - 1}$
  - (b)  $\frac{1}{e^\alpha e^{\frac{E_i}{k_B T}} - 1}$
  - (c)  $\frac{1}{e^{\alpha} e^{\frac{E_i}{k_B T}} + 1}$
  - (d)  $\frac{1}{1 - e^{\alpha} e^{\frac{E_i}{k_B T}}}$
11. The free electrons in a metal follow \_\_\_\_\_ distribution (0)
- (a) Maxwell–Boltzmann
  - (b) Fermi–Dirac
  - (c) Bose–Einstein
  - (d) None of the above

12. At 0K, the probability of an electron in Fermi energy level is ()  
 (a) 0 (b) 0.5  
 (c) 1.0 (d) less than 1
13. The probability of an electron in Fermi energy level at non-0K temperature is ()  
 (a) 0 (b) 0.5  
 (c) between 0.5 and 1 (d) 1.0
14. The expression for the density of electron states at energy  $E$  can be represented as [ $b = \text{Planck's constant}$ ] ()  
 (a)  $\frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}}$  (b)  $\frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E$  (c)  $\frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}}$  (d)  $\frac{\pi}{2} \left( \frac{8m}{b^2} \right)^{\frac{3}{2}} E$
15. Black body is ()  
 (a) a body that absorbs all wave lengths of radiation incident on it at low temperatures  
 (b) a body that emits different wave lengths of radiation at high temperatures  
 (c) Both a and b  
 (d) None of the above
16. If the temperature of a black body is increased then the intensity of radiation for each wave length of radiation ()  
 (a) remains constant  
 (b) decreases  
 (c) increases  
 (d) None of the above
17. In black body radiation, the wave length corresponds to maximum intensity moves towards \_\_\_\_\_ wave length region with increase of temperature. ()  
 (a) shorter  
 (b) longer  
 (c) both a and b  
 (d) none of the above
18. Wien's law explains the black body radiation in \_\_\_\_\_ region of the spectrum. ()  
 (a) the short wave length region  
 (b) the medium wave length region  
 (c) the longer wave length region  
 (d) None of the above
19. The planck's black body radiation distribution can be represented as ()  
 (a)  $\frac{\lambda^5}{8\pi cb} \left[ \frac{1}{e^{\frac{hc}{k_B T}} - 1} \right] d\lambda$  (b)  $\frac{8\pi cb}{\lambda^5} \left[ \frac{1}{e^{\frac{hc}{k_B T}} - 1} \right] d\lambda$  (c)  $\frac{\lambda^5}{8\pi cb} \left[ \frac{1}{e^{\frac{hc}{k_B T}} - 1} \right] d\lambda$  (d)  $\frac{8\pi cb}{\lambda^5} \left[ \frac{1}{e^{\frac{hc}{k_B T}} - 1} \right] d\lambda$
20. Rayleigh-Jeans explained black body radiation based on \_\_\_\_\_ of energy ()  
 (a) equipartition (b) kinetic theory (c) fifth power of wave length (d) All the above
21. Rayleigh-Jeans law is applicable to \_\_\_\_\_ wave length region of the spectrum ()



33. The spur in the curve drawn between the number of electrons collected against the angles of galvanometer with an incident beam in Davisson and Germer experiment is more clear for an anode voltage of: ()  
 (a) 40 V (b) 44 V (c) 54 V (d) 68 V
34. The diffraction angle for nickel crystal in Davisson and Germer experiment is: ()  
 (a)  $50^\circ$  (b)  $65^\circ$  (c)  $25^\circ$  (d)  $130^\circ$
35. Schrödinger's wave equation for a particle of mass  $m$  have energy  $E$ , moving along X-axis is: ()  
 (a)  $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$  (b)  $\frac{d\psi}{dt} + \frac{2m}{\hbar^2}(E - V)\psi = 0$   
 (c)  $\frac{d\psi}{dx} + \frac{2m}{\hbar^2}(E - V)\psi = 0$  (d)  $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(V - E)\psi = 0$
36. The wave function ' $\psi$ ' associated with a moving particle: ()  
 (a) is not an observable quantity (b) does not have direct physical meaning  
 (c) is a complex quantity (d) all
37. By solving one-dimensional Schrödinger's time-independent wave equation for a particle in the well gives: ()  
 (a) quantum numbers (b) discrete values of energy and zero point energy  
 (c) wave function associated with the particle (d) all
38. The energy possessed by a particle of mass ' $m$ ' in  $n$ th quantum state in a one-dimensional potential well of width ' $L$ ' is: ()  
 (a)  $\frac{n^2 h^2}{8mL^2}$  (b)  $\frac{nb}{8mL^2}$  (c)  $\frac{n^2 h^2}{8mL}$  (d)  $\frac{8mL^2}{n^2 h^2}$
39. In G.P. Thomson's experiment \_\_\_\_\_ particles are used for diffraction. ()  
 (a) slow neutrons (b) fast neutrons (c) slow electrons (d) fast electrons
40. In photoelectric effect, absorption or emission of energy takes place: ()  
 (a) in the form of packets of energy called quanta  
 (b) continuously  
 (c) both a and b  
 (d) none
41. When an electron is accelerated through a potential difference of 100 V, then it is associated with a wave of wavelength equal to: ()  
 (a) 0.112 nm (b) 0.1227 nm  
 (c) 1.227 nm (d) 12.27 nm
42. \_\_\_\_\_ proposed matter waves but he did not prove it experimentally. ()  
 (a) Thomson (b) Davisson and Germer  
 (c) de Broglie (d) Schrödinger
43. The interplanar spacing of gold foil obtained by G.P. Thomson's method agree very well with that obtained by \_\_\_\_\_ method. ()  
 (a) interference (b) X-ray  
 (c) diffraction (d) none

44. The thickness of gold foil used in G.P.Thomson experiment was: ( )  
 (a)  $10^{-3}$  m      (b)  $10^{-5}$  m      (c)  $10^{-7}$  m      (d)  $10^{-8}$  m
45. The original aim of Davisson and Germer experiment was to find the \_\_\_\_\_ by a metal target. ( )  
 (a) intensity of scattered electrons      (b) electron diffraction  
 (c) to find interplanar spacing      (d) none
46. The de Broglie wavelength of electrons obtained from Davisson and Germer experiment is: ( )  
 (a) 0.0165 nm      (b) 0.165 nm      (c) 1.65 nm      (d) 16.5 nm
47. Schrödinger's wave equation was derived based on \_\_\_\_\_ idea of matter waves. ( )  
 (a) de Broglie's      (b) Schrödinger's  
 (c) Thomson's      (d) Newton's
48. If  $\psi(x, y, z, t)$  represent wave function associated with a moving particle, then  $|\psi(x, y, z, t)|^2$  represents: ( )  
 (a) intensity      (b) amplitude  
 (c) probability density      (d) none
49. If  $E_1$  is the ground state energy of a particle, then the increase in energy from  $n$ th energy level to next higher level is: ( )  
 (a)  $(2n + 1)E_1$       (b)  $2nE_1$       (c)  $(2n - 1)E_1$       (d)  $(3n + 1)E_1$
50. The normalized wave function of a particle in a one-dimensional potential well of width  $L$  is: ( )  
 (a)  $\frac{2}{L} \sin \frac{n\pi x}{L}$       (b)  $\frac{L}{2} \sin \frac{n\pi x}{L}$       (c)  $\sqrt{\frac{L}{2}} \sin \frac{n\pi x}{L}$       (d)  $\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$
51. The most probable position of a particle in one-dimensional potential well of width 'L' in the first quantum state is: ( )  
 (a)  $L/4$       (b)  $L/3$       (c)  $L/2$       (d)  $2L/3$

## Answers

- |       |       |       |       |       |       |       |       |       |                |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|----------------|
| 1. d  | 2. a  | 3. c  | 4. a  | 5. b  | 6. b  | 7. b  | 8. b  | 9. a  | 10. b          |
| 11. b | 12. c | 13. b | 14. a | 15. c | 16. c | 17. a | 18. a | 19. b | 20. a          |
| 21. b | 22. a | 23. d | 24. a | 25. b | 26. c | 27. b | 28. c | 29. d | 30. b          |
| 31. a | 32. b | 33. c | 34. b | 35. a | 36. d | 37. d | 38. a | 39. c | 40. a          |
| 41. b | 42. c | 43. b | 44. d | 45. a | 46. b | 47. a | 48. c | 49. a | 50. d    51. c |

## Review Questions

- Derive an expression for the distribution of identical distinguishable particles based on classical concepts?
- Derive Maxwell–Boltzmann distribution expression?
- Derive Fermi–Dirac distribution equation for identical indistinguishable particles.
- Derive Bose–Einstein distribution for bosons.
- Distinguish between Maxwell–Boltzmann distribution, Fermi–Dirac distribution and Bose–Einstein distribution.

6. Write short notes on (i) electron gas (ii) photon gas and (iii) Fermi energy.
7. Derive an expression for density of available electron states between the energies  $E$  and  $E + dE$ .
8. Explain black body radiation.
9. What are matter waves? Explain their properties.  
(Set-1–Sept. 2006), (Set-1–May 2004), (Set-1–May 2003), (Set-4–Nov. 2003)
10. Derive the expression for de Broglie wavelength.  
(Set-1–Sept. 2006), (Set-1–May 2004), (Set-1–May 2003), (Set-4–Nov. 2003)
11. Explain the concept of matter waves.  
(Set-1, Set-3–May 2006), (Set-2, Set-3–June 2005), (Set-2–May 2004), (Set-4–May 2003)
12. Describe Davisson and Germer's experiment and explain how it enabled the verification of wave nature of matter.  
(Set-1, Set-3–May 2006), (Set-2, Set-3–June 2005), (Set-2–May 2004), (Set-4–May 2003)
13. Derive time-independent Schrödinger's wave equation for a free particle.  
(Set-2–Sept. 2006), (Set-4–June 2005), (Set-1–Nov. 2004), (Set-2–Nov. 2004), (Set-2, Set-3–May 2003)
14. Explain the physical significance of wave function.  
(Set-1, Set-3–Sept. 2008), (Set-4–June 2005), (Set-2, Set-3–Nov. 2004), (Set-3–May 2003), (Set-1–Nov. 2003)
15. Show that the wavelength ' $\lambda$ ' associated with an electron of mass ' $m$ ' and kinetic energy ' $E$ ' is given by  $\lambda = \frac{h}{\sqrt{2mE}}$ .  
(Set-2–Sept. 2006), (Set-3–Nov. 2004), (Set-2–May 2003)
16. Assuming the time-independent Schrödinger's wave equation, discuss the solution for a particle in one-dimensional potential well of infinite height.  
(Set-3–Nov. 2004), (Set-1–Nov. 2003)
17. Describe in detail, with a neat diagram, Davisson and Germer experiment to show that particles behave like waves.  
(Set-4–Sept. 2008), (Set-4–Nov. 2004), (Set-3–Nov. 2003)
18. Describe an experiment to establish the wave nature of electrons.  
(Set-4–May 2007), (Set-1–June 2005), (Set-4–May 2004)
19. Explain the difference between a matter wave and an electromagnetic wave.  
(Set-4–May 2007), (Set-1–June 2005), (Set-4–May 2004)
20. Show that the wavelength of an electron accelerated by a potential difference  $V$  volts is  $\lambda = \frac{1.227 \times 10^{-10}}{\sqrt{V}}$  m for non-relativistic case.  
(Set-4–May 2007), (Set-1–June 2005), (Set-4–May 2004)
21. Apply Schrödinger's equation to the case of a particle in a box and show that the energies of the particle are quantized.  
(Set-2–Nov. 2003),
22. Explain de Broglie hypothesis.  
(Set-1–May 2008), (Set-3–May 2004)
23. Explain G.P. Thomson's experiment in support of this hypothesis.  
(Set-3–May 2004)
24. Starting with the plane wave equation associated with a moving particle, formulate the time-independent Schrödinger's wave equation.  
(Set-2–Nov. 2003)
25. Explain in detail the properties of matter waves.  
(Set-2–May 2008)
26. Describe G.P. Thomson's experiment in support of de Broglie hypothesis.  
(Set-1–May 2008)

27. Describe Davisson and Germer experiment to verify the wave nature of matter. (Set-2–May 2008)
28. Distinguish between a matter wave and an electromagnetic wave. (Set-4–May 2008)
29. Describe G.P. Thomson's experiment to study electron diffraction. (Set-4–May 2008)
30. Discuss the de Broglie hypothesis of duality of matter particles. (Set-4–Sept. 2008), (Set-3–May 2008)
31. Describe G.P. Thomson's experiment to verify the wave nature of matter. (Set-3–May 2008)
32. Discuss, in detail, the physical significance of wave function. (Set-2–Sept. 2008)
33. Show that the energies of a particle in a 3-dimensional potential box, are quantized. (Set-2–Sept. 2008)
34. Deduce an expression for energy of an electron confined to a potential box of width ' $x$ '. (Set-1–Sept. 2008)
35. Derive 3-dimensional, time independent Schrödinger wave equation for an electron. (Set-1–Sept. 2008)
36. Derive one-dimensional, time independent Schrödinger wave equation for an electron. (Set-3–Sept. 2008)
37. What is de Broglie's hypothesis? Describe any one experiment by which the hypothesis was verified.
38. Show that the energies of a particle in a potential box are quantized.
39. Explain the concept of wave-particle duality and obtain an expression for the wavelength of matter waves.
40. Discuss the de Broglie's hypothesis of duality of material particles. Give in detail the experiment of Davisson and Germer in support of the hypothesis.
41. What are matter waves? Obtain an expression for the wavelength of matter waves.
42. Explain in detail the Davisson and Germer's experiment to prove the existence of matter waves.
43. Explain the dual nature of light. Describe G.P. Thomson's experiment to verify the dual nature of matter.
44. Obtain eigen values of energy, normalized wave functions and probability functions for a particle in one-dimensional potential box of side ' $L$ '.
45. Derive the Schrödinger's time-independent wave equation of an electron and write the significance of orthonormality condition of wave function.
46. Give the graphical presentation for the probability of metallic electron in its second allowed state as a function of length of potential box.
47. Show that for a quantum particle confined to an infinite deep potential box with finite length, the energy levels are quantized.
48. Write the time-independent Schrödinger's wave equation of electron and write the physical interpretation of  $\psi$ .
49. With suitable picturization of potential well and imposed boundary conditions, derive the Schrödinger's equation for metallic electron and prove that energy levels are unequally spaced.

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## C H A P T E R

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# 5

## Electron Theory of Metals

### 5.1 Introduction

The valence electrons of isolated metallic atoms are bound to the atoms, whereas in a metallic crystal they are not bound to any particular atom; they freely move in the spaces between the atoms. So, they are called free electrons. These free electrons participate in electrical conduction; hence they are called as conduction electrons. The metals possess some physical properties. They are:

- (i) Due to the existence of large number of free electrons, metals possess high electrical and thermal conductivities.
- (ii) They obey Ohm's law i.e., the current through a metal is proportional to the applied electric field.
- (iii) The resistivity ( $\rho$ ) is proportional to the fifth power of absolute temperature [i.e.,  $\rho \propto T^5$ ] at low temperatures, whereas resistivity is proportional to absolute temperature ( $\rho \propto T$ ) at high temperatures.
- (iv) In metals, the ratio of thermal conductivity to electrical conductivity is proportional to absolute temperature. This is known as Wiedmann-Franz law.
- (v) Near absolute zero of temperature, the resistivity of some metals drops to zero; hence they show superconductivity.
- (vi) The resistance of a metal increases with temperature as given below:

$$R(T) = R_0 + R_0\alpha T$$

where  $R(T)$  is the resistance at the temperature  $T^\circ C$

$R_0$  is the resistance at  $0^\circ C$

$\alpha$  is the temperature coefficient of resistance

$T$  is the temperature in  $^\circ C$ .

## 5.2 Classical free electron theory of metals

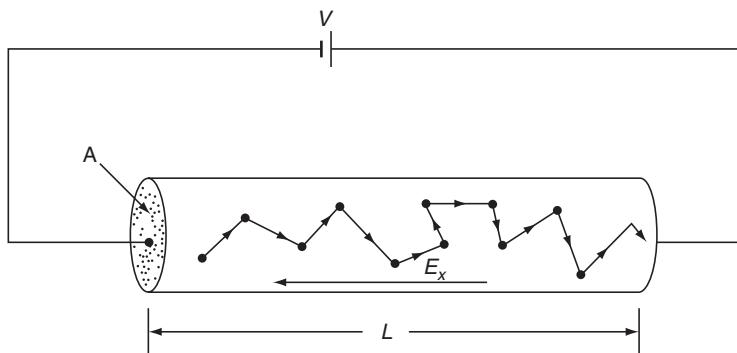
The classical free electron theory was introduced by P. Drude in 1900 and developed by Lorentz in 1909 to explain electrical conduction in metals. This theory has some assumptions; they are:

- (i) The valence electrons of metallic atoms are free to move in the spaces between ions from one place to another place within the metallic specimen similar to gaseous molecules so that these electrons are called free electron gas. These electrons also participate in electrical conduction; hence they are called conduction electrons.
- (ii) There is no interaction between these conduction electrons.
- (iii) The interaction of free electrons with ion cores is negligible.
- (iv) The free electrons find uniform electric field of positive ions and that of electrons in the metal.

### To study electrical conductivity

To obtain an expression for electrical conductivity, consider a metallic rod of length  $l$  and area of cross section ' $A$ ' as shown in Fig. (5.1). In the absence of an external electric field, the free electrons move in random directions, similar to gaseous molecules in a container so that there is no net resultant motion of electrons along any direction.

**Figure 5.1** Electron drifting in electric field ( $E_x$ )



The root mean square velocity of electrons is obtained by applying kinetic theory of gases and equipartition law of energy. The pressure ' $P$ ' of the gas is:

$$P = \frac{1}{3} \rho \bar{C}^2 = \frac{1}{3} mn \bar{C}^2 \quad (5.1)$$

where  $m$  is mass of an electron, ' $n$ ' is the number of free electrons per unit volume, ' $\rho$ ' is the density of an electron gas and  $\bar{C}$  is root mean square velocity.

For molar volume ( $V_m$ ) of the metal,

$$P = \frac{1}{3} \rho \bar{C}^2 = \frac{1}{3} m \frac{N_A}{V_m} \bar{C}^2 \quad (5.2)$$

where  $N_A$  is Avogadro's number

From Equation (5.2)

$$PV_m = \frac{1}{3} m N_A \bar{C}^2 = R_u T \quad (\text{or}) \quad m \bar{C}^2 = \frac{3R_u T}{N_A} = 3K_B T \quad (5.3)$$

where  $R_u$  is universal gas constant,  $T$  is absolute temperature and  $K_B$  is Boltzmann's constant.

From Equation (5.3)  $\bar{C} = \sqrt{\frac{3K_B T}{m}} \quad (5.4)$

Now a potential difference ( $V$ ) is applied across the ends of the rod, kept parallel to X-direction, then an electric field,  $E_x$  acts on the electrons, then the electrons acquire a constant velocity  $v_x$  in the opposite direction to that of electric field. This constant velocity is called drift velocity, this velocity is superimposed on the thermal velocity ( $\bar{C}$ ) of the electrons.

If ' $R_x$ ' is the resistance of the rod, then the current  $I_x$  through it is:

$$I_x = \frac{V_x}{R_x} = AJ_x \quad (5.5)$$

where  $J_x$  is the current density along X-direction

$$(\text{or}) \quad J_x = \frac{V_x}{AR_x} = \frac{E_x l}{A} \times \frac{A}{\rho_x l} = \frac{E_x}{\rho_x} = \sigma_x E_x \quad (5.6)$$

where  $E_x$  = intensity of electric field;  $\rho_x$  = resistivity and  $\sigma_x$  = electrical conductivity of the metal.

The field  $E_x$  produces a force  $-eE_x$  on each electron, due to this force the acceleration on  $i$ th electron is:

$$a_{ix} = \frac{dv_{ix}}{dt} = -\frac{eE_x}{m} \quad (5.7)$$

where  $v_{ix}$  is the drift velocity of  $i$ th electron along X-direction. Since the electrical force  $eE_x$  is the same on all electrons, so the average acceleration is:

$$\frac{d}{dt} \langle v_x \rangle = -\frac{eE_x}{m} \quad (5.8)$$

where  $\langle v_x \rangle$  is the average velocity of  $n$  free electrons in unit volume of metal, given by:

$$\langle v_x \rangle = \frac{1}{n} \sum_{i=1}^n v_{ix} \quad (5.9)$$

The current density along X-direction is:

$$J_x = n \langle v_x \rangle (-e) = -ne \langle v_x \rangle \quad (5.10)$$

The minus sign shows that  $J_x$  is in the opposite direction to that of  $\langle v_x \rangle$ . The average velocity  $\langle v_x \rangle$  can be obtained by considering the acceleration and retardation in steady state.

In addition to acceleration,  $\left( \frac{eE_x}{m} \right)$  the electrons get retarded due to collisions of electrons with lattice ions.

This is referred to as electron lattice scattering.

In steady state, the sum of acceleration and retardation is equal to zero.

$$\left[ \frac{d}{dt} \langle v_x \rangle \right]_{E_x} + \left[ \frac{d}{dt} \langle v_x \rangle \right]_{el-la} = 0 \quad (5.11)$$

## 5-4 | Applied Physics

The retardation,  $\left[ \frac{d}{dt} \langle v_x \rangle \right]_{el-la}$  can be calculated as follows: Let  $\langle v_x \rangle_0$  is the average drift velocity of

free electrons at  $t = 0$ , i.e., at the moment the electric field is removed, afterwards the drift velocity reduces exponentially to zero due to electron-lattice collisions.

$$\langle v_x \rangle = \langle v_x \rangle_0 e^{-t/\tau_x} \quad (5.12)$$

where  $\tau_x$  is known as relaxation time. It is defined as the time taken by an electron to decay its drift velocity to  $1/e$  of its initial value. Differentiating Equation (5.12) gives retardation.

$$\left[ \frac{d}{dt} \langle v_x \rangle \right]_{el-la} = -\frac{\langle v_x \rangle_0}{\tau_x} e^{-t/\tau_x} = -\frac{\langle v_x \rangle}{\tau_x} \quad (5.13)$$

substituting Equations (5.8) and (5.13) in Equation (5.11) gives:

$$\frac{-eE_x}{m} - \frac{\langle v_x \rangle}{\tau_x} = 0 \quad (\text{or}) \quad \langle v_x \rangle = -\left( \frac{e\tau_x}{m} \right) E_x \quad (5.14)$$

Equation (5.14) shows that the drift velocity acquired by the electron is proportional to applied electric field and the proportionality constant  $\frac{e\tau_x}{m}$  is known as their mobility ( $\mu_x$ ). It is defined as the drift velocity produced per unit applied electric field and it is given by:

$$\mu_x = \frac{\langle v_x \rangle}{E_x} = \frac{e\tau_x}{m} \quad (5.15)$$

Finally, comparing Equations  $J_x = \sigma_x E_x$  and  $J_x = -ne \langle v_x \rangle$ , we have:

$$\sigma_x E_x = -ne \langle v_x \rangle \quad (5.16)$$

Substituting Equation (5.14) in (5.16)

$$\begin{aligned} \sigma_x E_x &= -ne \left( -\frac{e\tau_x}{m} \right) E_x \\ \therefore \sigma_x &= \frac{ne^2}{m} \tau_x \end{aligned} \quad (5.17)$$

Substituting Equation (5.15) in (5.17) gives:

$$\sigma_x = ne\mu_x \quad (5.18)$$

$$(\text{or}) \quad \text{resistivity, } \rho_x = \frac{1}{\sigma_x} = \frac{1}{ne\mu_x} \quad (5.19)$$

Equations (5.17), (5.18) and (5.19) represent electrical conductivity and resistivity in a metal.

**Merits and drawbacks (or) failures of classical free electron theory:** Classical theory successfully explains electrical and thermal conductivities of metals, the increase of resistance with temperature, opacity, luster, etc., but fails to explain the following aspects.

- (1) According to classical theory, the electrical conductivity ( $\sigma$ ) of a metal is inversely proportional to its square root of its absolute temperature ( $T$ ). i.e.,  $\sigma \propto \frac{1}{\sqrt{T}}$ . But practically, it has been observed that the electrical conductivity is inversely proportional to its absolute temperature. i.e.,  $\sigma \propto \frac{1}{T}$ . Thus, classical theory failed to explain the electrical conductivity of metals.
- (2) Experimentally, it has been observed that the specific heat of a metal is proportional to its absolute temperature. But the classical theory predicts that the specific heat does not depend on temperature. Thus, classical theory failed to explain specific heat of metals.
- (3) According to classical free electron theory, the electrical conductivity ( $\sigma$ ) is proportional to the free electron concentration ( $n$ ) because,  $\sigma = \frac{ne^2\tau}{m}$ . The free electron concentration of divalent metals like Zn, Cd, etc., and trivalent metals like Al, Ga, etc., is larger than the metals like Cu and Ag. But the electrical conductivities of Cu and Ag are larger than that of the above divalent and trivalent metals. Thus, the classical free electron theory failed to explain electrical conductivity on the basis of free electron concentration of different metals.

### 5.3 Relaxation time, mean free path, mean collision time and drift velocity

**(i) Relaxation time ( $\tau$ ):** In the absence of an external electric field, the free electrons in a metallic substance will move in random directions, so that the resultant velocity of free electrons in any direction is equal to zero. By applying an external electric field on the specimen, the free electrons of the metal acquire a constant resultant velocity in the opposite direction to that of the applied electric field. If the field is turned off suddenly at  $t = 0$ , then the average drift velocity  $\langle v_x \rangle_0$  reduces exponentially to zero. The drift velocity after some time ' $t$ ' is:

$$\langle v_x \rangle = \langle v_x \rangle_0 e^{-t/\tau} \quad (5.20)$$

where  $\tau$  is called relaxation time. when  $t = \tau$  then Equation (5.20) becomes:

$$\langle v_x \rangle = \langle v_x \rangle_0 e^{-1} = \frac{\langle v_x \rangle_0}{e} \quad (5.21)$$

Thus, relaxation time may be defined as the time taken by an electron to reduce its velocity to  $1/e$  of its initial value. Differentiating Equation (5.20):

$$\frac{d \langle v_x \rangle}{dt} = \frac{-\langle v_x \rangle_0 e^{-t/\tau}}{\tau} = -\frac{\langle v_x \rangle}{\tau} \quad (5.22)$$

Equation (5.22) represents retardation.

**(ii) Mean free path ( $\lambda$ ):** It is the average distance travelled by a free electron between two successive collisions with lattice ions in a metallic crystal. The mean free path ( $\lambda$ ) of an electron is represented as  $\lambda = \bar{v}\tau_c$ , where  $\bar{v}$  is the root mean square velocity and  $\tau_c$  is the mean collision time of a conduction electron.

**(iii) Mean collision time ( $\tau_c$ ):** The time between two successive collisions of a free electron with lattice ions in a metallic crystal is called collision time. The average of successive collision times of a free electron is called

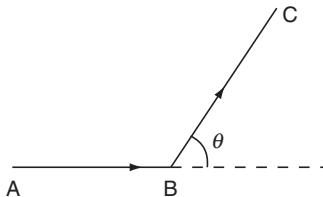
the mean collision time. If  $v$  is the resultant of thermal and drift velocities of a free electron, then the mean collision time ( $\tau_c$ ) is given by  $\tau_c = \frac{\lambda}{v}$ , where  $\lambda$  is the mean free path of an electron. If the drift velocity ( $v_d$ ) of an electron is very much lesser than the thermal velocity ( $v_{th}$ ) of the electron [i.e.,  $v_d \ll v_{th}$ ] then  $v \approx v_{th}$

$$\therefore \tau_c = \frac{\lambda}{v_{th}}$$

**(iv) Relation between  $\tau$  and  $\tau_c$ :** Consider a free electron moving with velocity  $v$  along AB direction inside a metallic crystal as shown in Fig.5.2. At 'B', the electron makes collision with a lattice point and travels along BC direction with same velocity, making an angle  $\theta$  with the original direction. Let  $\theta_1, \theta_2, \theta_3, \dots$  be the successive scattering angles in different collisions of an electron, then the average of  $\cos \theta_1, \cos \theta_2, \cos \theta_3, \dots$  is represented by  $\langle \cos \theta \rangle$ . The relaxation time  $\tau$  and mean collision time are related through the equation:

$$\tau = \frac{\tau_c}{1 - \langle \cos \theta \rangle}$$

**Figure 5.2** Movement of a free electron inside a metallic crystal



**(v) Expression for drift velocity:** In the absence of an applied electric field, the free electrons in a metal are moving in random directions so that the resultant motion of electrons in any direction is equal to zero. By the application of an electric field  $E$ , every electron experiences a force ( $F$ ) equal to  $-eE$ .

$$\text{i.e., } F = -eE \quad (5.23)$$

Due to this force, the velocities of free electrons should gradually increase, but this will not happen because of the collisions of conduction electrons with ion cores of the crystal. The velocities of free electrons increase up to a certain value called drift velocity  $v_d$ , afterwards their velocity does not increase because of retardation due to collisions with ions. If  $v_d$  is the steady state or drift velocity and  $\tau_c$  is the mean collision time of free electrons, then the resistive force,  $F_r$  offered to its motion is given by:

$$F_r = m \frac{v_d}{\tau_c} \quad (5.24)$$

In steady state,  $F_r = F$

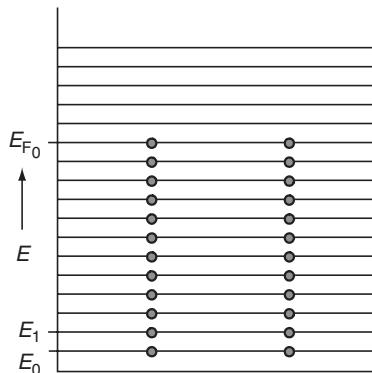
$$\text{i.e., } \frac{mv_d}{\tau_c} = -eE$$

Therefore, the drift velocity ( $v_d$ ) is given by  $v_d = -\frac{eE}{m} \tau_c$

## 5.4 Fermi-Dirac distribution

In a metallic crystal, the free electrons possess different energies except the restriction put forward by Pauli's exclusion principle. According to quantum theory, at absolute zero of temperature, the free electrons occupy different energy levels continuously without any vacancy in between filled states. This can be understood by dropping the free electrons of a metal one by one into the potential well. The first electron dropped would occupy the lowest available energy,  $E_0$  (say), and the next electron dropped also occupy the same energy level. The third electron dropped would occupy the next energy level. That is, the third electron dropped would occupy the energy level  $E_1 (>E_0)$  and so on because of Pauli's exclusion principle. If the metal contains  $N$  (even) number of electrons, they will be distributed in the first  $N/2$  energy levels and the higher energy levels will be completely empty as shown in Fig.5.3.

**Figure 5.3 Distribution of electrons in various energy levels at 0 K.**

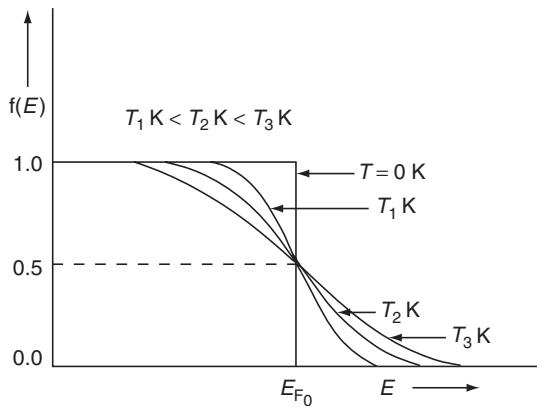


The highest filled level, which separates the filled and empty levels at 0 K is known as the Fermi level and the energy corresponding to this level is called Fermi energy ( $E_F$ ). Fermi energy can also be defined as the highest energy possessed by an electron in the material at 0 K. At 0 K, the Fermi energy  $E_F$  is represented as  $E_{F_0}$ . As the temperature of the metal is increased from 0 K to  $T$  K, then those electrons which are present up to a depth of  $K_B T$  from Fermi energy may take thermal energies equal to  $K_B T$  and occupy higher energy levels, whereas the electrons present in the lower energy levels i.e., below  $K_B T$  from Fermi level, will not take thermal energies because they will not find vacant electron states. The probability that a particular quantum state at energy  $E$  is filled with an electron is given by Fermi-Dirac distribution function  $f(E)$ , given by:

$$f(E) = \frac{1}{1 + \exp(E - E_F) / K_B T} \quad \text{where } K_B = \text{Boltzmann constant.}$$

A graph has been plotted between  $f(E)$  and  $E$ , at different temperatures 0 K,  $T_1$  K,  $T_2$  K,  $T_3$  K is shown in Fig. 5.4.

**Figure 5.4 Graph between  $f(E)$  and  $E$**



**Analytical Treatment At 0 K:** Substitute  $T = 0 \text{ K}$  in the Fermi-Dirac distribution, we have

$$\begin{aligned} f(E) &= \frac{1}{1 + \exp[(E - E_F)/K_B \times 0]} = 1 \text{ for } E < E_F \\ &= 0 \text{ for } E > E_F \end{aligned}$$

The curve has step-like character with  $f(E) = 1$  for energies below  $E_{F_0}$  and  $f(E) = 0$  for energies above  $E_{F_0}$ . This represents that all the energy states below  $E_{F_0}$  are filled with electrons and all those above it are empty.

At  $T > 0 \text{ K}$

$$\begin{aligned} f(E) &= \frac{1}{1 + \exp[(E - E_F)/K_B T]} < 1 \text{ for } E < E_F \\ &> 0 \text{ for } E > E_F \\ &= \frac{1}{2} \text{ for } E = E_F \end{aligned}$$

As the temperature is raised from absolute zero to  $T_1 \text{ K}$ , the distribution curve begins to depart from step-like function and tails off smoothly to zero. Again with a further increase in temperature to  $T_2 \text{ K}$  and to  $T_3 \text{ K}$ , the departure and tailing of the curves increases. This indicates that more and more electrons may occupy higher energy states with an increase of temperature and as a consequence the number of vacancies below the Fermi level increases in the same proportion. At non-zero temperatures, all these curves pass through a point whose  $f(E) = 1/2$ , at  $E = E_F$ . So  $E_F$  lies half way between the filled and empty states.

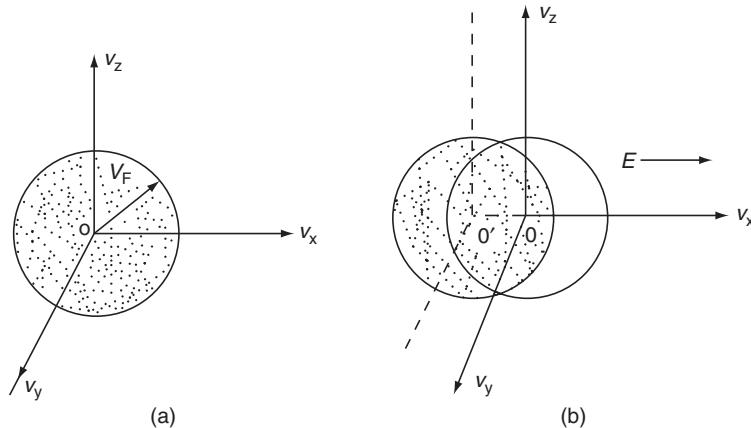
## 5.5 Quantum free electron theory of electrical conduction

Sommerfeld (1928) applied the principles of quantum mechanics to classical free electron theory.

According to classical theory, the free electrons in a metal have random motions with equal probability in all directions. But according to quantum theory, the free electrons occupy different energy levels,

Figure 5.5

(a) Distribution of velocities of free electrons of a metal at 0 K;  
 (b) Displacement of velocities sphere with electric field ( $E$ )



up to Fermi level at 0 K. So, they possess different energies and hence they possess different velocities. The different velocities of these free electrons of a metal can be seen in velocity space. At 0 K, the electrons present in Fermi level possess maximum velocity, represented as  $V_F$ . We assume a sphere of radius  $V_F$ , at the origin of velocity space as shown in Fig. 5.5a. Each point inside the sphere represents velocity of a free electron. This sphere is called Fermi sphere. The Fermi surface need not always be spherical. The vectors joining different points inside the sphere from the origin represent velocity vectors. In the absence of an external electric field, the velocity vectors cancel each other in pair-wise and the net velocity of electrons in all directions is zero.

Now if we apply an external electric field ( $E$ ) along X-direction on these electrons as shown in Fig. 5.5(b), then a force  $eE$  acts on each electron along negative X-direction. Only those electrons present near the Fermi surface can take electrical energy and occupy higher vacant energy levels. For rest of the electrons, the energy supplied by electrical force is too small so that they are unable to occupy higher vacant energy levels. Hence, the electric field causes the entire equilibrium velocity distribution to be shifted slightly by an amount in the opposite direction to the field as shown in Fig. 5.5(b).

In quantum theory, the velocity of a free electron can be represented in terms of propagation vector as:

$$\text{We know } K^2 = \frac{2mE}{\hbar^2}$$

$$\text{or } E = \frac{\hbar^2 K^2}{2m} = \frac{P^2}{2m}$$

$$\text{So, } P = \hbar K = mv$$

$$v = \frac{\hbar K}{m} \quad \text{--- (5.25)}$$

where  $\hbar = \frac{h}{2\pi}$  and  $K = \frac{2\pi}{\lambda}$  = propagation or wave vector.

Differentiating Equation (5.25) with respect to time gives acceleration ( $a$ ):

$$a = \frac{dv}{dt} = \frac{\hbar}{m} \frac{dK}{dt} \quad \text{_____ (5.26)}$$

The force on an electron due to an applied electric field is  $eE$ , and this is equated to the product of mass and acceleration [from Equation (5.26)] of the electron.

Hence,  $m \times \frac{\hbar}{m} \frac{dK}{dt} = eE$

$$\text{(or)} \quad \hbar \frac{dK}{dt} = eE \quad \text{_____ (5.27)}$$

$$\text{(or)} \quad dK = \frac{eE}{\hbar} dt \quad \text{_____ (5.28)}$$

Integrating Equation (5.28) gives:

$$K(t) - K(0) = \frac{eEt}{\hbar} \quad \text{_____ (5.29)}$$

Let the mean collision time and mean free path of a free electron present at Fermi surface is represented as  $\tau_F$  and  $\lambda_F$ , respectively then, we have:

$$\tau_F = \frac{\lambda_F}{v_F} \quad \text{_____ (5.30)}$$

For an electron at Fermi level, consider  $t = \tau_F$  and  $K(t) - K(0) = \Delta K$  in Equation (5.29).

$$\text{Then, } \Delta K = \frac{eE\tau_F}{\hbar} = \frac{eE}{\hbar} \left( \frac{\lambda_F}{v_F} \right) \quad \text{_____ (5.31)} \quad \text{using Equation (5.30).}$$

The applied electric field enhances the velocity of electrons present near the Fermi level. The increase in velocity ( $\Delta v$ ) causes current density ( $J$ ) in the material, given by:

$$J = ne\Delta v \quad \text{_____ (5.32)}$$

where  $n$  is the number of electrons that participate in conduction per unit volume of metal. Using Equation (5.25), the value of  $\Delta v$  is substituted in Equation (5.32), we have:

$$J = ne \frac{\hbar \Delta K}{m^*} \quad \text{_____ (5.33)} \quad \text{where } m^* \text{ is the effective mass of free electron.}$$

Substituting Equation (5.31) in Equation (5.33) gives:

$$J = \frac{ne\hbar}{m^*} \frac{eE}{\hbar} \frac{\lambda_F}{v_F} = \frac{ne^2}{m^*} \left( \frac{\lambda_F}{v_F} \right) E \quad \text{_____ (5.34)}$$

From Ohm's law,

$$J = \sigma E, \text{ where } \sigma = \text{Electrical conductivity.}$$

$$\text{So, } \sigma = \frac{ne^2}{m^*} \left( \frac{\lambda_F}{v_F} \right) = \frac{ne^2}{m^*} \tau_F \quad \text{_____ (5.35)}$$

Using Equation (5.35), electrical conductivity of a metal can be calculated.

A similar equation may be obtained from the band theory for electrical conductivity as:

$$\sigma = \frac{n_{\text{eff}} e^2}{m^*} \tau_F \quad \text{--- (5.36)}$$

where  $n_{\text{eff}}$  is the effective number of electrons per unit volume of material.

Thus, in case of quantum theory, the electrical conductivity is due to the electrons which are very close to Fermi surface only. This expression is in agreement with experimental conclusions.

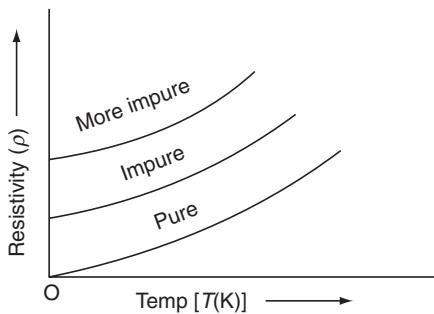
## 5.6 Sources of electrical resistance

In a metallic crystal, the electrons move through periodically varying electric potentials (or fields) of positive ions of the lattice. The cause for electrical resistance is the electron scattering and the cause for electron scattering is the non-periodicity of the lattice potentials. The causes for non-periodicity of lattice potentials are: (i) impurities in crystals, (ii) crystal defects (or imperfections) and (iii) thermal vibrations.

Freely moving electrons are associated with de Broglie [or matter] waves. In a perfect crystal, an electron moves similar to an electromagnetic wave without attenuation so that the mean free paths of electrons will be of several hundred Angstroms. This is in agreement with the observed values of mean free paths. According to classical free electron theory, the electrical resistance is due to collisions of free electrons with the positive ion cores of the crystal. From this concept, the mean free path will be a few Angstroms only. This is contradictory to the observed mean free paths of electrons, so the scattering of electrons by positive ions is ignored. Now, we will see in detail the causes of non-periodic potentials of lattice.

**(i) Presence of impurities in crystals:** The presence of impurities introduces electrical resistance in a metallic substance. With an increase of impurity concentration, the resistivity of a metal increases as shown in Fig. 5.6.

**Figure 5.6 Resistivity variation of impure metal with temperature**



The presence of impurity atomic site changes the periodicity of electrical potential. If the impurity concentration is more, then at large number of atomic sites non-periodic potentials exist and they cause large electron scattering and hence resistivity.

**(ii) Crystal defects:** The presence of imperfections such as vacancies and grain boundaries changes the periodic potentials. So, larger the number of defects, larger will be the non-periodic potentials and hence larger the electron scattering and resistivity.

**(iii) Thermal vibrations:** At high temperatures, the resistivity is linearly proportional to absolute temperature, whereas at low temperatures, the resistivity is proportional to the fifth power of temperature. Due to thermal vibrations, the positive ions move away from their ideal positions so that periodicity of potential changes. With an increase of temperature, the amplitude of thermal vibrations of positive ions will be more, so non-periodicity increases. Hence, resistivity increases.

Near absolute zero of temperature, some materials show zero resistivity or superconductivity. For some materials, the resistance is not equal to zero even at 0 K. The total resistivity ( $\rho$ ) of a metal is due to impurities and defects and also due to thermal vibrations.

$$\therefore \rho = \rho_i + \rho(T)$$

where  $\rho_i$  is the resistivity due to impurities and defects and  $\rho(T)$  = resistivity due to thermal vibrations.

## 5.7 Band theory of solids

### (a) Introduction

According to quantum free electron theory of metals, a conduction electron in a metal experiences constant (or zero) potential and free to move inside the crystal but will not come out of the metal because an infinite potential exists at the surface. This theory successfully explains electrical conductivity, specific heat, thermionic emission and paramagnetism. This theory fails to explain many other physical properties, for example: (i) it fails to explain the difference between conductors, insulators and semiconductors, (ii) positive Hall coefficient of metals and (iii) lower conductivities of divalent metals than monovalent metals.

To overcome the above problems, the periodic potentials due to the positive ions in a metal have been considered. As shown in Fig. 5.7(a), if an electron moves through these ions, it experiences varying potentials. The potential of an electron at the positive ion site is zero and is maximum in between two ions. The potential experienced by an electron, when it passes along a line through the positive ions is as shown in Fig. 5.7(b). We see that the potential experienced by an electron varies periodically with the same period as the lattice. The potential is negative because of an attractive force between electrons and positive ions. Along X-direction in the crystal, the potential function  $V(x)$  has the periodicity of the lattice given by:

$$V(x) = V(x + a) \quad \text{where 'a' is the periodicity of the lattice.} \quad (5.37)$$

The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice. The Schrödinger time-independent wave equation for the motion of an electron along X-direction is given by:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0 \quad (5.38)$$

Bloch showed a type of solution for Equation (5.38) given by:

$$\psi(x) = u_K(x) e^{iKx} \quad (5.39)$$

where  $u_K(x)$  represents periodic function given by:

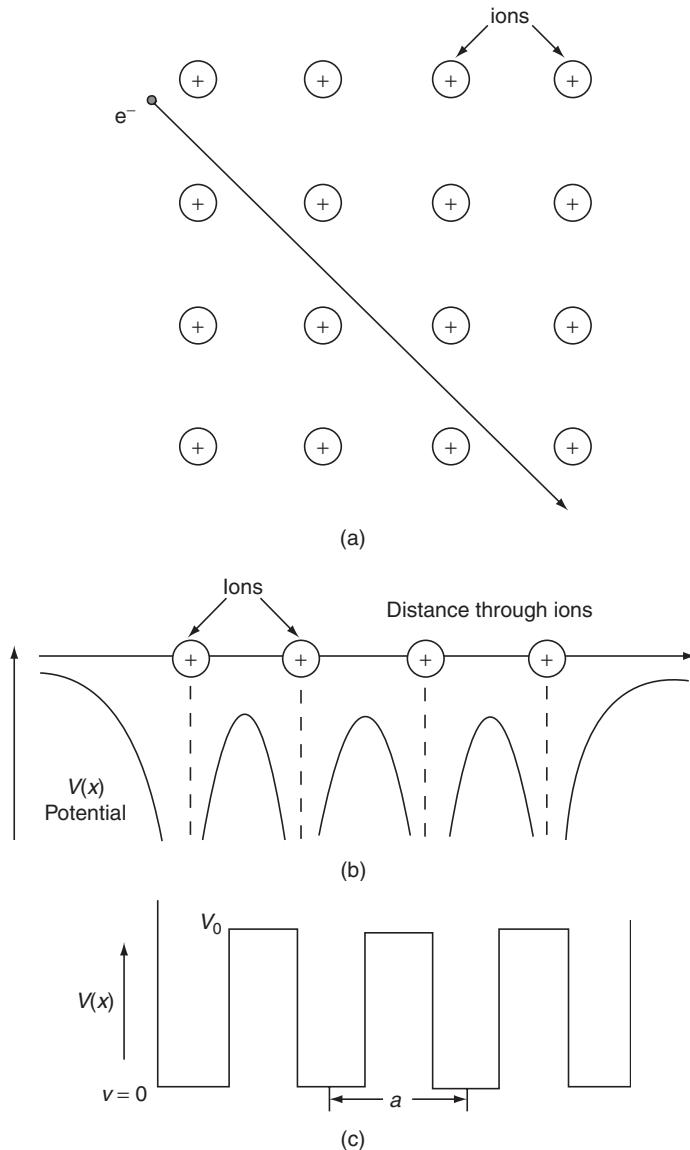
$$u_K(x) = u_K(x + a) \quad (5.40)$$

Here,  $K = \frac{2\pi}{\lambda}$  = propagation vector;  $\lambda$  = wavelength of de Broglie wave associated with the moving

electron,  $e^{iKx}$  represents a plane wave. Equation (5.39) is a solution to Schrödinger's wave Equation (5.38) in sinusoidal potential as shown in Fig. 5.7(b). It is not easy to solve Schrödinger's equation with

Figure 5.7

(a) Electron motion; (b) The potential experienced by an electron in a row of ions; (c) Rectangular potentials

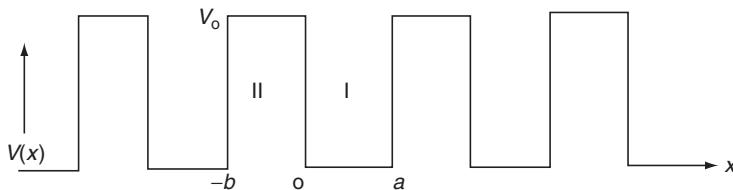


these potentials. So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. 5.7(c). This model is called Kronig-Penney model of potentials.

### (b) Kronig-Penney model – origin of energy bands

The rectangular potential wells and barriers, as assumed by Kronig and Penney for one-dimensional lattice in 1931, are best suited to solve Schrödinger's wave equation. These potentials are shown in Fig. 5.8, in which the

Figure 5.8 Kronig–Penney model of potentials



width of the potential well and potential barrier are ‘ $a$ ’ and ‘ $b$ ’, respectively. The potential energy of an electron in the well is zero; this corresponds to the potential in the vicinity of the nucleus and in barrier it possesses a constant value represented as  $V_0$ . The periodicity of the potential is  $(a + b)$ . This is an approximate model but close to reality.

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger’s wave equations for the two regions I and II as shown in Fig. 5.8.

The Schrödinger’s equations are:

$$\frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2}\right) E \psi = 0 \quad \text{for } 0 < x < a \quad (5.41)$$

$$\frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2}\right) (E - V_0) \psi = 0 \quad \text{for } -b < x < 0 \quad (5.42)$$

We define two real quantities (say)  $\alpha$  and  $\beta$  such that:

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2} (V_0 - E) \quad (5.43)$$

Hence, Equations (5.41) and (5.42) becomes:

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0 \quad \text{for } 0 < x < a \quad (5.44)$$

$$\frac{d^2\psi}{dx^2} - \beta^2 \psi = 0 \quad \text{for } -b < x < 0 \quad (5.45)$$

The solution that will be appropriate for both the regions will be of the form of a plane wave  $e^{ikx}$  modulated with a periodic function  $u_K(x)$ :

$$\psi(x) = e^{ikx} u_K(x) \quad (5.46)$$

where  $K = \frac{2\pi}{\lambda}$  = wave vector or propagation vector

Differentiating Equation (5.46) twice, we get:

$$\frac{d\psi}{dx} = iKe^{ikx} u_K(x) + e^{ikx} \frac{du}{dx}$$

$$\frac{d^2\psi}{dx^2} = -K^2 e^{iKx} u_K(x) + 2iKe^{iKx} \frac{du}{dx} + e^{iKx} \frac{d^2u}{dx^2}$$

Substituting these values in Equation (5.44) and (5.45), we get:

$$\begin{aligned} -K^2 e^{iKx} u_K(x) + 2iKe^{iKx} \frac{du}{dx} + e^{iKx} \frac{d^2u}{dx^2} + \alpha^2 e^{iKx} u_K(x) &= 0 \\ \frac{d^2u}{dx^2} + 2iK \frac{du}{dx} + (\alpha^2 - K^2) u_K(x) &= 0 \quad \text{for } 0 < x < a \end{aligned} \quad (5.47)$$

Similarly,

$$\frac{d^2u}{dx^2} + 2iK \frac{du}{dx} - (\beta^2 + K^2) u_k(x) = 0 \quad \text{for } -b < x < 0 \quad (5.48)$$

Now to solve these differential equations, assume the solution of the form:

$$u = e^{mx} \quad \text{so that} \quad \frac{du}{dx} = me^{mx} \quad \text{and} \quad \frac{d^2u}{dx^2} = m^2 e^{mx} \quad (5.49)$$

which on substitution in Equation (5.47) gives:

$$m^2 e^{mx} + 2iKm e^{mx} + (\alpha^2 - K^2) e^{mx} = 0$$

$$(or) \quad m^2 + 2iKm + (\alpha^2 - K^2) = 0 \quad \text{for } 0 < x < a$$

$$\begin{aligned} \therefore m &= \frac{-2iK \pm \sqrt{(-4K^2) - 4(\alpha^2 - K^2)}}{2} \\ &= -iK \pm i\alpha \end{aligned}$$

$$\text{i.e.,} \quad m_1 = i(\alpha - K) \quad \text{and} \quad m_2 = -i(\alpha + K)$$

Hence, the general solution is:

$$u_1 = Ae^{i(\alpha-K)x} + Be^{-i(\alpha+K)x} \quad \text{for } 0 < x < a$$

Similarly,

$$u_2 = Ce^{(\beta-iK)x} + De^{-(\beta+iK)x} \quad \text{for } -b < x < 0 \quad (5.50)$$

where  $u_1$  and  $u_2$  represent  $u_K(x)$  in region I and II, respectively.

Here, A, B, C and D are constants. These constants may be obtained by applying the following boundary conditions.

$$[u_1(x)]_{x=0} = [u_2(x)]_{x=0} \quad \text{and} \quad \left[ \frac{du_1}{dx} \right]_{x=0} = \left[ \frac{du_2}{dx} \right]_{x=0} \quad (5.51)$$

$$[u_1(x)]_{x=a} = [u_2(x)]_{x=-b} \quad \text{and} \quad \left[ \frac{du_1}{dx} \right]_{x=a} = \left[ \frac{du_2}{dx} \right]_{x=-b} \quad (5.52)$$

The boundary conditions represented in Equation (5.51) show that the wave functions and their first derivatives are equal at  $x = 0$  because of the continuity of wave functions at that point.

The boundary conditions represented in Equation (5.52) show that the wave function and its first derivative at  $x = a$  is equal to that at  $x = -b$ , because of the periodicity of wave functions.

Applying boundary conditions (5.51) and (5.52) on Equation (5.50) gives four equations involving the constants A, B, C and D.

$$A + B = C + D \quad (5.53)$$

$$Ai(\alpha - K) - Bi(\alpha + K) = C(\beta - iK) - D(\beta + iK) \quad (5.54)$$

$$Ae^{i(\alpha-K)a} + Be^{-i(\alpha+K)a} = Ce^{-(\beta-iK)b} + De^{(\beta+iK)b} \quad (5.55)$$

$$Ai(\alpha - K) e^{i(\alpha - K)a} - Bi(\alpha + K) e^{-i(\alpha + K)a} = C [\beta - iK] e^{-(\beta - iK)b} - D[\beta + iK] e^{(\beta + iK)b} \quad (5.56)$$

The constants A, B, C and D can be determined by solving Equations 5.53–5.56, and thus the wave function  $u_1$  and  $u_2$  can be obtained. The four Equations 5.53–5.56 have solution only if the determinant of the coefficients of A, B, C and D vanishes. The above condition leads to the following equation.

$$\frac{\beta^2 + \alpha^2}{2\alpha\beta} \sin h\beta b \sin \alpha a + \cos h\beta b \cos \alpha a = \cos K(a + b) \quad (5.57)$$

This equation is quite complicated. To express it in a more simplified form, Kronig and Penney suggested delta function such as  $V_0 \rightarrow \infty$  and  $b \rightarrow 0$  but the product  $V_0 b$  remains finite. Under these circumstances,  $\sin h\beta b \rightarrow \beta b$  and  $\cosh h\beta b \rightarrow 1$  as  $b \rightarrow 0$ . Hence, Equation (5.57) becomes:

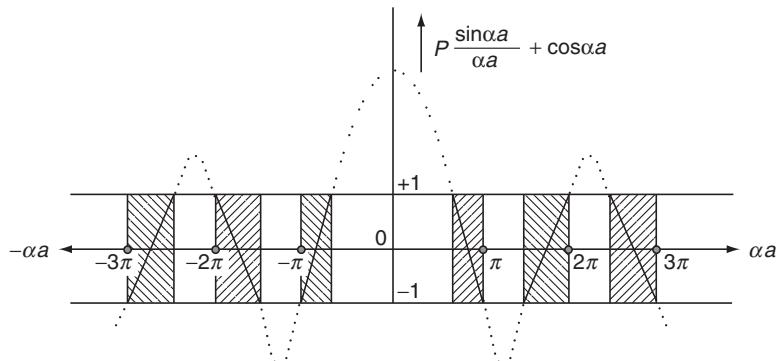
$$\left( \frac{mV_0 b}{\hbar^2 \alpha} \right) \sin \alpha a + \cos \alpha a = \cos K a \quad (5.58) \quad (\text{since } V_0 \gg E)$$

We define the quantity  $P = \frac{mV_0 ba}{\hbar^2}$ , then Equation (5.58) reduces to:

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos K a \quad (5.59)$$

Equation (5.59) represents a condition for the wave function. P is referred to as the scattering power of the potential barrier. It represents the strength with which electrons in a crystal are attracted to the ions. The term  $V_0 B$  is called barrier strength. With an increase of P, an electron is bound more strongly to a potential well, when  $P \rightarrow 0$ , the electrons are free. The right-hand side of Equation (5.59) can take values between  $\pm 1$ , But the left-hand side exceeds this value. By plotting the left-hand side of Equation (5.59) for a finite value of P ( say  $3\pi/2$ ) against  $\alpha a$ , it is possible to determine the allowed values of  $\alpha a$ .

**Figure 5.9** A graph plotted between  $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$  and  $\alpha a$  for  $P = 3\pi/2$



To find the allowed parts of the curve, horizontal lines are drawn at  $\pm 1$  on vertical line as shown in Fig. 5.9. The parts of the curve, which lies between the  $\pm 1$  horizontal line, are acceptable to the left-hand side of Equation (5.59).

From the graph, the following conclusions may be drawn.

- The allowed values of  $\alpha a$  [and hence energy, since  $\alpha^2 = \frac{2mE}{\hbar^2}$ ] for which wave mechanical solutions exist are shown by the shadow portions. From the graph, we know that the conduction electrons in periodic potentials of lattice ions possess the bands of allowed energy (shaded region) separated by forbidden regions [unshaded region].
- As the value of  $\alpha a$  increases, the width of allowed energy bands increases and the width of forbidden bands decreases.
- Now, we will see the effect of varying ' $P$ '. If  $P$  is large, then curve crosses  $\pm 1$  line steeply so that the allowed bands are narrower and forbidden bands are wider as shown in Fig. 5.10. In the limit  $P \rightarrow \infty$ ,

**Figure 5.10** Shows the decrease of allowed energy bands width for large value of  $P$

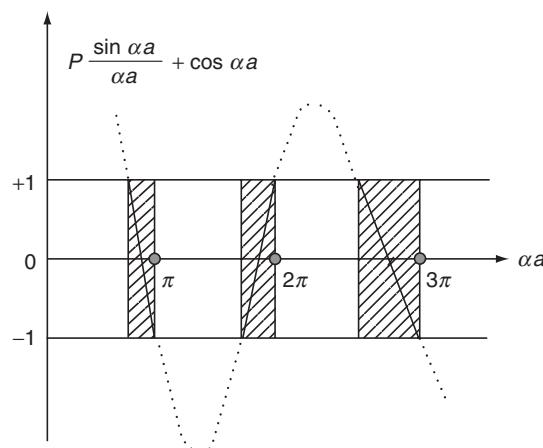


Figure 5.11

Shows that the allowed energy bands reduces to single energy levels as  $P \rightarrow \infty$

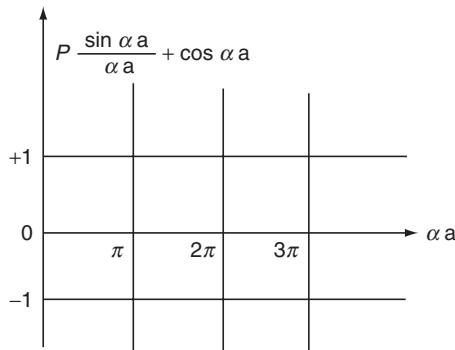
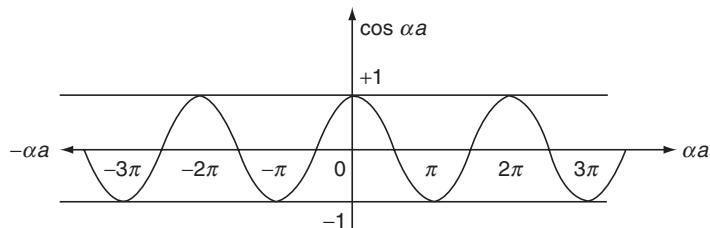


Figure 5.12

Shows that all energies are allowed to the electrons as  $P \rightarrow 0$



the allowed energy bands reduce to single energy levels as shown in Fig. 5.11. The energy levels in this case are discrete and similar to the energy levels of a particle in a constant potential box of atomic dimensions.

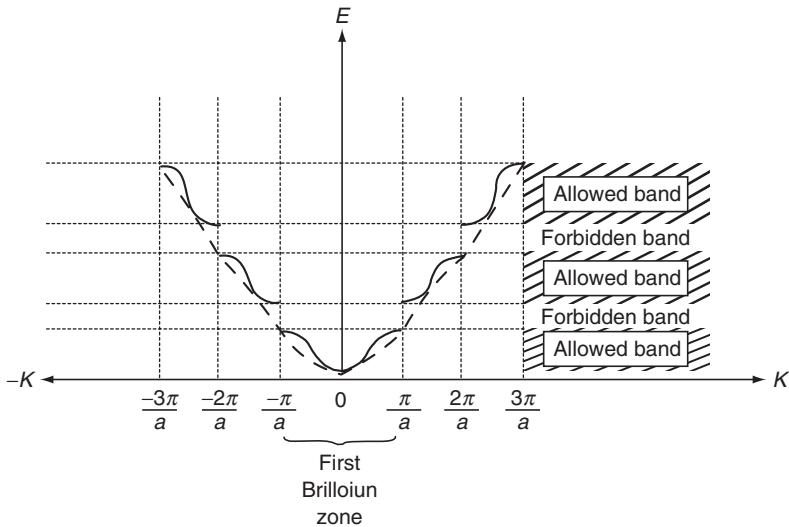
When  $P \rightarrow 0$ , then the left-hand side of Equation (5.59) will not cross  $\pm 1$  line as shown in Fig. 5.12. Hence, all the energies are allowed to the electrons. Thus, by varying  $P$  from zero to infinity, the energies of electrons will vary from continuous to bound, i.e., free electrons to bound electrons.

- (iv)  **$E-K$  diagram:** The free electrons moving in periodic potentials of lattice can have energy values only in the allowed regions or zones. It is possible to plot the total energies of free electrons versus their wave number or propagation vector  $K$  as shown in Fig. 5.13.

We observe that the curve is not continuous; it has discontinuities at  $K = \pm \frac{n\pi}{a}$ ,

where  $n = 1, 2, 3, \dots$ . The dotted parabolic curve shows  $E-K$  relation for completely free electrons. From the graph, we see that the electrons have allowed energy values in the region or zone extending from  $K = \frac{-\pi}{a}$  to  $\frac{+\pi}{a}$ . This is called the first Brillouin zone. After a break in the energy values, called the forbidden region or band, the electrons have another allowed zone of energy values in the region extended from  $K = \frac{-\pi}{a}$  to  $\frac{-2\pi}{a}$  and from  $\frac{\pi}{a}$  to  $\frac{2\pi}{a}$ . This zone is called the second Brillouin zone. Similarly, the higher order Brillouin zones can be defined.

Figure 5.13 E-K diagram



The discontinuities occur at the boundaries of the Brillouin zones. Each portion of the curve gives a number of allowed energies called allowed band of energies. The curves are horizontal at the top and bottom and they are parabolic near the top and bottom with curvatures in opposite directions. As 'P' decreases, the discontinuous  $E-K$  graph will reduce to a continuous parabolic graph as shown by the dotted lines and the forbidden bands disappear. Then, the energy values are practically continuous.

## 5.8 Bloch theorem

Suppose an electron passes along X-direction in a one-dimensional crystal having periodic potentials:

$$V(x) = V(x + a)$$

where 'a' is the periodicity of the potential. The Schrödinger wave equation for the moving electron is:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0 \quad (5.60)$$

The solution for Equation (5.60) is of the form:

$$\psi(x) = e^{ikx} u_k(x) \quad (5.61)$$

$$\text{where } u_k(x) = u_k(x + a) \quad (5.62)$$

Equation (5.62) represents periodic function and  $e^{ikx}$  represents plane wave. The above statement is known as Bloch theorem and Equation (5.62) is called Bloch function. The Bloch function has the property:

$$\psi(x + a) = \exp [ik(x + a)] u_k(x + a) = \psi(x) \exp ika \quad (5.63)$$

$$\text{or } \psi(x + a) = Q\psi(x) \text{ where } Q = \exp ika \quad (5.64)$$

**Proof:** Suppose  $g(x)$  and  $f(x)$  are two real independent solutions for the Schrödinger's equation 5.60, then  $f(x+a)$  and  $g(x+a)$  are also solutions of the above equation so that:

$$\begin{aligned} f(x+a) &= \alpha_1 f(x) + \alpha_2 g(x) \\ g(x+a) &= \beta_1 f(x) + \beta_2 g(x) \end{aligned} \quad (5.65)$$

where  $\alpha_1, \alpha_2, \beta_1$  and  $\beta_2$  are the real functions of energy ( $E$ ).  
The solution for Schrödinger wave equation is of the form:

$$\psi(x) = Af(x) + Bg(x) \quad (5.66)$$

where A and B are constants and

$$\psi(x+a) = Af(x+a) + Bg(x+a) \quad (5.67)$$

Substituting Equation (5.65) in Equation (5.67), we have:

$$\begin{aligned} \psi(x+a) &= A[\alpha_1 f(x) + \alpha_2 g(x)] + B[\beta_1 f(x) + \beta_2 g(x)] \\ &= [A\alpha_1 + B\beta_1]f(x) + [A\alpha_2 + B\beta_2]g(x) \end{aligned} \quad (5.68)$$

From the property of Bloch function, Equation (5.64), and using Equation (5.66), we have:

$$\psi(x+a) = Q\psi(x) = QAf(x) + QBg(x) \quad (5.69)$$

Comparing Equations (5.68) and (5.69), we have:

$$\begin{aligned} A\alpha_1 + B\beta_1 &= QA \\ \text{and } A\alpha_2 + B\beta_2 &= QB \end{aligned} \quad (5.70)$$

In Equations (5.70), A and B have non-vanishing values only if the determinant of the coefficients of A and B is equal to zero.

$$\text{i.e., } \begin{vmatrix} \alpha_1 - Q & \beta_1 \\ \alpha_2 & \beta_2 - Q \end{vmatrix} = 0$$

$$\text{or } Q^2 - (\alpha_1 + \beta_2)Q + \alpha_1\beta_2 - \alpha_2\beta_1 = 0 \quad (5.71)$$

From the above equation, we can show  $\alpha_1\beta_2 - \alpha_2\beta_1 = 1$ . Then the Equation (5.71) becomes:

$$Q^2 - (\alpha_1 + \beta_2)Q + 1 = 0 \quad (5.72)$$

The above quadratic equation has two roots say  $Q_1$  and  $Q_2$ . So, we have two values for  $\psi(x)$  i.e.,  $\psi_1(x)$  and  $\psi_2(x)$ . Also note that  $Q_1 Q_2 = 1$ . For certain values of energy corresponding to  $(\alpha_1 + \beta_2)^2 < 4$ , the two roots are complex and can be written as:

$$Q_1 = e^{iK_a} \quad \text{and} \quad Q_2 = e^{-iK_a} \quad (5.73)$$

The wave functions  $\psi_1(x)$  and  $\psi_2(x)$  can be represented as  $\psi_1(x+a) = e^{ika} \psi_1(x)$  and

$$\psi_2(x+a) = e^{-ika} \psi_2(x) \quad (5.74)$$

For other regions of energy corresponding to  $(\alpha_1 + \beta_2)^2 > 4$ , the roots  $Q_1$  and  $Q_2$  are real and reciprocal to each other. These two roots corresponding to Schrödinger's equation of the type:

$$\psi_1(x) = e^{\mu x} u(x) \quad \text{and} \quad \psi_2(x) = e^{-\mu x} u(x) \quad (5.75)$$

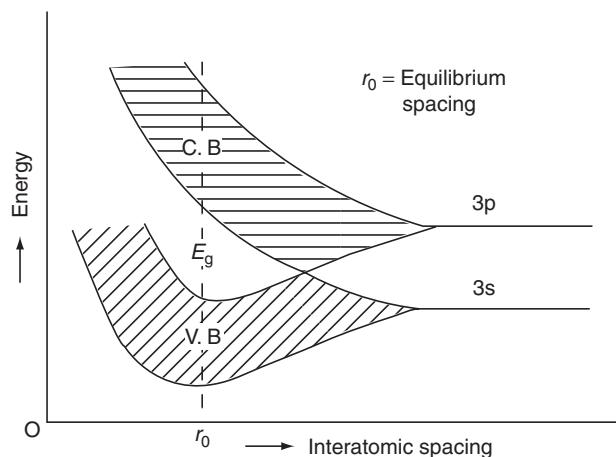
where  $\mu$  is a real quantity. Mathematically, the above solutions are sound but not accepted as wave functions describing electrons. This leads to the energy spectrum of an electron in a periodic potential consists of allowed and forbidden energy regions or bands.

## 5.9 Origin of energy bands formation in solids

An isolated atom possesses discrete energies of different electrons. Suppose two isolated atoms are brought to very close proximity, then the electrons in the orbits of two atoms interact with each other. So, that in the combined system, the energies of electrons will not be in the same level but changes and the energies will be slightly lower and larger than the original value. So, at the place of each energy level, a closely spaced two energy levels exists. If 'N' number of atoms are brought together to form a solid and if these atoms' electrons interact and give 'N' number of closely spaced energy levels in the place of discrete energy levels, it is known as bands of allowed energies. Between the bands of allowed energies, there are empty energy regions, called forbidden band of energies. Kronig-Penney model supports the existence of these bands of energies (allowed bands and forbidden bands). The mathematical solution for Schrödinger's wave equation is very tedious but it provides a clue in understanding the origin of energy bands.

The formation of energy bands has been explained taking Sodium (Na) metal as an example. When isolated sodium atoms are brought together to form a solid, then the energy levels of the valence electrons spread into bands. The 3S and 3P orbitals electrons energies are shown in Fig. 5.14. These bands are seen to overlap strongly at the interatomic spacing of sodium.

**Figure 5.14 Spreading of energy levels into energy bands in sodium metal**



## 5.10 Velocity and effective mass of an electron

According to de Broglie hypothesis, a moving electron is associated with a wave. The velocity of an electron ( $v$ ) is equal to the group velocity ( $v_g$ ) of the associated wave. The group velocity is given by:

$$v = v_g = \frac{d\omega}{dK} \quad (5.76)$$

where  $\omega$  is the angular frequency ( $2\pi\nu$ ) and  $K$  is the propagation vector  $\left(= \frac{2\pi}{\lambda}\right)$  of the wave.

In quantum mechanics, the energy, 'E' of an electron is given by:

$$E = \hbar\omega \quad \text{_____} \quad (5.77)$$

Differentiating Equation (5.77) with respect to 'K', we get:

$$\frac{dE}{dK} = \hbar \frac{d\omega}{dK} \quad \text{or} \quad \frac{d\omega}{dK} = \frac{1}{\hbar} \frac{dE}{dK} \quad \text{_____} \quad (5.78)$$

From Equations (5.76) and (5.78), we have:

$$v = \frac{1}{\hbar} \left( \frac{dE}{dK} \right) \quad \text{_____} \quad (5.79)$$

In quantum theory, the momentum of an electron is given by:

$$p = \hbar K \quad \text{and energy,} \quad E = \frac{\hbar^2 K^2}{2m} \quad \text{_____} \quad (5.80)$$

The above equation can be proved as follows:

Differentiating Equation (5.80) w.r.t 'K', gives:

$$\frac{dE}{dK} = \frac{\hbar^2}{2m} 2K = \frac{\hbar^2 K}{m} \quad \text{_____} \quad (5.81)$$

Substituting Equation (5.81) in (5.79), we have:

$$v = \frac{1}{\hbar} \frac{\hbar^2 K}{m} = \frac{\hbar K}{m} = \frac{p}{m} \times \frac{2\pi}{\lambda m} = \frac{p}{\lambda m} = \frac{p}{m} \quad \text{_____} \quad (5.82)$$

[using de Broglie hypothesis]

From the above equation, we know that velocity is linearly related with momentum. Also from Equation (5.80) we know,  $E \propto K^2$ .

From band theory of solids, we know  $E$  is not proportional to  $K^2$ . The variation of  $E$  with  $K$  is shown in Fig. 5.15(a). Using the type of variation of  $E$  with  $K$  from Fig. 5.15(a) in Equation (5.79), one can plot  $v$  versus  $K$  as shown in Fig. 5.15(b). At the bottom of the energy band, the velocity of an electron is zero and as the value of  $K$  increases, the velocity increases and attains a maximum value at  $K = K_0$ , known as the point of inflection on the  $E-K$  curve. Beyond this point, the velocity decreases and attains zero at  $K = \frac{\pi}{a}$ , which is the top of the band. The negative values of the wave vector exhibit a similar behaviour. Thus, a feature, which is altogether different from the behaviour of free electrons, is observed.

## Effective mass of an electron

The mass of an electron in the periodic potentials of a crystal is different from the free electron mass and is usually referred to as the effective mass.

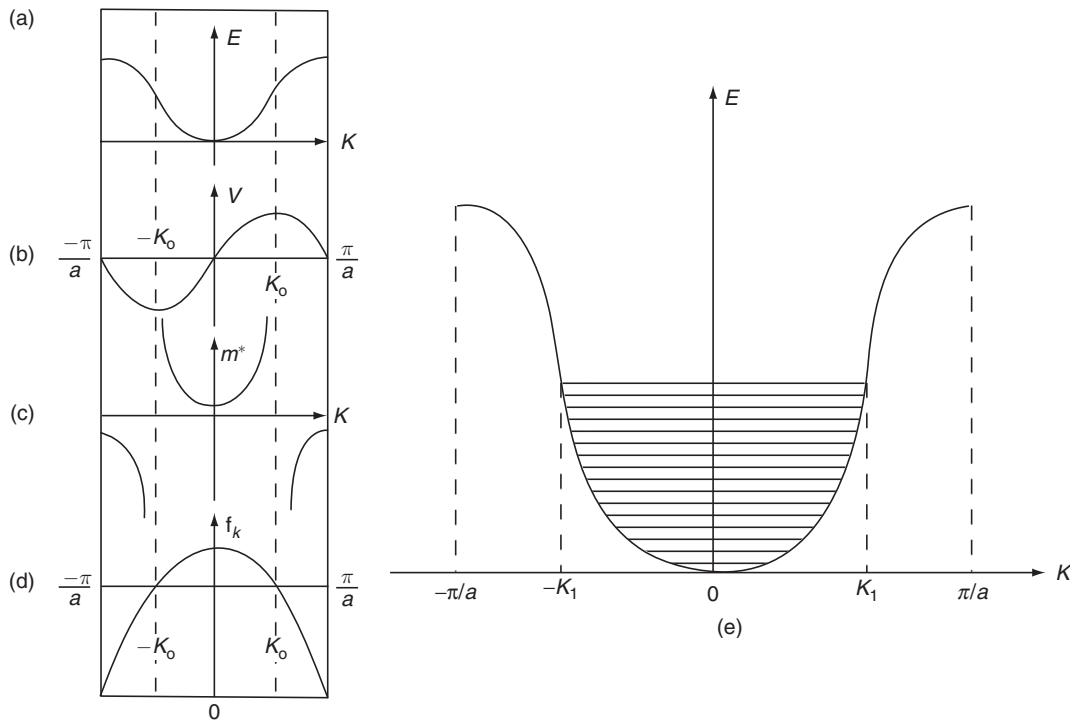
To find an expression for an effective mass, consider an external electric field ' $\epsilon$ ' act on an electron present initially in state  $K$  in a Brillouin zone of one-dimensional crystal for a time  $dt$ . The electron gains acceleration and some amount of energy  $dE$  equal to the work done on the electron by the electric field during the time  $dt$ .

$$\text{i.e. } dE = e\epsilon dx = e\epsilon v dt \quad \text{_____} \quad (5.83)$$

where  $dx$  is the resultant displacement in time  $dt$ .

Figure 5.15

(a)  $E$ - $K$  diagram; (b) Velocity versus  $K$ ; (c) Effective mass of an electron;  
 (d) Degree of freedom of an electron; (e)  $E$ - $K$  diagram



Substituting Equation (5.79) in Equation (5.83), we have:

$$dE = e\varepsilon \left( \frac{1}{\hbar} \frac{dE}{dK} \right) dt \quad \text{_____} \quad (5.84)$$

$$\text{(or)} \quad \frac{dK}{dt} = \frac{e\varepsilon}{\hbar} \quad \text{_____} \quad (5.85)$$

Acceleration ' $a$ ' of the electron can be obtained by differentiating Equation (5.79) with respect to ' $t$ :

$$a = \frac{dv}{dt} = \frac{d}{dt} \left[ \frac{1}{\hbar} \frac{dE}{dK} \right] = \frac{1}{\hbar} \left( \frac{d^2 E}{dK^2} \right) \left( \frac{dK}{dt} \right) \quad \text{_____} \quad (5.86)$$

substitute of Equation (5.85) in (5.86) gives:

$$a = \frac{e\varepsilon}{\hbar^2} \frac{d^2 E}{dK^2} \quad \text{_____} \quad (5.87)$$

The acceleration ' $a$ ' of a free electron of mass ' $m$ ' in an external electric field  $\varepsilon$  is given by:

$$a = \frac{e\varepsilon}{m} \quad \text{_____} \quad (5.88)$$

Equations (5.87) and (5.88) represent acceleration. Equating these two equations, we obtain the mass of an electron based on band theory. This mass of an electron is called the effective mass of an electron, denoted as  $m^*$ . So, we have:

$$\frac{e\varepsilon}{m^*} = \frac{e\varepsilon}{\hbar^2} \frac{d^2E}{dK^2} \quad (\text{or}) \quad m^* = \frac{\hbar^2}{(d^2E/dK^2)} \quad (5.89)$$

The effective mass is thus determined by  $d^2E/dK^2$ .

The effective mass is represented as a function of  $K$  in Fig. 5.15(c). For the lower portion of  $E-K$  curve,  $d^2E/dK^2$  is positive so  $m^*$  is positive, and increases with increase of  $K$ , attains a maximum value at the point of inflection  $K_0$ . For further higher values of  $K$ ,  $\frac{d^2E}{dK^2}$  is negative, hence  $m^*$  is negative. As  $K \rightarrow \frac{\pi}{a}$ , the effective mass approaches to a smaller negative value. At the point of inflection [ $(d^2E/dK^2) = 0$ ],  $m^*$  becomes infinite.

Physically, that in the upper half of the band, the electron behaves as having negative mass or as behaving like particles with positive charges. Suppose an electron starts at  $K = 0$ , when an electric field is applied, the wave vector increases linearly with time. Until the velocity reaches its maximum value, the electron is accelerated by the field, beyond this maximum velocity the same field produces a decrease in velocity, i.e., the mass must become negative in the upper part of the band.

The effective mass of an electron has been experimentally determined from electron specific heat and also using cyclotron resonance experiments.

The degree of freedom of an electron is generally defined by a factor:

$$f_K = \frac{m}{m^*} = \frac{m}{\hbar^2} \left( \frac{d^2E}{dK^2} \right) \quad (5.90)$$

Here,  $f_K$  is a measure of the extent to which an electron in state  $K$  is free.  $f_K$  is positive in the lower half of the band and negative in the upper half of the band as shown in Fig. 5.15(d).

If  $m^*$  is large  $f_K$  is small, so the particle behaves as a heavy particle. When  $f_K = 1$ , the electron behaves as a free electron.

## 5.11 Distinction between metals, semiconductors and insulators

The differences between metals, semiconductors and insulators can be made based on the availability of number of free electrons that participate in electrical conduction per unit volume when an electric field is applied. These free electrons are called effective electrons. The number of effective electrons per unit volume ( $N_{\text{eff}}$ ) for a material can be calculated using band theory of solids. According to band theory, the electrons in a solid can possess bands of energies called allowed bands of energies and these electrons may not possess some other bands of energies called forbidden bands of energies. The allowed bands of energies and forbidden bands of energies are present alternatively one after another for the electrons of a solid. The top-most fully filled (with electrons) band at absolute zero of temperature (0K) is known as the valence band and next allowed band is called the conduction band. These two bands are separated by forbidden band.

To find the difference between metals, semiconductors and insulators, we consider  $E-K$  diagram of a solid material as shown in Fig. 5.15(e). Let us consider the band filled with electrons up to a certain value  $K_1$ ,

which is lesser than  $\frac{\pi}{a}$ . Now by knowing the number of effective electrons per unit volume, one can conclude the conductivity of the material. The number of effective electrons per unit volume of material ( $N_{\text{eff}}$ ) is equal to:

$$N_{\text{eff}} = \sum f_K dn \quad (5.91)$$

$$\text{where } f_K = \frac{m}{m^*} = \frac{m}{\hbar^2} \frac{d^2 E}{dK^2} = \text{degree of freeness of an electron}$$

The summation has been taken in all the occupied states of the band. The number density of states ( $dn$ ) in the interval  $dK$  of one-dimensional crystal of length  $L$  is:

$$dn = \frac{L}{2\pi} dK \quad (5.92)$$

For each positive  $K$  value of an electron, negative  $K$  value also exists, so the number of effective electrons from  $-K_1$  to  $K_1$  state is:

$$\begin{aligned} N_{\text{eff}} &= \frac{L}{2\pi} \int_{-K_1}^{K_1} f_k dK \times 2 = \frac{L}{\pi} \int_{-K_1}^{K_1} f_k dK \\ &= \frac{L}{\pi} \frac{m}{\hbar^2} \int_0^{K_1} \frac{d^2 E}{dK^2} dK \times 2 = \frac{2L}{\pi} \frac{m}{\hbar^2} \int_0^{K_1} \frac{d^2 E}{dK^2} dK \\ &= \left( \frac{2mL}{\pi\hbar^2} \right) \int_0^{K_1} \frac{d^2 E}{dK^2} dK = \left( \frac{2mL}{\pi\hbar^2} \right) \left( \frac{dE}{dK} \right)_{K=K_1} \quad (5.93) \end{aligned}$$

From the above equation, we can draw the following conclusions:

- (1) For the fully filled top-most band,  $\frac{dE}{dK} = 0$  at the top of the band. So, the effective number of electrons

in the material is zero [ $N_{\text{eff}} = 0$ ]. Hence, the material possesses very poor electrical conductivity, and it is an insulator. Usually in case of insulators, the top-most completely filled band [valence band] and next allowed band [conduction band] are separated by large energy gap, so practically it is impossible to excite an appreciable number of electrons present in the top-most energy levels of valence band to the lowest energy levels of conduction band by an electric field or by thermal energy. In insulators, the energy gap varies from 5 eV to 10 eV. In case of diamond, the energy gap is 6 eV as shown in Fig. 5.16(a).

- (2) For the partially filled top-most band,  $\frac{dE}{dK} \neq 0$  at the top-most filled state. So, the effective number

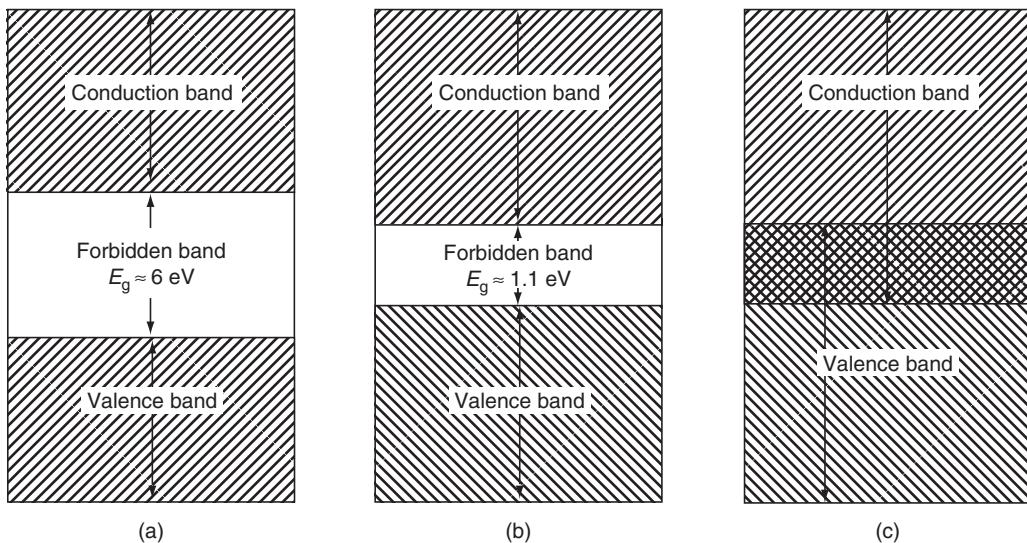
of electrons in the material is not zero [i.e.,  $N_{\text{eff}} \neq 0$ ]. Hence, the material possesses electrical conductivity proportional to  $\frac{dE}{dK}$ . If  $\frac{dE}{dK}$  is small for a material, then the material possesses small electrical

conductivity. Such materials are known as semiconductors. At 0K, they are insulators. The energy gap between valence band and conduction band is very less; it is about 1 eV. So even at room temperature, the conduction band possesses effective electrons for conduction.

Examples for semiconductors are Ge [ $E_g = 0.72$  eV] and Si [ $E_g = 1.1$  eV]. The energy band diagram for silicon is shown in Fig. 5.16(b).

Figure 5.16

(a) Band diagram of diamond; (b) Band diagram of silicon; (c) Band diagram of a metal



If the partially filled top-most band is filled up to a point of inflection ( $K_1$ ), then  $\frac{dE}{dK}$  is maximum. The

material possesses very large number of effective electrons and hence electrical conductivity of the material is very large. So, the material is known as a good conductor. Usually, metals possess very good electrical and thermal conductivity. In metals, the valence band and conduction band are merged, so that there is no energy gap. The electrons that are present in valence band will be present also in conduction band. The band diagram for metals is shown in Fig. 5.16c. Examples for metals are gold, silver, copper, etc.

## Formulae

$$1. \quad \bar{C} = \sqrt{\frac{3K_B T}{m}}$$

$$2. \quad J = nev = ne\mu E = \sigma E$$

$$3. \quad \frac{dJ_x}{dt} = \frac{ne^2}{m} E_x$$

$$4. \quad \langle V_x \rangle = \langle V_x \rangle_0 e^{-t/\tau_x}$$

$$5. \quad \mu_x = \frac{e\tau_x}{m}$$

$$6. \quad \sigma_x = \frac{ne^2 \tau_x}{m} = ne\mu_x = \frac{1}{\rho_x}$$

$$7. \quad \lambda = \bar{C} \tau_c$$

$$8. \quad \tau_c = \frac{\lambda}{V_{th}}$$

$$9. \quad \tau = \frac{\tau_c}{1 - \langle \cos \theta \rangle}$$

$$10. \quad V_d = \frac{e\tau_c E}{m} = \mu E$$

$$11. \quad f(x) = \frac{1}{1 + \exp((E - E_F)/K_B T)}$$

$$12. \quad \tau_F = \frac{\lambda_F}{v_F}$$

$$13. \quad J = ne \Delta v = \frac{ne^2}{m^*} \left( \frac{\lambda_F}{v_F} \right) E$$

$$14. \quad \sigma_{\text{eff}} = \frac{n_{\text{eff}} e^2 \tau_F}{m^*}$$

$$15. \quad \rho = \rho_i + \rho(T)$$

$$16. \quad \Psi(x) = e^{ikx} u_k(x)$$

$$17. \quad P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos K a$$

$$18. \quad P = \frac{m V_0 b a}{\hbar^2}$$

$$19. \quad v_g = \frac{d\omega}{dK}$$

$$20. \quad v = \frac{1}{\hbar} \left[ \frac{dE}{dK} \right]$$

$$21. \quad m^* = \frac{\hbar^2}{(d^2E/dK^2)}$$

$$22. \quad f_K = \frac{m}{m^*} = \frac{m}{\hbar^2} \left( \frac{d^2E}{dK^2} \right)$$

## Solved Problems

1. Find the temperature at which there is 1% probability that a state with energy 0.5 eV above Fermi energy.

(Set-1, Set-3, Set-4–May 2007), (Set-1, Set-2, Set-3–Sept. 2006),  
(Set-2, Set-3–May 2006), (Set-1, Set-4–June 2005), (Set-1–May 2003)

**Sol:** Probability,  $f(E) = 1\% = 1/100$

$$E - E_F = 0.5 \text{ eV}$$

$$T = ?$$

$$F(E) = \frac{1}{1 + \exp((E - E_F)/K_B T)}$$

$$K_B = 1.381 \times 10^{-23} \text{ J/K} = 1.381 \times 10^{-23} \times 6.24 \times 10^{18} \text{ eV/K}$$

$$= 8.61744 \times 10^{-5} \text{ eV/K}$$

Substituting the values, we get:

$$\frac{1}{100} = \frac{1}{1 + \exp \left[ \frac{0.5}{8.61744 \times 10^{-5} T} \right]}$$

$$100 = 1 + \exp \left[ \frac{0.5}{8.61744 \times 10^{-5} T} \right]$$

$$100 = 1 + \exp \left[ \frac{5801.87}{T} \right]$$

$$100 \approx \exp \left[ \frac{5801.87}{T} \right]$$

Taking ln on both sides, we get:

$$\ln 100 = \frac{5801.87}{T}$$

$$T = \frac{5801.87}{4.605} = 1259.98 \text{ K.}$$

2. Fermi energy of copper is 7 eV at room temperature. What is the total number of free electrons/unit volume at the same temperature?

(Set-2-May 2003)

**Sol:** Fermi energy,  $E_F = 7 \text{ eV} = 7 \times 1.602 \times 10^{-19} \text{ J} = 11.214 \times 10^{-19} \text{ J}$

$$E_F = \left( \frac{\hbar^2}{8m} \right) \left( \frac{3}{\pi} \right)^{2/3} n^{2/3}$$

$$11.214 \times 10^{-19} = \frac{[6.63 \times 10^{-34}]^2}{8 \times 9.11 \times 10^{-31}} \times \left[ \frac{3 \times 7}{22} \right]^{3/2} n^{2/3}$$

$$11.214 \times 10^{-19} = \frac{43.9569 \times 10^{-68}}{72.88 \times 10^{-31}} \times 0.9326 \times n^{2/3}$$

$$n^{2/3} = \frac{11.214 \times 72.88}{43.9569 \times 0.9326 \times 10^{-18}} = 19.9364 \times 10^{18}$$

$$n = [19.9364 \times 10^{18}]^{3/2} \text{ electrons/m}^3 = 8.9106 \times 10^{28} \text{ electrons/m}^3$$

3. Find the relaxation time of conduction electrons in a metal of resistivity  $1.54 \times 10^{-8} \Omega\text{-m}$ , if the metal has  $5.8 \times 10^{28}$  conduction electrons/ $\text{m}^3$ .

(Set-3-Sept. 2007), (Set-2-May 2007), (Set-1-May 2006), (Set-4-Sept. 2006),  
(Set-1-Nov. 2004), (Set-2-May 2004), (Set-2-Nov. 2003), (Set-4-Nov. 2003)

**Sol:** Given data are:

Resistivity of the metal,  $\rho = 1.54 \times 10^{-8} \Omega\text{-m}$

Number of conduction electrons,  $n = 5.8 \times 10^{28}/\text{m}^3$

Relaxation time,  $\tau = ?$

$$\begin{aligned} \sigma &= \frac{ne^2\tau}{m} \quad \text{or} \quad \tau = \frac{\sigma m}{ne^2} = \frac{m}{ne^2\rho} \\ &= \frac{9.11 \times 10^{-31}}{5.8 \times 10^{28} \times [1.602 \times 10^{-19}]^2 \times 1.54 \times 10^{-8}} \\ &= \frac{9.11 \times 10^{-31}}{5.8 \times (1.602)^2 \times 1.54 \times 10^{-18}} = \frac{9.11 \times 10^{-13}}{22.92} \\ &= \frac{911 \times 10^{-15}}{22.92} = 39.747 \times 10^{-15} \text{ s} \end{aligned}$$

4. For the metal having  $6.5 \times 10^{28}$  conduction electrons/m<sup>3</sup>. Find the relaxation time of conduction electrons if the metal has resistivity  $1.43 \times 10^{-8} \Omega\text{-m}$ .

(Set-4–Sept. 2008), (Set-3–Nov. 2003)

**Sol:** Number of conduction electrons,  $n = 6.5 \times 10^{28}/\text{m}^3$

Resistivity of the metal,  $\rho = 1.43 \times 10^{-8} \Omega\text{-m}$

Relaxation time,  $\tau = ?$

$$\begin{aligned}\sigma &= \frac{ne^2 \tau}{m} \quad \text{or} \quad \tau = \frac{\sigma m}{ne^2} = \frac{m}{ne^2 \rho} \\ &= \frac{9.1 \times 10^{-31}}{6.5 \times 10^{28} \times (1.6 \times 10^{-19})^2 \times 1.43 \times 10^{-8}} \text{ s} = 3.82 \times 10^{-14} \text{ s}\end{aligned}$$

5. Calculate the free electron concentration, mobility and drift velocity of electrons in aluminium wire of length of 5 m and resistance of 0.06 Ω carrying a current of 15 A, assuming that each aluminium atom contributes 3 free electrons for conduction.

Given: [Resistivity for aluminium] =  $2.7 \times 10^{-8} \Omega\text{-m}$

[Atomic weight] = 26.98

[Density] =  $2.7 \times 10^3 \text{ Kg/m}^3$

[Avagadro number] =  $6.025 \times 10^{23}$

(Set-1, Set-2, Set-4–Sept. 2007), (Set-4–May 2006), (Set-2, Set-3–June 2005)

**Sol:** Given data are:

Aluminium wire length,  $L = 5 \text{ m}$

Resistance of wire,  $R = 0.06 \Omega$

Current in wire,  $I = 15 \text{ A}$

Number of conduction electrons of Al atom = 3

Resistivity of aluminium,  $\rho = 2.7 \times 10^{-8} \Omega\text{-m}$

Atomic weight of aluminium,  $w = 26.98$

Density of aluminium,  $D = 2.7 \times 10^3 \text{ Kg/m}^3$

Avogadro's Number,  $N_A = 6.025 \times 10^{26}$  per k-mol

Free electron concentration,  $n = ?$

Mobility of electrons,  $\mu = ?$

Drift velocity of electrons,  $v_d = ?$

Number of conduction electrons per  $\text{m}^3$ ,  $n = \frac{\text{no. of electrons per atom} \times N_A \times D}{\text{atomic weight}}$

$$= \frac{3 \times 6.025 \times 10^{26} \times 2.7 \times 10^3}{26.98} = 1.8088 \times 10^{29}/\text{m}^3$$

We know  $\rho = \frac{1}{ne\mu}$  or  $\mu = \frac{1}{ne\rho}$

$$\text{mobility, } \mu = \frac{1}{1.8088 \times 10^{29} \times 1.6 \times 10^{-19} \times 2.7 \times 10^{-8}} = 0.00128 \text{ m}^2/\text{VS}$$

$$\text{Drift velocity, } v_d = \left( \frac{eE}{m} \right) \times \tau$$

$$E = \frac{V}{L} = \frac{IR}{L}$$

$$\text{and } \sigma = \frac{ne^2\tau}{m} \quad \text{or} \quad \tau = \frac{\sigma m}{ne^2} = \frac{m}{\rho ne^2}$$

$$\therefore v_d = \frac{e}{m} \times \frac{IR}{L} \times \frac{m}{\rho ne^2} = \frac{IR}{L\rho ne}$$

$$= \frac{15 \times 0.06}{5 \times 2.7 \times 10^{-8} \times 1.8088 \times 10^{29} \times 1.6 \times 10^{-19}}$$

$$= \frac{0.9 \times 10^{-2}}{39.07} = 2.3 \times 10^{-4} \text{ m/s.}$$

6. Calculate the mobility of the electrons in copper obeying classical laws. Given that the density of copper =  $8.92 \times 10^3 \text{ kg/m}^3$ , Resistivity of copper =  $1.73 \times 10^{-8} \text{ ohm-m}$ , atomic weight of copper = 63.5 and Avogadro's number =  $6.02 \times 10^{26} \text{ per K-mol}$

(Set-3–May 2008)

**Sol:** Density of copper,  $D = 8.92 \times 10^3 \text{ kg/m}^3$

Resistivity of copper,  $\rho = 1.73 \times 10^{-8} \text{ ohm-m}$

Atomic weight of copper,  $W = 63.5$

Avogadro number,  $N_A = 6.02 \times 10^{26} \text{ per K-mol}$

Mobility  $\mu = ?$

$$\text{Number of free electrons per m}^3, n = \frac{\text{No. of free electrons per atom} \times N_A \times D}{\text{Atomic weight}}$$

$$n = \frac{1 \times 6.02 \times 10^{26} \times 8.92 \times 10^3}{63.5} \text{ per m}^3$$

$$= 8.456 \times 10^{28} \text{ per m}^3$$

$$\rho = \frac{1}{n e \mu} \quad \text{where } \mu = \text{mobility}$$

$$\mu = \frac{1}{n e \rho} = \frac{1}{8.456 \times 10^{28} \times 1.6 \times 10^{-19} \times 1.73 \times 10^{-8}}$$

$$= 0.0427 \text{ m}^2/\text{Vs.}$$

7. Calculate the mobility of electrons in copper, considering that each atom contributes one electron for conduction. Resistivity of copper =  $1.721 \times 10^{-8} \Omega\text{-m}$ , Atomic weight is 63.54, density of copper is  $8.95 \times 10^3 \text{ kg/m}^3$  and Avogadro number is  $6.025 \times 10^{23}/\text{mole}$ .

**Sol:** Given data are:

$$\text{Resistivity of copper, } \rho = 1.721 \times 10^{-8} \Omega\text{-m}$$

$$\text{Atomic weight of copper, } W = 63.54$$

$$\text{Density of copper, } D = 8.95 \times 10^3 \text{ kg/m}^3$$

$$\text{Avogadro's number, } N_A = 6.025 \times 10^{26} \text{ per K-mol}$$

$$\text{Number of free electrons per atom} = 1$$

$$\text{Mobility of conduction electrons of copper, } \mu = ?$$

$$\text{Number of conduction electrons per m}^3, n = \frac{\text{no. of electrons per atom} \times N_A \times D}{\text{At.weight}}$$

$$n = \frac{1 \times 6.025 \times 10^{26} \times 8.95 \times 10^3}{63.54} / \text{m}^3$$

$$= 8.487 \times 10^{28} / \text{m}^3$$

$$\text{we know that } \rho = \frac{1}{ne\mu}$$

$$\text{or } \mu = \frac{1}{nep} = \frac{1}{8.487 \times 10^{28} \times 1.6 \times 10^{-19} \times 1.721 \times 10^{-8}}$$

$$\frac{1}{23.37 \times 10} = 0.0428 \text{ m}^2/\text{Vs.}$$

8. Find the relaxation time of conduction electrons in a metal contains  $6.5 \times 10^{28}$  conduction electrons per m<sup>3</sup>. The resistivity of the metal is  $1.50 \times 10^{-8} \Omega\text{-m}$ .

**Sol:** Given data are:

$$\text{Number of conduction electrons, } n = 6.5 \times 10^{28} / \text{m}^3$$

$$\text{Resistivity of the metal, } \rho = 1.50 \times 10^{-8} \text{ ohm-m}$$

$$\text{Relaxation time, } \tau = ?$$

$$\text{we know that } \sigma = \frac{ne^2\tau}{m}$$

$$\begin{aligned} \tau &= \frac{\sigma m}{ne^2} = \frac{m}{ne^2\rho} \\ &= \frac{9.11 \times 10^{-31}}{6.5 \times 10^{28} \times [1.602 \times 10^{-19}]^2 \times 1.50 \times 10^{-8}} \end{aligned}$$

$$= \frac{9.11 \times 10^{-31}}{25.022 \times 10^{-18}} = 0.364 \times 10^{-13} \text{ s}$$

$$= 3.64 \times 10^{-14} \text{ s}$$

9. A uniform silver wire has a resistivity of  $1.54 \times 10^{-8} \Omega\text{-m}$  at a temperature 300 K. For an electric field along the wire of 1 V/cm. Calculate:

- (i) the drift velocity
- (ii) the mobility and relaxation time of electrons assuming that there are  $5.8 \times 10^{28}$  conduction electrons per  $\text{m}^3$  of the material and
- (iii) calculate the thermal velocity of conduction electrons.

**Sol:** Given data are:

Resistivity of silver wire,  $\rho = 1.54 \times 10^{-8} \Omega\text{-m}$

Electric field,  $E = 1 \text{ V/cm} = 10^2 \text{ V/m}$

Number of electrons per unit volume,  $n = 5.8 \times 10^{28} / \text{m}^3$

Relaxation time,  $\tau = ?$

Drift velocity,  $v_d = ?$

Mobility of conduction electrons,  $\mu = ?$

$$\sigma = \frac{ne^2\tau}{m} \quad \text{or} \quad \tau = \frac{\sigma m}{ne^2} = \frac{m}{ne^2\rho}$$

$$\begin{aligned}\text{Relaxation time, } \tau &= \frac{9.11 \times 10^{-31}}{5.8 \times 10^{28} \times [1.602 \times 10^{-19}]^2 \times 1.54 \times 10^{-8}} \\ &= \frac{9.11 \times 10^{-31}}{22.93 \times 10^{-18}} = 3.97 \times 10^{-14} \text{ s}\end{aligned}$$

$$\begin{aligned}\text{Drift velocity, } v_d &= \left( \frac{eE}{m} \right) \times \tau \\ &= \left[ \frac{1.602 \times 10^{-19} \times 10^2}{9.11 \times 10^{-31}} \right] \times 3.97 \times 10^{-14} = 0.7 \text{ m/s}\end{aligned}$$

$$\text{Mobility, } \mu = \frac{v_d}{E} = \frac{0.7}{10^2} = 0.7 \times 10^{-2} \text{ m}^2/\text{Vs}$$

$$\frac{3}{2} K_B T = \frac{1}{2} m v_{th}^2$$

$$\begin{aligned}\text{so, thermal velocity, } V_{th} &= \sqrt{\frac{3K_B T}{m}} = \sqrt{\frac{3 \times 1.381 \times 10^{-23} \times 300}{9.11 \times 10^{-31}}} \\ &= 1.17 \times 10^5 \text{ m/s}\end{aligned}$$

10. The Fermi energy of silver is 5.5 eV, and the relaxation time of electrons is  $3.97 \times 10^{-14} \text{ s}$ . Calculate the Fermi velocity and the mean free path for the electrons in silver.

**Sol:** The given data are:

The Fermi energy of silver,  $E_F = 5.5 \text{ eV} = 5.5 \times 1.602 \times 10^{-19} \text{ J}$

The relaxation time of electrons in silver,  $\tau = 3.97 \times 10^{-14} \text{ s}$

Fermi velocity,  $V_F = ?$

Mean free path,  $\lambda = ?$

We know that  $\frac{1}{2}mv_F^2 = E_F$

$$\text{or } V_F = \sqrt{\frac{2E_F}{m}} = \sqrt{\frac{2 \times 5.5 \times 1.602 \times 10^{-19}}{9.11 \times 10^{-31}}}$$

$1.39 \times 10^6 \text{ m/s}$

The mean free path,  $\lambda = V_F \tau$

$$\begin{aligned} &= 1.39 \times 10^6 \times 3.97 \times 10^{-14} \\ &= 5.52 \times 10^{-8} \text{ m} \end{aligned}$$

11. Calculate the Fermi energy in eV for silver at 0 K, given that the density of silver is  $10500 \text{ kg/m}^3$ , its atomic weight is 107.9 and it has one conduction electron per atom.

**Sol:** The given data are:

Density of silver,  $D = 10500 \text{ kg/m}^3$

Atomic weight of silver,  $M = 107.9$

Number of free electrons per atom = 1

$$\begin{aligned} \text{Electronic concentration, } n &= \frac{\text{number of free electrons per atom} \times N_A \times D}{M} \\ &= \frac{1 \times 6.025 \times 10^{26} \times 10500}{107.9} = 5.863 \times 10^{28} \text{ per m}^3 \end{aligned}$$

$$\begin{aligned} \text{Fermi energy, } E_F &= \frac{n^2}{8m} \left( \frac{3}{\pi} \right)^{2/3} n^{2/3} \\ &= \frac{[6.63 \times 10^{-34}]^2}{8 \times 9.11 \times 10^{-31}} \times \left( \frac{3 \times 7}{22} \right)^{2/3} \times (5.863 \times 10^{28})^{2/3} \\ &= 5.85 \times 10^{-38} \times 1.5091 \times 10^{19} = 8.83 \times 10^{-19} \text{ J} \end{aligned}$$

12. Find the drift velocity of free electrons in a copper wire of cross sectional area  $10 \text{ mm}^2$ . When the wire carries a current of 100 A. Assume that each copper atom contributes one electron to the electron gas. [Density of copper =  $8.92 \times 10^3 \text{ kg/m}^3$ , Atomic weight of copper = 63.5 and Avogadro's number =  $6.02 \times 10^{26} \text{ per K-mol}$ ]

**Sol:** Area of cross section of wire,  $A = 10 \text{ mm}^2$

$$= 10 \times 10^{-6} \text{ m}^2$$

Current through the wire,  $I = 100 \text{ amperes}$

Number of free electrons per atom = 1

Density of copper,  $D = 8.92 \times 10^3 \text{ kg/m}^3$

Atomic weight of copper,  $W = 63.5$

Avogadro's number,  $N_A = 6.02 \times 10^{26} \text{ per K-mol}$

Drift velocity of free electron,  $v_d = ?$

$$\text{Current density, } J = \frac{I}{A} = \frac{100}{10 \times 10^{-6}} = 10^7 \text{ Amp/m}^2$$

But  $J = nev_d$  where  $n$  = free electron concentration

$$\text{No. of free electrons per m}^3, n = \frac{\text{No. of electrons per atom} \times N_A \times D}{\text{Atomic weight}}$$

$$n = \frac{1 \times 6.02 \times 10^{26} \times 8.92 \times 10^3}{63.5} \text{ per m}^3$$

$$v_d = \frac{J}{ne} = \frac{10^7 \times 63.5}{6.02 \times 10^{26} \times 8.92 \times 10^3 \times 1.6 \times 10^{-19}}$$

$$= 0.7391 \times 10^{-3} \text{ m/s}$$

### Multiple Choice Questions

1. Metals possess: ( )  
 (a) high electrical and thermal conductivities  
 (b) obey Ohm's law  
 (c) at high temperatures, resistivity is proportional to temperature  
 (d) all
2. According to classical free electron theory, ( )  
 (a) there is no interaction between conduction electrons  
 (b) the interaction of free electrons with ion cores is negligible  
 (c) the free electrons find uniform electric field of positive ions and that of electrons in metal  
 (d) all
3. At absolute temperature  $T$  K, the root mean square velocity ( $\bar{C}$ ) of an electron of mass ' $m$ ' is [ $K_B$  = Boltzmann constant] ( )  
 (a)  $\sqrt{\frac{3K_B T}{m}}$   
 (b)  $\frac{3K_B T}{m}$   
 (c)  $\frac{m}{3K_B T}$   
 (d)  $\sqrt{\frac{m}{3K_B T}}$
4. If  $\tau_x$  is the relaxation time of an electron of mass ' $m$ ' moving along X-direction, the mobility of the electrons ( $\mu_x$ ) is [e = charge on electron] ( )  
 (a)  $\frac{e\tau_x}{\sqrt{m}}$   
 (b)  $\frac{e\tau_x}{m}$   
 (c)  $\frac{e\tau_x}{m^2}$   
 (d)  $\frac{m^2}{e\tau_x}$
5. If  $m, e, \tau$  and  $n$  are the mass, charge, relaxation time and number of free electrons per unit volume, respectively, then the electrical conductivity is: ( )  
 (a)  $\frac{ne^2\tau}{m}$   
 (b)  $\frac{ne^2}{m\tau}$   
 (c)  $\frac{n\tau}{me^2}$   
 (d)  $\frac{m}{ne^2\tau}$

6. The drift velocity produced by applying electric field of intensity ' $E$ ' on an electron of mass ' $m$ ' having charge ' $e$ ' is [ $\tau_c$  = mean collision time] ( )
- (a)  $\frac{-eE}{m\tau_c}$  (b)  $\frac{-eE\tau_c}{m}$  (c)  $\frac{-m\tau_c}{eE}$  (d)  $\frac{-eEm}{\tau_c}$
7. At non-zero temperatures, the probability of filling Fermi energy level of a metal with electrons is: ( )
- (a) 1/3 (b) 2/3 (c) 1/2 (d) '0'
8. The cause for electrical resistance of a metal is: ( )
- (a) impurities and crystal defects  
 (b) thermal vibrations  
 (c) electron scattering and non-periodicity of lattice potentials  
 (d) all
9. The observed mean free paths of electrons in a metal are of: ( )
- (a) few Angstroms (b) ten Angstroms  
 (c) several hundred Angstroms (d) none
10. Quantum free electron theory of metals successfully explains: ( )
- (a) electrical conductivity  
 (b) specific heat and thermionic emission  
 (c) paramagnetism  
 (d) all
11. Quantum free electron theory of metals fails to explain: ( )
- (a) the difference between conductors, semiconductors and insulators  
 (b) positive Hall coefficient of metals  
 (c) lower conductivities of divalent metals than monovalent metals  
 (d) all
12. Kronig-Penney model is: ( )
- (a) approximate model (b) real model  
 (c) both a and b (d) none
13. If  $a$  and  $b$  are the widths of potential well and barrier,  $V_0$  is the height of barrier. If an electron of mass  $m$  is present in such potentials, then  $\frac{mV_0ba}{\hbar^2}$  represent  $\left[ \hbar = \frac{b}{2\pi} \right]$  ( )
- (a) scattering power of the potential barrier  
 (b) the strength with which electrons in a crystal are attracted to the ions  
 (c) both a and b  
 (d) none
14. In  $E-K$  diagram, ( )
- (a) each portion of the curve represents allowed band of energies  
 (b) the curves are horizontal at the top and bottom  
 (c) the curves are parabolic near the top and bottom with curvatures in opposite directions  
 (d) all

15. The velocity of a free electron in a metal is maximum when: ( )
- it is present in the bottom energy levels of an allowed band
  - it is present in the top energy levels of an allowed band
  - it is present in a energy level corresponding to a point of inflection in an allowed band
  - none
16. The effective mass of an electron is maximum when it is: ( )
- in the lower energy levels of an allowed band
  - in the higher energy levels of an allowed band
  - in the energy level corresponding to a point of inflection in a allowed band
  - none
17. The valence electrons of metallic atoms are \_\_\_\_\_ in the spaces between the atoms. ( )
- freely move
  - difficult to move
  - will not move
  - none
18. At very low temperatures, the resistivity of a metal is proportional to \_\_\_\_\_ power of absolute temperature. ( )
- first
  - second
  - third
  - fifth
19. Classical free electron theory of metals was introduced by: ( )
- P. Drude
  - G.P. Thomson
  - Albert Einstein
  - Newton
20. Relaxation time may be defined as the time taken by an electron to reduce its velocity to \_\_\_\_\_ of its initial value. ( )
- half
  - one-third
  - $(1/e)$
  - $1/2e$
21. The average distance travelled by a free electron between two successive collisions with lattice ions of a metallic crystal is called: ( )
- mean free path
  - free path
  - drift velocity
  - mean collision time
22. The time between two successive collisions of a free electron with lattice ions in a metallic crystal is called: ( )
- mean collision time
  - collision time
  - mean free path
  - free path
23. According to Pauli's exclusion principle, an energy level can accommodate not more than \_\_\_\_\_ electrons. ( )
- one
  - two
  - three
  - four
24. At absolute zero of temperature, the highest filled energy level of a metal is called: ( )
- Fermi energy level
  - de Broglie energy level
  - Maxwell energy level
  - none
25. At absolute temperature  $T_K$ , the free electrons of a metal present in the energy levels below  $K_B T$  from Fermi energy level \_\_\_\_\_ go to higher energy levels [ $K_B$  = Boltzmann constant]. ( )
- may not
  - may
  - both a and b
  - none
26. As the temperature of a metal is raised from absolute zero temperature, the Fermi-Dirac distribution curve begins to depart from \_\_\_\_\_ function. ( )
- wave-like
  - tail-like
  - step-like
  - none
27. The Fermi surface need not always be: ( )
- spherical
  - cubic
  - parallelopiped
  - none
28. The applied electric field on a metal \_\_\_\_\_ the velocity of electrons present near the Fermi level. ( )
- decreases
  - enhances
  - both (a) & (b)
  - none



**Answers**

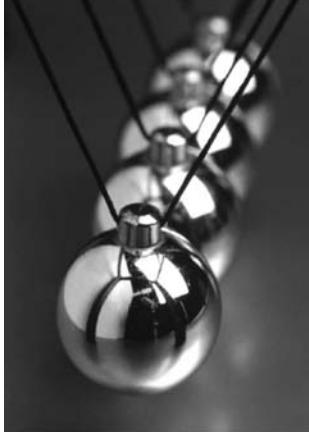
1. d	2. d	3. a	4. b	5. a	6. b	7. c	8. d	9. c	10. d	11. d
12. a	13. c	14. d	15. c	16. c	17. a	18. d	19. a	20. c	21. a	22. b
23. b	24. a	25. a	26. c	27. a	28. b	29. a	30. d	31. d	32. a	33. a
34. a	35. b	36. b	37. a	38. c	39. a	40. d				

**Review Questions**

- What is Fermi level? Explain the Fermi-Dirac distribution function for electrons in a metal. Discuss the variation with temperature.  
(Set-1, Set-2, Set-4–Sept. 2007), (Set-4–May 2006), (Set-2, Set-3–June 2005)
- Explain the origin of energy bands in solids.  
(Set-1, Set-3, Set-4–May 2007), (Set-1, Set-2, Set-3–Sept. 2006),  
(Set-2, Set-3–May 2006), (Set-1, Set-4–June 2005), (Set-1–May 2003)
- Assuming the electron-lattice interaction to be responsible for the scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons.  
(Set-1, Set-3, Set-4–May 2007), (Set-1, Set-2, Set-3–Sept. 2006),  
(Set-2, Set-3–May 2006), (Set-1, Set-4–June 2005), (Set-1–May 2003)
- Explain drift velocity, mobility and relaxation time, effective mass and Bloch theorem.  
(Set-3–Nov. 2004), (Set-4–May 2004), (Set-4–May 2003)
- What are the salient features of the ‘free electron gas’ model? Obtain Ohm’s law based on it.  
(Set-4–Nov. 2004), (Set-3–May 2004), (Set-3–May 2003)
- Explain the salient features of quantum free electron theory. Discuss the Kronig–Penney model for the motion of an electron in a periodic potential.  
(Set-2–May 2003)
- How does the electrical resistance of the metal change with temperature?  
(Set-3–Sept. 2007), (Set-2–May 2007), (Set-1–May 2006)
- Discuss the motion of an electron in a periodic lattice.  
(Set-3–Sept. 2007), (Set-2–May 2007) (Set-1–May 2006), (Set-4–Nov. 2003)
- Explain the concept of ‘effective mass’.  
(Set-2, Set-4–Nov. 2004), (Set-1–May 2004),  
(Set-3–May 2004), (Set-3–May 2003), (Set-1–Nov. 2003)
- Discuss the motion of an electron in a periodic potential field and explain the formation of energy bands.  
(Set-2–Nov. 2004), (Set-1–May 2004), (Set-1–Nov. 2003)
- Discuss the origin of electrical resistance in metals.  
(Set-3–Sept. 2008) (Set-3–May 2008), (Set-4–Sept. 2006), (Set-1–Nov. 2004), (Set-2–May 2004), (Set-2–Nov. 2003)
- Show that the resistivity of a metal above room temperature varies directly with temperature.  
(Set-4–Sept. 2006), (Set-1–Nov. 2004), (Set-2–May 2004), (Set-2–Nov. 2003)
- Elucidate the difference between the classical free electron theory and quantum free electron theory.  
(Set-3–Nov. 2003)
- Distinguish between conductors, insulators and semiconductors on the basis of band theory of solids.  
(Set-3–Nov. 2003)

15. Distinguish between metal, insulator and semiconductors. (Set-2–June 2005)
16. Distinguish between Drude-Lorentz theory and Sommerfeld's theory of metals. (Set-1–May 2008), (Set-4–Sept. 2008)
17. Define Fermi level of electron. (Set-1–May 2008)
18. Distinguish between classical free electron theory and quantum free electron theory of metals. (Set-2–May 2008)
19. Explain the Fermi-Dirac distribution function of electrons. Explain the effect of temperature on the distribution. (Set-2–May 2008)
20. Explain the terms (i) mean free path, (ii) relaxation time and (iii) drift velocity of an electron in a metal. (Set-3–Sept. 2008), (Set-3–May 2008)
21. Explain the following (i) Electrical resistivity and (ii) Fermi energy. (Set-4–May 2008)
22. Explain briefly the quantum free electron theory of metals. (Set-4–May 2008)
23. On the basis of band theory, how the crystalline solids are classified into metals, semiconductors and insulators? (Set-4–May 2008)
24. Discuss with suitable mathematical expressions, the Kronig Penney model for the energies of an electron in a metal. (Set-1, Set-2–Sept. 2008)
25. Explain the classification of metals, semiconductors and insulators based on band theory. (Set-1, Set-2–Sept. 2008)
26. Explain the Fermi-Dirac distribution function of electrons. (Set-4–Sept. 2008)
27. Derive an expression for electrical conductivity on the basis of classical free electron theory.
28. Derive the expression for the electrical conductivity of a metal. How is it affected by temperature?
29. Discuss the various drawbacks of classical free electron theory of metals and explain the assumptions made in quantum theory to overcome the drawback.
30. Describe the salient features of Kronig-Penney model.
31. Give an account of the band theory of solids based on the Kronig-Penney model. Distinguish between semiconductors and insulators.
32. What are the important features of the free electron gas model?
33. Discuss the salient features of Kronig-Penney model of a crystal.
34. Explain the concept of effective mass of an electron.
35. What are the main sources of electrical resistance in a metal? How does the conductivity of a metal vary with rise of temperature and added impurity content?
36. Write short notes on relaxation time, mean free path, collision time and drift velocity.
37. Distinguish between metals, semiconductors and insulators.
38. Starting with the plane wave equation associated with a moving particle, formulate the time-independent Schrödinger's wave equation.
39. Apply Schrödinger's equation to the case of a particle in a box and show that the energies of the particle are quantized.
40. Describe with essential picturization, potential encountered by an electron in a crystal and hence the origin for band spectrum.
41. Write a brief account of effective mass of an electron.

42. Derive an expression for the current density in metals following classical free electron concept.
43. State the drawbacks of classical free electron theory of metals. Derive an expression for the conductivity using F-D statistics in metals.
44. Detail the dynamics (velocity and acceleration) of an electron confined to a periodic lattice in its first allowed band.
45. Discuss the consequences of applying F-D statistics to classical free electron theory of metals and detail the relevant source mechanism behind electrical resistance.
46. Prove that the number of allowed states in any energy bands in a solid is equal to the number of primitive unit cells.
47. Write short notes on effective mass of an electron.
48. Discuss the formation of allowed and forbidden energy bands on the basis of the Kronig–Penney model.
49. What is meant by the effective mass of an electron? Discuss the conditions when the effective mass of an electron becomes positive and negative.
50. What are the failures of the Drude–Lorentz free electron theory?
51. Obtain an expression for electrical conductivity on the basis of band theory.
52. Explain with theory the formation of allowed and forbidden energy bands on the basis of the Kronig–Penney model.
53. List the differences between metals, semiconductors and insulators based on band structure.
54. Explain Fermi–Dirac distribution for electrons in a semiconductor.
55. Discuss the theory of free electron gas in one-dimensional box. Explain the energy levels.



## CHAPTER

# 6

## Dielectric Properties

### 6.1 Introduction

Dielectrics are insulating materials. So, there are no free charge carriers in them. The dielectrics are of two types: (i) non-polar and (ii) polar dielectrics. In non-polar materials, the molecules are usually diatomic and composed of same type of atoms; each atom possesses a positive nucleus of charge  $q$  and surrounded by a symmetrically distributed negative electron cloud of charge  $-q$ . In the absence of an applied electric field, the centres of the positive and negative charge distribution coincide with each other. When external electric field is applied, then the centres of positive and negative charges move apart by a very small distance ( $10^{-10}$  m), then the molecules and atoms are said to be polarized. Next, the polar dielectric molecules are normally composed of two or more different types of atoms. They have dipole moments even in the absence of an external applied electric field. Usually, these molecular dipoles are oriented in random directions, so that the average dipole moment over the volume element is zero. In the presence of an externally applied electric field, the molecular dipoles tend to rotate certain extent in the direction of an applied electric field so that the material has some resultant dipole moment. Not only the rotation of molecular dipoles but also the centres of positive and negative charges of atoms are separated by small distance and it is called a dipole. It possess dipole moment ( $p$ ). The electric dipole moment is defined as the product of one of the charge ( $q$ ) and separation between the charges ( $d$ ) [i.e.,  $p = q d$ ]. The resultant dipole moment per unit volume of material is called polarization ( $P$ ).

Dielectrics find applications in electrical and in electronic equipment. They are used for insulation purposes. In capacitors, dielectric material is used between the capacitor plates to increase capacitance.

### 6.2 Dielectric constant

The permittivity of free space has been represented as  $\epsilon_0$  and is equal to  $8.85 \times 10^{-12}$  F/m. The permitivity of any dielectric material can be represented as  $\epsilon$  and it is equal to  $\epsilon_r \epsilon_0$  i.e.,

$$\epsilon = \epsilon_0 \epsilon_r \quad (\text{or}) \quad \epsilon_r = \frac{\epsilon}{\epsilon_0} \quad \text{_____} \quad (6.1)$$

where  $\varepsilon_r$  is called the relative permittivity or dielectric constant of the dielectric material. It is a dimensionless quantity.

The dielectric constant can also be obtained from electric flux density ( $D$ ) and an applied electric field ( $E$ ). The number of electric force lines passing per unit area perpendicular to field is called electric flux density ( $D$ ). It is proportional to the applied electric field ( $E$ ).

$$\text{So } D \propto E \quad \text{or} \quad D = \varepsilon_0 \varepsilon_r E \quad (6.2)$$

If  $P$  is the polarisation of the dielectric material due to the applied electric field ( $E$ ), Then the flux density ' $D'$  is equal to flux density in vacuum plus polarisation of the material. Therefore, we have:

$$D = \varepsilon_0 E + P \quad (6.3)$$

From Equations (6.2) and (6.3), we have:

$$P = \varepsilon_0 (\varepsilon_r - 1) E \quad (6.4)$$

The electric susceptibility  $\chi$  is:

$$\chi = \frac{P}{\varepsilon_0 E} \quad \text{or} \quad P = \chi \varepsilon_0 E \quad (6.5)$$

From Equations (6.4) and (6.5), we have:

$$\chi \varepsilon_0 E = \varepsilon_0 (\varepsilon_r - 1) E$$

$$\therefore \chi = \varepsilon_r - 1 \quad (\text{or}) \quad \varepsilon_r = 1 + \chi \quad (6.6)$$

Experimentally, the dielectric constant can be obtained easily using parallel plate capacitor. If  $C$  and  $C'$  are the capacitances of a capacitor without and with dielectric, respectively between the capacitor plates, Then, we have:

$$\varepsilon_r = \frac{C'}{C} \quad (6.7)$$

### 6.3 Internal or local field

In dielectric solids, the atoms or molecules experience not only the external applied electric field but also the electric field produced by the dipoles. The resultant electric field acting on the atoms or molecules of dielectric substance is called the local field or an internal field.

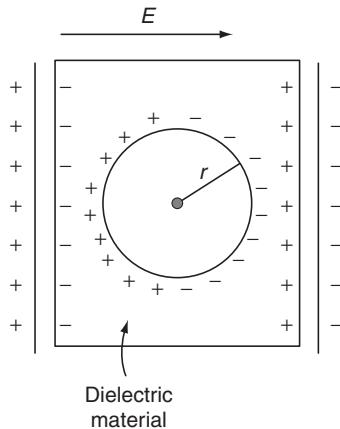
To find an expression for local electric field on a dielectric molecule or an atom, we consider a dielectric material in the electric field of intensity  $E$ , between the capacitor plates so that the material is uniformly polarized, as a result opposite type of charges are induced on the surface of the dielectric near the capacitor plates. The local field is calculated by using the method suggested by Lorentz.

According to this method, consider a small spherical region of the dielectric with an atom at the centre of the sphere for which the local field is to be calculated. The radius of the sphere is chosen large enough so that the region outside the sphere is a continuum while inside the sphere as the actual structure of the substance. The part of the dielectric external to the sphere maybe represented by a system of charges induced and also at the spherical surface as shown in Fig. 6.1.

The electric field at the centre of the sphere may be written as:

$$E_{\text{loc}} = E_0 + E_p + E_s + E_m \quad (6.8)$$

**Figure 6.1 Local field**



where  $E_0$  is the intensity of the electric field due to the charge 'q' on the plates,  $E_p$  is the field due to the polarization charges at the plate dielectric interface,  $E_s$  is the field due to the charges induced on the spherical surface and  $E_m$  due to all the dipoles of the atoms inside the spherical region. The macroscopic electric field ( $E$ ) inside the dielectric is:

$$E = E_0 + E_p$$

Hence  $E_{\text{loc}} = E + E_s + E_m$  \_\_\_\_\_ (6.9)

For high symmetric crystals,  $E_m = 0$ . So, we write:

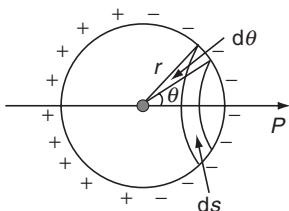
$$E_{\text{loc}} = E + E_s$$
 \_\_\_\_\_ (6.10)

Equation (6.10) is not applicable to anisotropic materials. So, we consider isotropic materials only so that Equation (6.10) holds good. To evaluate  $E_s$ , an enlarged view of the spherical region in dielectric is shown in Fig. 6.2.

The charge element on a surface element  $ds$  of the sphere is equal to the parallel component of the polarization times the surface element i.e.,  $P \cos \theta \cdot ds$ .

Hence, the intensity of the electric field  $dE_s$  at the centre due to this charge element in the direction of 'r' is:

**Figure 6.2 Enlarged spherical region of dielectric**



$$dE_s = \frac{P \cos \theta \, ds}{4\pi \epsilon_0 r^2} \quad (6.11)$$

The components of  $dE_s$ , perpendicular to the direction of  $P$  will be cancelled due to an equal contribution from another symmetrically situated surface element. Only components of  $dE_s$  parallel to  $P$  will contribute to the integral of Equation (6.11) over the entire surface. Thus,

$$E_s = \int dE_s \cos \theta = \frac{\int P \cos \theta \, ds \times \cos \theta}{4\pi \epsilon_0 r^2} = \frac{\int P \cos^2 \theta \, ds}{4\pi \epsilon_0 r^2} \quad (6.12)$$

The surface element  $ds$  is the ring shown in Fig. 6.2 so that  $ds = 2\pi r \sin \theta (r \, d\theta) = 2\pi r^2 \sin \theta \, d\theta$  and the limits of integration with respect to  $\theta$  are from 0 to  $\pi$ . Thus, we have:

$$\begin{aligned} E_s &= \frac{\int_0^\pi P \cos^2 \theta \times 2\pi r^2 \sin \theta \, d\theta}{4\pi \epsilon_0 r^2} \\ &= \frac{2\pi P}{4\pi \epsilon_0} \int_0^\pi \cos^2 \theta \sin \theta \, d\theta = \frac{P}{2\epsilon_0} \int_0^\pi \cos^2 \theta \sin \theta \, d\theta \end{aligned}$$

This can be evaluated making the substitution  $Z = \cos \theta$  and  $dZ = -\sin \theta \, d\theta$   
So that,

$$E_s = \frac{-P}{2\epsilon_0} \int_{+1}^{-1} Z^2 \, dZ = \frac{P}{2\epsilon_0} \left[ \frac{Z^3}{3} \right]_{-1}^{+1} = \frac{P}{3\epsilon_0} \quad (6.13)$$

Thus, equation (6.10) becomes:

$$E_{\text{loc}} = E + \frac{P}{3\epsilon_0} \quad (6.14)$$

Equation (6.14) is known as the Lorentz relation for local field.

## 6.4 Clausius–Mosotti relation

Clausius–Mosotti relation makes relation between microscopic and macroscopic quantities of polarization. A dielectric material can be polarized by applying an external field on it. Dipole moment per unit volume of material is called polarization. The dipole moment ' $p$ ' is equal to the product of one of the charges and separation between the opposite charges of atoms or molecules. This dipole moment is proportional to the local electric field,  $E_{\text{loc}}$ , so that:

$$p = \alpha E_{\text{loc}} \quad (6.15)$$

where ' $\alpha$ ' is the electrical polarizability. If there are ' $n$ ' atoms per unit volume of the dielectric, then polarization ' $P$ ' is:

$$P = np = n\alpha E_{\text{loc}} \quad (6.16)$$

Substituting the equation for local electric field,  $E_{\text{loc}} = E + P/3\epsilon_0$  in the above equation,

$$P = n\alpha \left[ E + \frac{P}{3\epsilon_0} \right] \quad (\text{or}) \quad P = n\alpha E + \frac{n\alpha P}{3\epsilon_0} \quad (\text{or}) \quad P \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right] = n\alpha E$$

$$(\text{or}) \quad P = \frac{n\alpha E}{1 - \frac{n\alpha}{3\epsilon_0}} \quad (6.17)$$

Polarization per unit electric flux density in vacuum is called electric susceptibility, represented as  $\chi_e$ .

$$\chi_e = \frac{P}{\epsilon_0 E} \quad (6.18),$$

where  $\epsilon_0$  is the permittivity of free space.

Substituting Equation (6.17) in (6.18) gives:

$$\chi_e = \frac{n\alpha E}{\left[ 1 - \frac{n\alpha}{3\epsilon_0} \right] \epsilon_0 E} = \frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} \quad (6.19)$$

The expression for electric susceptibility can also be obtained from electric flux density. Let the number of electric force of lines per unit area of the surface perpendicular to the force of lines or the electric flux density 'D' is proportional to the intensity of the applied electric field.

The relation between the flux density and intensity of the applied electric field is:

$$D = \epsilon E = \epsilon_0 \epsilon_r E \quad (6.20)$$

where  $\epsilon$  is the permittivity of the dielectric material and  $\epsilon_r$  is its relative permittivity or dielectric constant of the material. The relation between  $D$  and  $P$  is:

$$D = \epsilon_0 E + P \quad (6.21)$$

Equations (6.20) and (6.21) are same:

$$\text{so, } \epsilon_0 \epsilon_r E = \epsilon_0 E + P \quad (\text{or}) \quad P = \epsilon_0 (\epsilon_r - 1) E \quad (6.21a)$$

From Equation (6.18), we have:

$$P = \chi_e \epsilon_0 E \quad (6.22)$$

Substituting Equation (6.22) in (6.21) gives:

$$D = \epsilon_0 E + \chi_e \epsilon_0 E = \epsilon_0 E [1 + \chi_e] \quad (6.23)$$

Equating Equations (6.20) and (6.23), we have:

$$\epsilon_0 \epsilon_r E = \epsilon_0 E [1 + \chi_e] \quad (\text{or}) \quad \epsilon_r = 1 + \chi_e$$

$$(\text{or}) \quad \chi_e = \epsilon_r - 1 \quad (6.24)$$

## 6-6 | Applied Physics

Equations (6.19) and (6.24) are equal, so:

$$\chi_e = \epsilon_r - 1 = \frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} \quad (6.25)$$

Adding 3 on both sides of Equation (6.25), we have:

$$\epsilon_r + 2 = \frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} + 3 \quad (6.26)$$

Dividing Equation (6.25) by Equation (6.26) gives:

$$\begin{aligned} \frac{\epsilon_r - 1}{\epsilon_r + 2} &= \frac{\frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]}}{\frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} + 3} = \frac{\frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]}}{\frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} + 3 \cdot \frac{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]}} \\ &= \frac{n\alpha}{n\alpha + 3\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} = \frac{n\alpha}{n\alpha + 3\epsilon_0 - n\alpha} = \frac{n\alpha}{3\epsilon_0} \quad (6.27) \end{aligned}$$

If there are  $N$  different types of atoms in the dielectric such that  $n_1, n_2, n_3, \dots, n_N$  are the number of first, second, third ...  $N$ th kind of atoms and  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_N$  are the polarizabilities of first, second, third ...  $N$ th kind of atoms, respectively.

Then, Equation (6.27) becomes:

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{\sum_{i=1}^N n_i \alpha_i}{3\epsilon_0} \quad (6.28)$$

Here,  $\sum_{i=1}^N n_i = n$  and  $\alpha_i$  is the polarizability of  $i$ th kind of atoms. If  $\rho$  is the density,  $N_A$  is Avogadro number

and  $M$  is molecular weight of the crystal, then  $\rho = \frac{nM}{N_A}$  (or)  $n = \frac{\rho N_A}{M}$ , so Equation (6.27) becomes:

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{1}{3\epsilon_0} \frac{\rho N_A \alpha}{M} \quad (\text{or}) \quad \frac{M}{\rho} \left( \frac{\epsilon_r - 1}{\epsilon_r + 2} \right) = \frac{1}{3\epsilon_0} N_A \alpha \quad (6.29)$$

Equation (6.28) or (6.29) is called Clausius-Mosotti equation. It can be used to determine the polarizabilities of the atoms if the dielectric constant is known. Further, the dielectric constants of new materials can be predicted from a knowledge of polarizabilities. This relation thus provides the necessary relation between the microscopic and macroscopic quantities of polarization.

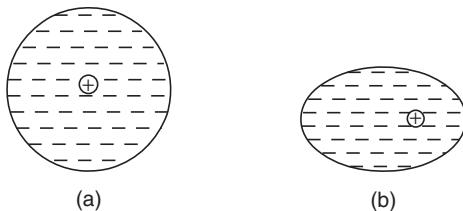
## 6.5 Orientational, ionic and electronic polarizations

When an electric field is applied on a dielectric crystal, then the positive charges of atoms and molecules are displaced along the field while the negative charges in a direction opposite to that of the applied field. This is the basis for polarization of a dielectric substance.

If a molecule has permanent dipole moment, then it is a dipolar molecule and the substance is a dipolar substance. Example is H<sub>2</sub>O molecule. In the absence of an external electric field, the dipoles are randomly oriented, so that polarization is zero. But when the electric field is applied, these dipoles tend to rotate different extents in the direction of an applied electric field giving rise to dipolar or orientational polarization. The applied field also tends to displace the positive and negative ions of molecule in opposite directions causing a change in the ionic bond length. This change in bond length is to produce a net dipole moment in the crystal. This dipole moment per unit volume of material is known as ionic polarization.

The individual ions or atoms of a crystal are themselves polarized in the electric field. Fig. 6.3 shows the polarization of an atom, the electrons in its various shells are displaced relative to the nucleus and produce an electric dipole moment. This dipole moment per unit electric field of the material is called electric polarizability.

**Figure 6.3 (a) Unpolarized atom; (b) Polarized atom**



The total polarizability ( $\alpha$ ) is the sum of the various polarizabilities such as the electronic polarizability ( $\alpha_e$ ), ionic polarizability ( $\alpha_i$ ) and dipolar polarizability ( $\alpha_d$ ). Therefore, we write  $\alpha = \alpha_e + \alpha_i + \alpha_d$ . Now, we study each polarization in detail.

### (a) Dipolar or orientational polarization

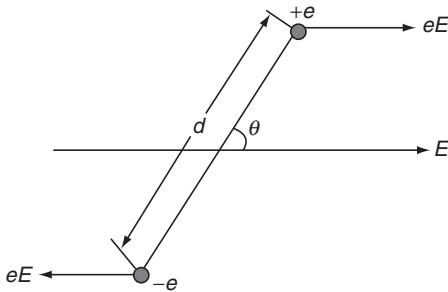
The expression for dipolar polarization can be obtained from Langevin-Debye theory as given below. According to Debye, oriental polarization is due to the rotation of polar molecules in dielectric substance. In the absence of an applied electric field, the dipoles of the substance are randomly oriented in all directions with equal probability and the resultant polarization is zero. In the presence of an applied electric field ( $E$ ), the torque ( $\vec{\tau}$ ) acting on a dipole to rotate it in the direction of  $E$  is given as:

$$|\vec{\tau}| = |\vec{F} \times \vec{d}| = eEd \sin \theta = pE \sin \theta$$

where  $p$  is the dipole moment of a molecule [Fig. 6.4]. The only force that prevents permanent dipoles from complete alignment with the field is thermal agitation.

Therefore, an equilibrium state will reach in which different dipoles will make 0 to  $\pi$  radian angles with field direction, producing a net resultant polarization in the direction of the field. The potential energy ( $V$ ) of a dipole corresponding to an angle  $\theta$  between  $p$  and  $E$  direction is:

Figure 6.4 Torque acting on a dipole



$$V = \int_{\pi/2}^{\theta} \tau \, d\theta = \int_{\pi/2}^{\theta} pE \sin \theta \, d\theta = -pE \cos \theta \quad (6.30)$$

According to Boltzmann distribution law, the probability for a dipole to make an angle between  $\theta$  and  $\theta + d\theta$  with the field is proportional to:

$$2\pi \sin \theta \, d\theta \exp \left[ \frac{pE \cos \theta}{K_B T} \right]$$

where  $2\pi \sin \theta \, d\theta$  is the solid angle between  $\theta$  and  $\theta + d\theta$ . Hence, the average component of the dipole moment along the field direction is equal to:

$$\langle \cos \theta \rangle = \frac{\int_0^\pi p \cos \theta \cdot 2\pi \sin \theta \, d\theta \exp \left[ \frac{pE \cos \theta}{K_B T} \right]}{\int_0^\pi 2\pi \sin \theta \, d\theta \exp \left[ \frac{pE \cos \theta}{K_B T} \right]} \quad (6.31)$$

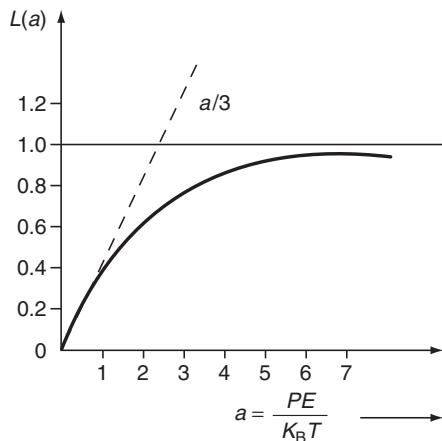
$\theta = 0$  corresponds to parallel alignment and  $\theta = \pi$  to anti-parallel alignment of the dipoles. Dividing numerator and denominator by  $2\pi$  and putting  $a = \frac{pE}{K_B T}$ ,  $x = a \cos \theta = \frac{pE}{K_B T} \cos \theta$  and  $dx = -a \sin \theta \, d\theta$ .

Substituting the above values in Equation (6.31), we have:

$$\langle \cos \theta \rangle = \frac{1}{a} \frac{\int_{-a}^a x e^x \, dx}{\int_{-a}^a e^x \, dx} = \frac{e^a + e^{-a}}{e^a - e^{-a}} - \frac{1}{a} = \cot ha - \frac{1}{a} = L(a) \quad (6.32)$$

$L(a)$  is called Langevin function, because this formula was derived by Langevin in 1905 in connection with paramagnetism.

A graph of  $L(a)$  versus ' $a$ ' has been plotted as shown in Fig. 6.5. Near the origin, the Langevin function increases linearly so that  $L(a) = a/3$ . As ' $a$ ' increases, the function continues to increase and approaching the saturation value unity as  $a \rightarrow \infty$  i.e., for high field strengths. This saturation corresponds to complete alignment of the dipoles in the field direction, so that  $\langle \cos \theta \rangle = 1$

Figure 6.5 A graph plotted between  $L(a)$  and 'a'

For moderate field strengths (when  $a \ll 1$ ),  $L(a) = a/3$

$$\text{so that } \langle p \cos \theta \rangle = \frac{a}{3} = \left( \frac{p^2}{3K_B T} \right) E \quad (6.32a)$$

If there are  $N$  molecules per unit volume of the crystal, then the dipolar polarization ( $P_d$ ) is:

$$P_d = N \langle p \cos \theta \rangle = \frac{N p^2 E}{3K_B T} \quad (6.33)$$

The average dipolar dipole moment [  $\langle p \cos \theta \rangle$  ] is proportional to the intensity of the applied electric field [  $E$  ] i.e.,  $\langle p \cos \theta \rangle \propto E$  (or)  $\langle p \cos \theta \rangle = \alpha_d E$ , where the proportionality constant  $\alpha_d$  is called the dipolar polarizability given as:

$$\alpha_d = \frac{\langle p \cos \theta \rangle}{E} = \frac{p^2}{3K_B T} \quad (6.34) \quad [\text{using Equation (6.32a)}]$$

Equation (6.34) is actually applicable to liquids and gases, because in these substances only the molecular dipoles may rotate continuously and freely, as has been assumed in its derivation. In solids, a dipole may move back and forth between certain limits, which depends on the temperature and electric field. Therefore, the total polarizability of a dipolar molecule can be written as:

$$\alpha = \alpha_{ei} + \frac{p^2}{3K_B T} \quad (6.35)$$

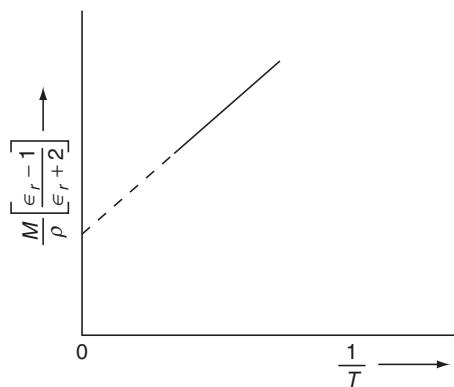
where  $\alpha_{ei}$  is the combined polarizability from electronic and ionic contributions. The Clausius–Mosotti equation for a dipolar system is:

$$\frac{M}{\rho} \left( \frac{\epsilon_r - 1}{\epsilon_r + 2} \right) = \frac{1}{3\epsilon_0} N_A \left[ \alpha_{ei} + \frac{p^2}{3K_B T} \right] \quad (6.36)$$

Equation (6.36) is known as Debye formula. A plot can be drawn between  $\frac{M}{\rho} \left( \frac{\epsilon_r - 1}{\epsilon_r + 2} \right)$  versus  $1/T$  as shown in Fig. 6.6

The graph is a straight line, the slope of this line is proportional to  $p^2$  and its intercept is proportional to  $\alpha_{ei}$ . This formula leads to the determination of both the dipole moment and  $\alpha_{ei}$ .

**Figure 6.6 Temperature versus dielectric constant**



### (b) Ionic polarization

Polarization in ionic crystals arises due to the displacement of ions from their equilibrium positions by the force of an applied electric field.

Ionic polarization can be calculated by considering NaCl crystal. Let the masses of  $\text{Na}^+$  and  $\text{Cl}^-$  ions are  $m$  and  $M$ , respectively. In the absence of an applied electric field, the  $\text{Na}^+$  and  $\text{Cl}^-$  ions are at equilibrium positions and the equilibrium separation between these ions is equal to  $r_0$  (say). After application of the electric field of intensity  $E$ , on the NaCl crystal, some amount of force equal to  $eE$  acts on each  $\text{Na}^+$  and  $\text{Cl}^-$  ions in opposite directions, so that the ions get displaced by  $x_1$  and  $x_2$  distances from equilibrium position. These displacements of ions produce dipole moment in the molecules. The induced dipole moment ( $p$ ) per molecule is:

$$p = e(x_1 + x_2) \quad (6.37)$$

Even though the electric field is continuously acting on the ions, the displacement between the ions will not continuously increase because of the restoring force between the oppositely charged ions. At equilibrium conditions the restoring force ( $F$ ) between the ions is:

$$F = K_1 x_1 = K_2 x_2 \quad \text{where } K_1 \text{ and } K_2 \text{ are force constants}$$

From the above equation, for  $\text{Na}^+$  ion of mass ' $m$ ',

$$x_1 = \frac{F}{K_1} = \frac{eE}{m\omega_0^2} \quad (6.38) \quad [\text{Since } K_1 = m\omega_0^2 = \text{force constant}]$$

where  $\omega_0$  is the natural frequency of NaCl molecule. For  $\text{Cl}^-$  ion of mass ' $M$ ',

$$x_2 = \frac{F}{K_2} = \frac{eE}{M\omega_0^2} \quad \text{--- (6.39)} \quad [\text{Since } K_2 = M\omega_0^2 = \text{force constant}]$$

From Equations (6.38) and (6.39), we have

$$\text{The total displacement } (x) = x_1 + x_2 = \frac{eE}{\omega_0^2} \left[ \frac{1}{m} + \frac{1}{M} \right] \quad \text{--- (6.40)}$$

Substituting Equation (6.40) in (6.37) gives:

$$p = e(x_1 + x_2) = \frac{e^2 E}{\omega_0^2} \left[ \frac{1}{m} + \frac{1}{M} \right] \quad \text{--- (6.41)}$$

This is the induced dipole moment in NaCl molecule. If  $N$  number of NaCl molecules are present per unit volume of the crystal, then polarization  $P$  is:

$$P = Np = Nex = \frac{Ne^2 E}{\omega_0^2} \left( \frac{1}{m} + \frac{1}{M} \right) \quad \text{--- (6.42)}$$

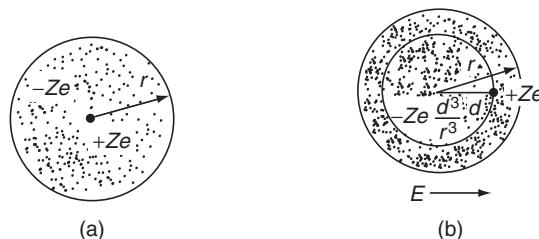
$$\text{The ionic polarizability, } \alpha_i \text{ is} \quad \alpha_i = \frac{p}{E} = \frac{e^2}{\omega_0^2} \left( \frac{1}{m} + \frac{1}{M} \right) \quad \text{--- (6.43)}$$

Substituting the various values in the above equation, we get  $\alpha_i = 9.75 \times 10^{-24} \text{ F-m}^2$ , but the experimental value is  $3.3 \times 10^{-24} \text{ F-m}^2$ . The poor agreement between these values is that the effective ionic charge on an ion was assumed as  $e$ , but in fact it turned out to be  $0.7e$ .

### (c) Electronic polarization

Electronic polarization can be calculated by considering the atoms of a given substance. In the absence of an applied electric field, an atom will be spherical as shown in Fig. 6.6(a). The atom consists of a point nucleus of charge  $+Ze$ , surrounded symmetrically by an electron cloud of charge  $-Ze$  in a sphere of radius  $r$ . If an electric field  $E$  is applied on the atom, then a force of  $|ZeE|$  acts on the nucleus in the direction of the applied electric field and on the electron cloud in the opposite direction, so that they shift with respect to each other by a distance ' $d$ ' as shown in Fig. 6.6(b). The electron cloud is assumed to remain spherical for simplicity.

**Figure 6.6** Electric polarization



The distance of separation ‘ $d$ ’ between the centre of electron cloud and nucleus is such that the restoring force on the nucleus and electron cloud is equal to the force of attraction between the nucleus and the fraction of the charge inside the sphere of radius ‘ $d$ ’. Applying Coulomb’s law for restoring force,

$$F = \frac{1}{4\pi\epsilon_0} \frac{Ze \left( Ze \frac{d^3}{r^3} \right)}{d^2} \quad (6.44)$$

This is equal to force by electric field,

$$F = ZeE \quad (6.45)$$

Equating these forces, we have:

$$\frac{1}{4\pi\epsilon_0} \frac{Ze \left( Ze \frac{d^3}{r^3} \right)}{d^2} = ZeE$$

$$\text{gives } d = \frac{r^3 E \times 4\pi\epsilon_0}{Ze} \quad (6.46)$$

The induced dipole moment ‘ $p_e$ ’ is:

$$p_e = Zed = r^3 E \times 4\pi\epsilon_0 \quad (6.47)$$

The dipole moment per unit volume is polarization.

If ‘ $N$ ’ number of atoms are present in unit volume of material, then electronic polarization  $P_e$  is:

$$P_e = Np_e = N4\pi\epsilon_0 r^3 E \quad (6.48)$$

and the polarizability  $\alpha_e$  is:

$$\alpha_e = \frac{p_e}{E} = 4\pi\epsilon_0 r^3 \quad (6.49)$$

Using Equation (6.49), electronic polarizability can be calculated.

For monoatomic gas,  $P_e = N4\pi\epsilon_0 r^3 E = \epsilon_0(\epsilon_r - 1) E$

Hence, we have:

$$\epsilon_r = 1 + 4\pi r^3 N$$

The value  $4\pi r^3 N$  is of the order of  $10^{-4}$ . Hence,  $\epsilon_r \approx 1$  for gases. In solids,  $\epsilon_r$  varies from 2 to 10.

## 6.6 Frequency dependence of polarizability: (Dielectrics in alternating fields)

In this topic, the variation of polarizability, polarization and dielectric constant of the dielectric with the frequency of the applied electric field has been explained. The permittivity of a dielectric material is equal to  $\epsilon_0 \epsilon_r$ , where  $\epsilon_r$  is called the relative permittivity or dielectric constant of the material and  $\epsilon_0$  is the permittivity of the free space. Also from Clausius–Mosotti relation, we know that the dielectric constant is related to

polarizability of the material. So, we can see the variation of permittivity and hence relative permittivity or dielectric constant, in turn polarizability of a dielectric material with the frequency of the applied electric field. When an alternating electric field of frequency less than  $10^6$  Hz is applied on a dielectric material, then the orientation of the electric dipoles and hence polarization will reverse every time as the polarity of the field reverses. The polarization of the material follows the field without any lag so that the permittivity remains constant. As the frequency of the applied electric field is increased from  $10^6$  Hz to  $10^{11}$  Hz (radiowave frequencies), the electric dipoles present in the material unable to follow the field, hence they lag behind the field and orientational polarization ceases. So, the dielectric constant changes whereas ionic and electronic polarizations are present. Again if the frequency of the applied electric field is increased from  $10^{11}$  Hz to  $10^{14}$  Hz [infrared frequencies], the heavy positive and negative ions present in the material cannot follow the field variations; hence ionic polarization ceases.

This leads against to the change in dielectric constant. The electronic polarization exists up to a frequency of nearly  $10^{15}$  Hz, because electrons are light particles and easily follow the variations of the applied voltage.

To know the dependence of electronic polarizability with the frequency of the applied electric field in the optical region, we consider an atomic model with a nucleus of charge  $+e$  and an electron. The electron has been represented as a cloud having radius  $r_0$ . In the absence of an applied electric field, the centre of electron cloud coincides with the nucleus. After applying static electric field, the centre of electron cloud displaces by small distance  $x$  (say) relative to the nucleus.

$$\text{Then, the restoring force } (F) = \frac{-e^2 x}{4\pi\epsilon_0 r_0^3} = -fx \quad \dots \quad (6.50)$$

$$\text{where } f = \frac{e^2}{4\pi\epsilon_0 r_0^3} = \text{restoring force constant.}$$

If there is no damping, then the equation of motion is:

$$m \left( \frac{d^2 x}{dt^2} \right) = -fx \quad \dots \quad (6.51)$$

or

$$\frac{d^2 x}{dt^2} + \frac{f}{m} x = 0 \quad \dots \quad (6.52)$$

The solution for Equation (6.52) is of the form  $x = x_0 \sin(\omega_0 t + \delta)$ , where  $x_0$  = maximum displacement,  $\delta$  is the integrating constant and  $\omega_0 = \sqrt{f/m}$  is the natural or resonance frequency of the electron cloud. If we consider damping in the motion of electrons, then Equation (6.51) becomes:

$$m \frac{d^2 x}{dt^2} = -fx - 2b \frac{dx}{dt} \quad \dots \quad (6.53)$$

where  $2b$  is the damping constant.

Instead of static electric field, an alternating electric field  $E = E_0 \cos \omega t$  is applied on the electron, then the Lorentz force,  $-eE_0 \cos \omega t$  acts on the electron cloud and the equation of motion is:

$$m \frac{d^2 x}{dt^2} = -fx - 2b \frac{dx}{dt} - eE_0 \cos \omega t \quad \dots \quad (6.54)$$

where  $E_0$  is the maximum electric field.

(or)

$$\frac{d^2x}{dt^2} + \frac{2b}{m} \frac{dx}{dt} + \frac{f}{m}x + \frac{eE_0}{m} \cos \omega t = 0 \quad (6.55)$$

The solution for Equation (6.55) is of the form:

$$x(t) = \text{Real}[A^* e^{i\omega t}] \quad (6.56)$$

where  $A^*$  is complex amplitude

$$\text{Here, } \text{Real}[E_0 e^{i\omega t}] = E_0 \cos \omega t$$

Equation (6.56) is differentiated twice and substituted in Equation (6.55)

$$\frac{dx}{dt} = \text{Real}[A^* i\omega e^{i\omega t}]$$

$$\frac{d^2x}{dt^2} = \text{Real}[A^* (i\omega)^2 e^{i\omega t}] = \text{Real}[-A^* \omega^2 e^{i\omega t}]$$

Substituting these in Equation (6.55)

$$\text{Real} \left[ \left\{ -\omega^2 A^* + i \left( \frac{2b\omega}{m} \right) A^* + \left( \frac{f}{m} \right) A^* + \left( \frac{e}{m} \right) E_0 \right\} e^{i\omega t} \right] = 0 \quad (6.57)$$

As the exponential value in the above equation is not equal to zero, so the value in curling bracket is equal to zero.

$$\text{That is } -\omega^2 A^* + i \left( \frac{2b}{m} \right) \omega A^* + \left( \frac{f}{m} \right) A^* + \left( \frac{e}{m} \right) E_0 = 0$$

$$\text{Substitute } \frac{f}{m} = \omega_0^2$$

we have:

$$A^* \left[ \omega_0^2 - \omega^2 + i \left( \frac{2b}{m} \right) \omega \right] = \frac{-eE_0}{m}$$

$$\text{or } A^* = \frac{-eE_0/m}{\left( \omega_0^2 - \omega^2 \right) + i \left( \frac{2b}{m} \right) \omega} \quad (6.58)$$

Substitute Equation (6.58) in Equation (6.56)

$$x(t) = \text{Real} \left[ \frac{-\left( eE_0/m \right) e^{i\omega t}}{\left( \omega_0^2 - \omega^2 \right) + i \left( \frac{2b}{m} \right) \omega} \right] \quad (6.59)$$

The induced dipole moment  $p_{\text{ind}}(t) = -ex(t)$

$$= \text{Real} \left[ \frac{(e^2/m) E_0 e^{i\omega t}}{(\omega_0^2 - \omega^2) + i \left( \frac{2b}{m} \right) \omega} \right] \quad (6.60)$$

Under static electric field, the electronic induced dipole moment ( $p_{\text{ind}}$ ) is proportional to the applied electric field  $E$ ,

So,

$$p_{\text{ind}} \propto E \quad \text{or} \quad p_{\text{ind}} = \alpha_e E \quad (6.61), \quad \text{where } \alpha_e \text{ is electronic polarizability.}$$

Comparing Equations (6.60) and (6.61), the coefficient of electric field  $E_0 e^{i\omega t}$  is the electronic polarizability. So,

$$p_{\text{ind}}(t) = \text{Real} [\alpha_e^* E_0 e^{i\omega t}]$$

where  $\alpha_e^*$  is the complex electronic polarizability and is equal to:

$$\alpha_e^* = \frac{(e^2/m)}{(\omega_0^2 - \omega^2) + i \left( \frac{2b}{m} \right) \omega} \quad (6.62)$$

To separate real and imaginary parts of Equation (6.62), multiply and divide with  $(\omega_0^2 - \omega^2) - i \left( \frac{2b}{m} \right) \omega$ , We have:

$$\alpha_e^* = \left( \frac{e^2}{m} \right) \left[ \frac{(\omega_0^2 - \omega^2)}{\left( \omega_0^2 - \omega^2 \right)^2 + \left( \frac{4b^2 \omega^2}{m^2} \right)} - \frac{i \left( \frac{2b}{m} \right) \omega}{\left( \omega_0^2 - \omega^2 \right)^2 + \frac{4b^2 \omega^2}{m^2}} \right] \quad (6.63)$$

The above equation can be represented in the form as  $\alpha_e^* = \alpha'_e - i\alpha''_e$  (6.64)

Here,  $\alpha'_e$  and  $\alpha''_e$  are the real and imaginary parts of polarizability, respectively. The induced electronic dipole moment per unit volume of the material is the electronic polarization of the material. This can be represented as:

$$P_e(t) = \text{Real} [N \alpha_e^* E_0 e^{i\omega t}] \quad (6.65)$$

where  $N$  is the number of atoms per unit volume of the material

$$P_e(t) = \text{Real} [N (\alpha'_e - i\alpha''_e) E_0 (\cos \omega t + i \sin \omega t)]$$

$$= N \alpha'_e E_0 \cos \omega t + N \alpha''_e E_0 \sin \omega t \quad (6.66)$$

Substituting  $\alpha'_e$  and  $\alpha''_e$  in Equation (6.66), we have:

$$P_e(t) = \left( \frac{Ne^2}{m} \right) \begin{bmatrix} (\omega_0^2 - \omega^2) E_0 \cos \omega t \\ (\omega_0^2 - \omega^2)^2 + \frac{4b^2\omega^2}{m^2} \end{bmatrix} + \left( \frac{Ne^2}{m} \right) \begin{bmatrix} \left( \frac{2b\omega}{m} \right) E_0 \sin \omega t \\ \left( \omega_0^2 - \omega^2 \right) + \frac{4b^2\omega^2}{m^2} \end{bmatrix} \quad (6.67)$$

The first part of polarization is in phase with the applied electric field, whereas the second part of polarization lags  $90^\circ$  with the applied field.

Equation (6.65) can also be represented in terms of dielectric constant as:

$$P_e(t) = \text{Real} [N\alpha_e^* E_0 e^{i\omega t}] = \text{Real} [\varepsilon_0 (\varepsilon_r^* - 1) E_0 e^{i\omega t}]$$

So,

$$\varepsilon_0 (\varepsilon_r^* - 1) = N\alpha_e^* \quad (6.68)$$

Substitute  $\alpha_e^*$  from Equation (6.63) in the above Equation 6.68, we have:

$$\varepsilon_0 (\varepsilon_r^* - 1) = \frac{N(e^2/m)}{(\omega_0^2 - \omega^2) + i\left(\frac{2b}{m}\right)\omega}$$

or

$$\varepsilon_r^* = 1 + \frac{Ne^2/m}{\varepsilon_0 \left[ (\omega_0^2 - \omega^2) + i\left(\frac{2b}{m}\right)\omega \right]} \quad (6.69)$$

A graph has been plotted for the real and imaginary parts of  $\alpha_e^*$  (Equation (6.63)) with  $\omega$  as shown in Fig. 6.7.

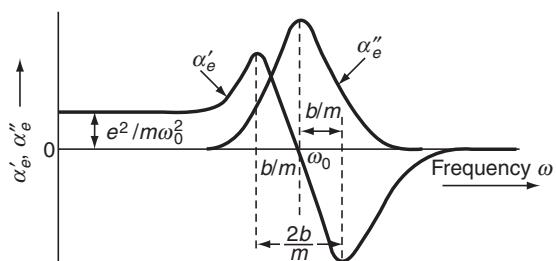
In Equation (6.62) for  $\omega = 0$  (i.e., dc field), the imaginary part becomes zero and the real part is:

$$\alpha'_e = \frac{e^2}{m \omega_0^2}$$

For  $\omega < \omega_0$ , the real and imaginary parts of electronic polarizabilities are positive.

For  $\omega > \omega_0$ , the real part is negative and the imaginary part is positive.

**Figure 6.7 Variation of  $\alpha'_e$  and  $\alpha''_e$  with  $\omega$  for a single electron**

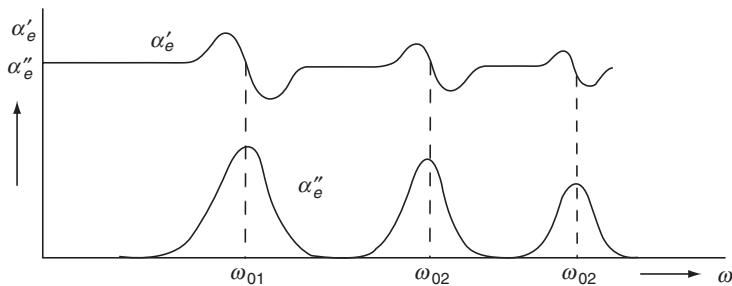


At  $\omega = \omega_0$ , the real part is zero and the imaginary part has maximum value. From the graph, it has been observed that the real part of polarizability is almost constant up to large frequencies from zero frequency, whereas the imaginary part vanishes at  $\omega = 0$  and when  $\omega \rightarrow \infty$ .

So far, we have discussed with an atomic model in which there is only one electron in the atom. Actually, majority of atoms have several electrons and each electron has its own restoring force constant ( $f$ ) and damping constant ( $b$ ). In multielectron atoms, there are several values of  $\omega_0$  (natural frequencies of different atoms). For multielectron atom, plots have been drawn for  $\alpha'_e$  and  $\alpha''_e$  versus  $\omega$  and are shown in Fig. 6.8.

Figure 6.8

A graph has been drawn between,  $\alpha'_e$ ,  $\alpha''_e$ , versus  $\omega$  for multielectron atom



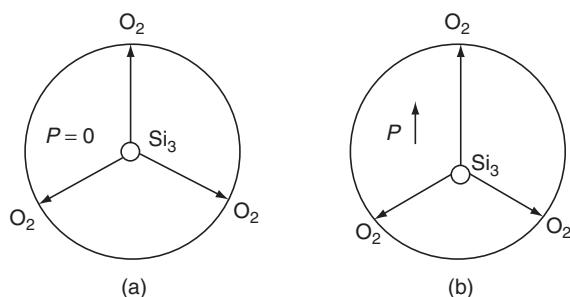
## 6.7 Piezoelectricity

The word 'Piezo' means 'pressure' in Greek. So, 'piezoelectricity' means 'pressure electricity'. Piezoelectric phenomenon was discovered by Curie brothers in 1880. Piezoelectric effect is shown by certain non-centrosymmetric crystals, such as quartz, rochelle salt, tourmaline and barium titanate. Electric polarization develops opposite charges on their surfaces by stress. On these substances, a mechanical stress produces an electric polarization and reciprocally, an applied electric field produces a mechanical strain. These effects are called the direct and inverse piezoelectric effects. Crystals with centres of inversion do not exhibit piezoelectricity.

A crystal can exhibit piezoelectricity only if its unit cell lacks centre of inversion. Fig. 6.9(a) shows the three-fold symmetry axis of an unstressed quartz crystal. The arrows represent the dipole moments. The sum

Figure 6.9

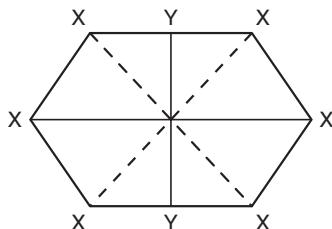
Three-fold symmetry of quartz crystal: (a) when it is unstressed and (b) when it is stressed



of three dipole moments at the vertex is zero. When subjected to stress, it gets polarization ( $P$ ) in the direction indicated because of the distortion of the charge symmetry.

Piezoelectric effect in quartz crystal is explained here. Quartz crystallizes in hexagonal crystal system. A section cut perpendicular to Z-axis (optic axis) is shown in Fig. 6.10. Optic axis in a crystal is a direction along which the velocity of ordinary and extraordinary rays is the same. The lines joining the opposite corners are called X-axis and the lines perpendicular to the opposite faces are known as Y-axis. A plate of quartz crystal with its faces perpendicular to X-axis is called X-cut quartz crystal. Similarly, a plate with its faces perpendicular to the Y-axis is called Y-cut crystal. Quartz crystal will not show piezoelectric effect along the optic axis, piezoelectricity is maximum along Y-axis and is medium along X-axis.

**Figure 6.10** Quartz crystal: Section cut perpendicular to Z-axis



#### Applications:

- (1) Piezoelectric effect is used in detection and to produce sound waves.
- (2) Quartz crystal responds to pressure variations; so, it is used as a pressure transducer.
- (3) The natural frequency of quartz crystal does not vary with temperature. Using this property, quartz crystal is used to produce highly stable RF oscillations for broadcasting purposes and in quartz watches to maintain accurate time.

## 6.8 Ferroelectricity

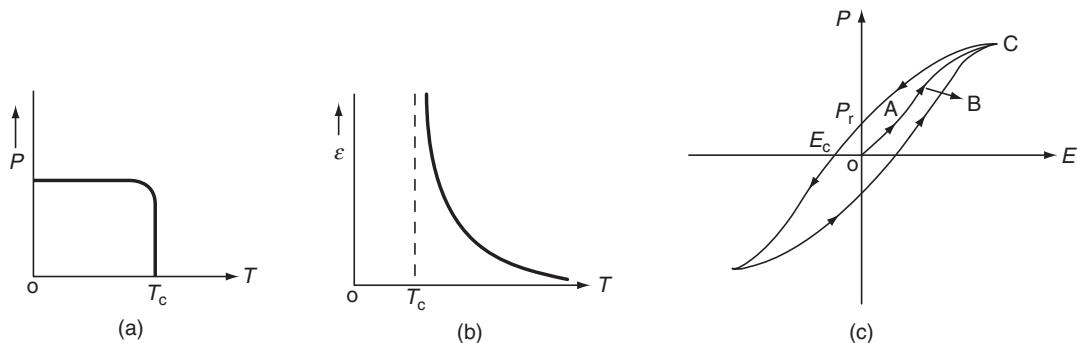
Few dielectric substances such as barium titanate  $[\text{BaTiO}_3]$ , rochelle salt, KDP  $(\text{KH}_2\text{PO}_4)$ , ADP  $[\text{NH}_4\text{H}_2\text{PO}_4]$ ,  $\text{LiNbO}_3$ ,  $\text{KNbO}_3$ , etc. called ferroelectric materials show spontaneous electric polarization ( $P$ ) below Curie temperature ( $T < T_c$ ) is known as ferroelectricity. This is shown in Fig. 6.11(a). Polarization of a material without any applied external electric field on it below Curie temperature is known as spontaneous polarization.

The dielectric constant of a ferroelectric material increases enormously as the temperature of the material reduces to its Curie temperature. The variation of dielectric constant with temperature is shown in Fig. 6.11(b) and is given by Curie-Weiss law  $\epsilon_r = \frac{C}{T - T_c}$ , where  $C$  is the Curie constant and  $T_c$  is Curie temperature.

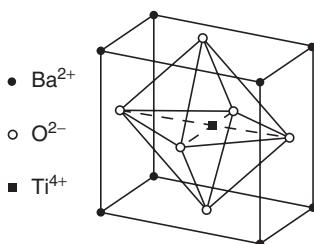
Another important property of ferroelectrics is that they show hysteresis similar to magnetic materials under the action of alternating voltages as shown in Fig. 6.11(c). When an electric field is applied on the specimen, the polarization increases along the curve OABC. And when the field is reduced to zero, then a certain amount of polarization called remanent polarization,  $P_r$  is still present in the material. To remove this polarization, electric field in the opposite direction must be applied. The amount of field required to remove remanent polarization is called coercive field ( $E_c$ ).

Figure 6.11

(a) Spontaneous polarization; (b) Variation of dielectric constant with temperature; (c) Hysteresis of a ferroelectric material



The spontaneous polarization of ferroelectric material is due to asymmetrical ionic displacements in the crystal structure as it is cooled through  $T_c$ . This can be explained by considering  $\text{BaTiO}_3$  as an example. The structure of  $\text{BaTiO}_3$  above  $T_c$  ( $=120^\circ \text{C}$ ) is shown in Fig. 6.12. The unit cell of  $\text{BaTiO}_3$  above Curie temperature is cubic. Oxygen ions are present at the centres of six cube faces. These six oxygen ions form an octahedron configuration.

Figure 6.12  $\text{Ba TiO}_4$  unit cell

The  $\text{Ti}^{4+}$  ion is present at the centre of this octahedron. Barium ions occupy the corners of the cube. The centre of the negative charges coincide with that of the centre of positive charges. So, the net dipole moment is zero. As it is cooled through  $T_c$ , the  $\text{Ti}^{4+}$  and  $\text{Ba}^{2+}$  ions move with respect to  $\text{O}^{2-}$  ions. X-ray and neutron diffraction studies show that the titanium and barium ions move up by 2.8% and oxygen ions move down by 1%. This favours spontaneous polarization of the material. The direction of spontaneous polarization may lie along any one of the cube edges, giving six possible directions of polarization; the material expands in the direction of polarization and contracts perpendicular to that direction. Thus, the unit cell changes from cubic to tetragonal structure. Now, the centre of positive charges is no longer coincident with the centre of negative charges. This explains spontaneous polarization.

**Applications:**

- (i) The ferroelectric material possesses very high value of dielectric constant, so they are used in the manufacture of small-sized and large-capacitance capacitors.
- (ii) Because of the hysteresis property of ferroelectric materials, they are used in the construction of memory devices used in computers.
- (iii) The ferroelectric materials show piezoelectric property, so they are used to produce and detect sound waves.
- (iv) The ferroelectric materials also show pyroelectric property, so they are used to detect infrared radiation.

## 6.9 Frequency dependence of dielectric constant

The permittivity ( $\epsilon$ ) of a dielectric material is equal to  $\epsilon_0 \epsilon_r$ . Where  $\epsilon_r$  is called relative permittivity or dielectric constant of the material and  $\epsilon_0$  is the permittivity of free space. Also from Clausius-Mosotti relation, we know that the dielectric constant is related to polarizability of the material. So, we can see the variation of permittivity and hence relative permittivity or, dielectric constant, in turn, polarizability of a dielectric material with the frequency of the applied electric field. The fall in the permittivity of a dielectric material with increasing frequency of the applied electric field is usually referred to as anomalous dispersion.

The behaviour of a dielectric material in alternating electric field shows that the dielectric constant is a complex quantity. The imaginary part of this dielectric constant represents the dielectric loss of the material. When an alternating electric field of frequency less than  $10^6$  Hz is applied on a dielectric material, then the orientation of the electric dipoles and hence the polarization will reverse every time as the polarity of the field reverses. The polarization of the material follows the field without any lag so that the permittivity remains constant. As the frequency of the applied electric field is increased from  $10^6$  Hz to  $10^{11}$  Hz [radiowave frequencies], the electric dipoles present in the material are unable to follow the field, hence they lag behind the field and orientational polarization ceases. So, the dielectric constant changes whereas ionic and electronic polarizations are present. Dispersion arising during the transition from full orientational polarization at zero or low frequencies to negligible orientational polarization at high radio frequencies is referred to as dielectric relaxation. Again, if the frequency of the applied electric field is increased from  $10^{11}$  Hz to  $10^{14}$  Hz [infrared wave frequencies], the heavy positive and negative ions present in the material cannot follow the field variations, hence ionic polarization ceases. This leads again to the change in dielectric constant. The dispersion arising during the transition from full atomic polarization at radio-frequencies to negligible atomic polarization at optical frequencies is referred to as resonance absorption. The electronic polarization exists up to a frequency of nearly  $10^{15}$  Hz, because electrons are light particles and easily follow the variations of applied voltage. Above this frequency, all polarizations ceases.

Now, we will see the variation of the real part and the imaginary part of dielectric constant in orientational, ionic and electronic polarizations.

### Orientational polarization

The complex dielectric constant can be expressed as:

$$\epsilon(\omega) = \epsilon'(\omega) - i\epsilon''(\omega)$$

As shown in Fig. 6.13(a), the real part of dielectric constant  $\epsilon'_r(\omega)$  is constant equal to  $\epsilon(0)$  for all frequencies in the range  $\omega << \frac{1}{\tau}$ , where  $\tau$  is the orientational relaxation time and  $\omega$  is the frequency of the applied voltage.

This frequency range usually covers all frequencies up to the microwave region. In the frequency range  $\omega \geq 1/\tau$ , the real part of dielectric constant decreases to a constant value equal to  $n_2$  [called optical dielectric constant], where  $n$  = refractive index of the material. The imaginary part,  $\epsilon''(\omega)$  has its maximum value at  $\omega = 1/\tau$  [or  $\omega\tau = 1$ ] and decreases as the frequency departs from this value (i.e., increases or decreases), and represents dissipation of electrical energy in the form of heat in the dielectric material. The rate of dissipation is proportional to  $\epsilon''(\omega)$  and is maximum at  $\omega = 1/\tau$ .

## Ionic polarization

In the high frequency range (IR), the ionic contribution vanishes because at high frequencies, the ions cannot follow the oscillations of the field.

## Electronic polarization

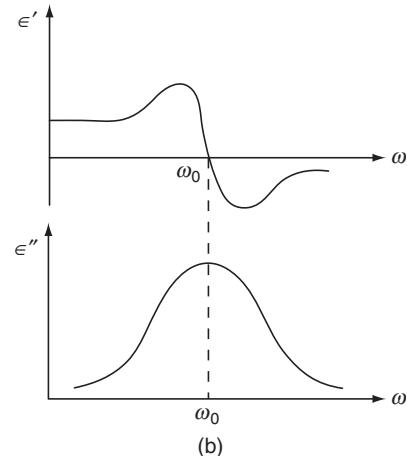
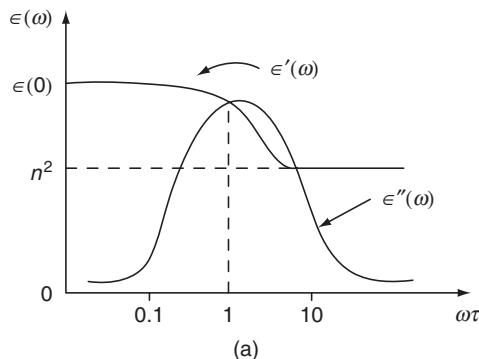
The real part of the dielectric constant  $\epsilon'(\omega)$  gives the value of the dielectric constant and  $\epsilon''(\omega)$  gives the power dissipated and hence the damping loss, the variations of these are shown in Fig. 6.13(b).  $\epsilon''(\omega)$  has a maximum at  $\omega = \omega_0$ , this means that the material absorbs energy at the natural frequency. This is called resonance absorption.  $\epsilon'(\omega)$  is strongly frequency-dependent and the susceptibility undergoes a change in sign is called anomalous dispersion.

Since the dielectric constant of a material is related with the polarizability 'α' of a dielectric substance. The variation of polarizability with frequency is shown in Fig. 6.14.

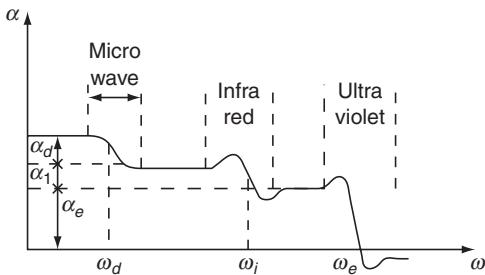
## 6.10 Important requirements of insulators

Insulating materials with different properties are required in electrical, thermal, mechanical and chemical applications.

**Figure 6.13** Real and imaginary parts of dielectric constant with frequency of alternating voltage: (a) Upto microwave region and (b) At optical frequencies



**Figure 6.14 Variation of polarizability with frequency of alternating voltage**



### (a) Electrical requirements

High-resistivity insulating materials are required to reduce leakage current. To withstand at high voltages, high dielectric strength materials are used. Dielectric strength is defined as the ability of a material to withstand up to a certain maximum electric field without breakdown. An insulator should have, low loss factor, high thermal stability, good mechanical strength, high resistivity and high dielectric strength. Mostly, polymeric materials like polystyrene, polyethylene, polyvinyl chloride, acrylic plastic, kapron, etc. are used.

Insulating materials used in capacitors should have high permittivity, low loss factors, high resistivity values, low frequency dependence of loss factor, good thermal stability, high dielectric strength and dielectric constant in the frequency range of operation. Good capacitor materials are  $\text{TiO}_2$ ,  $\text{SnO}_2$  (or)  $\text{ZrO}_2$ ,  $\text{CaO}$ ,  $\text{MgO}$  or their mixtures.

Phenolics are widely used as insulating varnishes. Laminated sheets are used as insulating components of generators, transformers, etc. Teflon is one of the best insulators, as it has high resistivity.

### (b) Thermal requirements

Some insulating materials such as transformer oil, hydrogen, helium, etc. are used for insulation and cooling purposes. Good thermal conductivity is desired for the materials which are used as coolants. The insulators should possess small coefficients of thermal expansion to prevent mechanical damage. The insulators should be non-ignitable, if ignitable it should be self-extinguishable.

### (c) Mechanical requirements

Depending on the use, the insulating materials should have some required mechanical properties. For example, when an insulator is used in electric machine, it should have sufficient mechanical strength to withstand vibrations and shock. Insulators are used on the basis of volume and not on weight, hence a low-density insulator is preferred.

### (d) Chemical requirements

Chemically insulating materials should be resistant to oils, acids, alkalies, gas fumes and liquids. Insulators should be non-absorbant of water, because by absorbing water the insulating resistance and dielectric strength of the material is reduced.

## Formulae

1.  $E_{\text{loc}} = E_0 + E_p + E_s + E_m$
2.  $E = E_0 + E_p$
3.  $E_{\text{loc}} = E + E_s + E_m$
4.  $E_{\text{loc}} = E + E_s$  for symmetric crystals  $= E + \frac{P}{3\epsilon_0}$
5.  $p = \alpha E_{\text{loc}}$
6.  $P = np = n\alpha E_{\text{loc}} = \chi_e \epsilon_0 E$
7.  $\chi_e = \frac{P}{\epsilon_0 E} = \frac{n\alpha}{\epsilon_0 \left[ 1 - \frac{n\alpha}{3\epsilon_0} \right]} = \epsilon_r - 1$
8.  $D = \epsilon E = \epsilon_0 \epsilon_r E = \epsilon_0 E + P$
9.  $\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{n\alpha}{3\epsilon_0} = \frac{\sum_{i=1}^n n_i \alpha_i}{3\epsilon_0}$
10.  $\frac{M}{\rho} \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right] = \frac{N_A \alpha}{3\epsilon_0}$
11.  $\alpha = \alpha_e + \alpha_i + \alpha_d$
12.  $L(a) = \cot h a - \frac{1}{a} = \langle \cos \theta \rangle$
13.  $P_d = Np \langle \cos \theta \rangle = \frac{Np^2 E}{3K_B T}$
14.  $\alpha_d = \frac{p \langle \cos \theta \rangle}{E} = \frac{p^2}{3K_B T}$
15.  $\alpha = \alpha_{ei} + \frac{p^2}{3K_B T}$
16.  $\frac{M}{\rho} \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right] = \frac{N_A}{3\epsilon_0} \left[ \alpha_{ei} + \frac{p^2}{3K_B T} \right]$
17.  $p = e[x_1 + x_2] = \frac{e^2 E}{\omega_0^2} \left[ \frac{1}{m} + \frac{1}{M} \right]$
18.  $P_i = Np = \frac{Ne^2 E}{\omega_0^2} \left[ \frac{1}{m} + \frac{1}{M} \right]$
19.  $\alpha_i = \frac{p}{E} = \frac{e^2}{\omega_0^2} \left[ \frac{1}{m} + \frac{1}{M} \right]$
20.  $P_e = Np_e = N 4\pi \epsilon_0 r^3 E$
21.  $\alpha_e = \frac{p_e}{E} = 4\pi \epsilon_0 r^3$
22.  $\epsilon_r = \frac{C}{T - T_c}$
23.  $\epsilon(\omega) = \epsilon'(\omega) - i\epsilon''(\omega)$
24.  $\alpha_e = \frac{\epsilon_0 [\epsilon_r - 1]}{N}$
25.  $P = \epsilon_0 (\epsilon_r - 1) E$

## Solved Problems

1. A solid elemental dielectric with  $3 \times 10^{28}$  atoms/m<sup>3</sup> shows an electronic polarizability of  $10^{-40}$  F-m<sup>2</sup>. Assuming the internal electric field to be a Lorentz field, calculate the dielectric constant of the material.  
(Set-3–Sept. 2007), (Set-1–May 2004), (Set-4–Nov. 2004), (Set-1–May 2003)

**Sol:** Number density of dielectric atoms,  $N = 3 \times 10^{28}/\text{m}^3$

Electronic polarizability,  $\alpha_e = 10^{-40}$  F-m<sup>2</sup>

Calculate the dielectric constant,  $\epsilon_r = ?$

$$\alpha_e = \frac{\epsilon_0 (\epsilon_r - 1)}{N}$$

$$(or) \quad \epsilon_r = \frac{\alpha_e N}{\epsilon_0} + 1 = \frac{10^{-40} \times 3 \times 10^{28}}{8.85 \times 10^{-12}} + 1 = \frac{3}{8.85} + 1 = 1.339$$

2. A parallel plate capacitor has an area of  $100 \text{ cm}^2$ , a plate separation of  $1 \text{ cm}$  and is charged to a potential of  $100 \text{ V}$ . Calculate the capacitance of the capacitor and the charge on the plates.

(Set-4–May 2007), (Set-4–May 2004), (Set-3–Nov. 2004), (Set-4–May 2003)

**Sol:** Area of the capacitor plates,  $A = 100 \text{ cm}^2 = 10^{-2} \text{ m}^2$

Separation between the plates,  $d = 1 \text{ cm} = 10^{-2} \text{ m}$

Potential between the plates,  $V = 100 \text{ V}$

Capacitance,  $C = ?$  and charge on plates,  $Q = ?$

We know that:

$$C = \frac{\epsilon_0 A}{d} \quad \text{and} \quad Q = CV$$

$$C = \frac{8.85 \times 10^{-12} \times 10^{-2}}{10^{-2}} = 8.85 \times 10^{-12} \text{ F}$$

$$Q = 8.85 \times 10^{-12} \times 100 = 8.85 \times 10^{-10} \text{ C}$$

3. The dielectric constant of He gas at NTP is  $1.0000684$ . Calculate the electronic polarizability of He atoms if the gas contains  $2.7 \times 10^{25}$  atoms per  $\text{m}^3$ .

(Set-1–Sept. 2007), (Set-4–June 2005), (Set-2–May 2004), (Set-2–May 2003), (Set-4–Nov. 2003)

**Sol:** The dielectric constant,  $\epsilon_r = 1.0000684$

Number density of He atoms,  $N = 2.7 \times 10^{25}/\text{m}^3$

Electronic polarizability,  $\alpha_e = ?$

$$\begin{aligned} \alpha_e &= \frac{\epsilon_0 (\epsilon_r - 1)}{N} \\ &= \frac{8.85 \times 10^{-12} [1.0000684 - 1]}{2.7 \times 10^{25}} = 2.242 \times 10^{-41} \text{ F}\cdot\text{m}^2. \end{aligned}$$

4. A parallel plate of area  $650 \text{ mm}^2$  and a plate separation of  $4 \text{ mm}$  has a charge of  $2 \times 10^{-10} \text{ C}$  on it. When a material of dielectric constant  $3.5$  is introduced between the plates. What is the resultant voltage across the capacitor?

(Set-1–May 2007), (Set-1–Nov. 2003)

**Sol:** Area of the capacitor plates,  $A = 650 \text{ mm}^2 = 650 \times 10^{-6} \text{ m}^2$

Distance of separation between the plates,  $d = 4 \text{ mm} = 4 \times 10^{-3} \text{ m}$

Charge on the plates,  $Q = 2 \times 10^{-10} \text{ C}$

Dielectric constant of the material between the plates,  $\epsilon_r = 3.5$

Voltage across the capacitor,  $V = ?$

$$C = \frac{\epsilon_0 \epsilon_r A}{d} \quad \text{and} \quad C = \frac{Q}{V}$$

$$\text{So, } \frac{Q}{V} = \frac{\epsilon_0 \epsilon_r A}{d}$$

$$\text{or } V = \frac{Qd}{\epsilon_0 \epsilon_r A} = \frac{2 \times 10^{-10} \times 4 \times 10^{-3}}{8.85 \times 10^{-12} \times 3.5 \times 650 \times 10^{-6}} \text{ V} = 39.73 \text{ V.}$$

5. A parallel plate capacitor having an area  $6.45 \times 10^{-4} \text{ m}^2$  and a plate separation of  $2 \times 10^{-3} \text{ m}$ , across which a potential of 12 V is applied. If a material having a dielectric constant 5.0 is positioned within the region between the plates, compute the polarization.  
 (Set-3, Set-4–May 2006), (Set-2–Nov. 2003)

**Sol:** Area of the plates,  $A = 6.45 \times 10^{-4} \text{ m}^2$

Separation between the plates,  $d = 2 \times 10^{-3} \text{ m}$

Potential across the plates,  $V = 12 \text{ V}$

Dielectric constant,  $\epsilon_r = 5$

Polarization,  $P = ?$

$$\text{Intensity of the electric field, } E = \frac{V}{d}$$

$$P = \epsilon_0 [\epsilon_r - 1] E = \epsilon_0 [\epsilon_r - 1] \frac{V}{d}$$

$$= 8.85 \times 10^{-12} [5 - 1] \times \frac{12}{2 \times 10^{-3}} = 212.4 \times 10^{-9} \text{ C-m}$$

6. The relative dielectric constant of sulphur is 3.75 when measured at  $27^\circ \text{ C}$ . Assuming the internal field constant  $\gamma = 1/3$ , calculate the electronic polarizability of sulphur if its density at this temperature is  $2050 \text{ Kg/m}^3$ . The atomic weight of sulphur being 32.  
 (Set-1–June 2005), (Set-3–May 2004), (Set-3–May 2003)

**Sol:** The dielectric constant of sulphur,  $\epsilon_r = 3.75$

$$\text{Internal field constant, } \gamma = \frac{1}{3}$$

Density of sulphur,  $D = 2050 \text{ Kg/m}^3$

Atomic weight of sulphur,  $M = 32$

Electronic polarization  $\alpha_e = ?$

$$\text{Number of atoms/m}^3, N = \frac{N_A \times D}{M} \quad \text{where } N_A = \text{Avogadro number}$$

$$= \frac{6.02 \times 10^{26} \times 2050}{32} = 385.66 \times 10^{26} \text{ atoms/m}^3$$

$$E_{\text{loc}} = E + \frac{\gamma P}{\epsilon_0} = E + \frac{P}{3\epsilon_0}$$

Hence, from Clausius-Mosotti relation  $\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha_e}{3\epsilon_0}$

$$\begin{aligned} \text{(or)} \quad \alpha_e &= \left( \frac{\epsilon_r - 1}{\epsilon_r + 2} \right) \frac{3\epsilon_0}{N} \\ &= \left( \frac{3.75 - 1}{3.75 + 2} \right) \left( \frac{3 \times 8.85 \times 10^{-12}}{385.66 \times 10^{26}} \right) = \left( \frac{2.75}{5.75} \right) \left( \frac{25.65}{385.66} \right) 10^{-38} \\ &= 3.18 \times 10^{-40} \text{ F-m}^2 \end{aligned}$$

7. There are  $1.6 \times 10^{20}$  NaCl molecules/m<sup>3</sup> in a vapour. Determine the orientational polarization at room temperature if the vapour is subjected to a dielectric field 5000 V/Cm. Assume that the NaCl molecule consists of sodium and chlorine ions separated by 0.25 nm.

(Set-2-June 2005)

**Sol:** Number of NaCl molecules,  $N = 1.6 \times 10^{20}/\text{m}^3$

Room temperature,  $T = 300 \text{ K}$

Intensity of electric field,  $E = 5000 \text{ V/Cm} = 5 \times 10^5 \text{ V/m}$

Separation between ions,  $x = 0.25 \text{ nm} = 0.25 \times 10^{-9} \text{ m}$

Orientation polarization,  $P_d = ?$

$$P_d = \frac{N p^2 E}{3K_B T}; \text{ dipole moment, } p = ex$$

where  $K_B = \text{Boltzmann constant} = 1.381 \times 10^{-23} \text{ J/K}$

$$\therefore P_d = \frac{N(ex)^2 E}{3K_B T} = \frac{1.6 \times 10^{20} \times (1.6 \times 10^{-19})^2 \times (0.25 \times 10^{-9})^2 \times 5 \times 10^5}{3 \times 1.381 \times 10^{-23} \times 300}$$

$$= 1.0298 \times 10^{-11} \text{ C-m.}$$

8. The dielectric constant of helium, measured at 0° C and 1 atmosphere is  $\epsilon_r = 1.0000684$ . Under these conditions the gas contains  $2.7 \times 10^{25}$  atoms/m<sup>3</sup>. Calculate the radius of the electron cloud. Also calculate the displacement when a helium atom is subjected to an electric field of  $10^6 \text{ V/m}$ .

(Set-3-Sept. 2006)

**Sol:** The dielectric constant,  $\epsilon_r = 1.0000684$

Number density of He atoms,  $N = 2.7 \times 10^{25} \text{ atoms/m}^3$

Electronic polarizability,  $\alpha_e = ?$

$$\begin{aligned} \alpha_e &= \frac{\epsilon_0 (\epsilon_r - 1)}{N} = \frac{8.85 \times 10^{-12} [1.0000684 - 1]}{2.7 \times 10^{25}} \\ &= 2.242 \times 10^{-41} \text{ F-m}^2 \end{aligned}$$

Electric field applied,  $E = 10^6 \text{ V/m}$

Radius of electron cloud,  $r = ?$

Displacement of centres of charges,  $d = ?$

$$\alpha_e = 4\pi \epsilon_0 r^3$$

$$\text{or } r^3 = \frac{\alpha_e}{4\pi \epsilon_0} = \frac{2.242 \times 10^{-41} \times 7}{4 \times 22 \times 8.85 \times 10^{-12}} \\ = 0.02 \times 10^{-29} = 200 \times 10^{-33} \\ \therefore r = 5.848 \times 10^{-11} \text{ m}$$

$$d = \frac{r^3 E \times 4\pi \epsilon_0}{Ze} = \frac{\alpha_e}{4\pi \epsilon_0} \times \frac{E \times 4\pi \epsilon_0}{Ze} \\ = \frac{\alpha_e E}{Ze} = \frac{2.242 \times 10^{-41} \times 10^6}{2 \times 1.6 \times 10^{-19}} \\ = 0.7 \times 10^{-16} \text{ m}$$

9. A parallel plate capacitor of area  $750 \text{ mm}^2$  possess a charge of  $2.5 \times 10^{-10} \text{ C}$  when the plates are separated by 5 mm and the space between plates is filled with a material of dielectric constant of 3.5. Find the voltage across the capacitor plates.

**Sol:** Area of plates,  $A = 750 \text{ mm}^2 = 750 \times 10^{-6} \text{ m}^2$

Separation of plates,  $d = 5 \text{ mm} = 5 \times 10^{-3} \text{ m}$

Charge on plates,  $Q = 2.5 \times 10^{-10} \text{ C}$

Dielectric constant of material,  $\epsilon_r = 3.5$

Voltage across the plates,  $V = ?$

$$C = \frac{\epsilon_0 \epsilon_r A}{d} \quad \text{(1)} \quad \text{and} \quad C = \frac{Q}{V} \quad \text{(2)}$$

Equation (1) = (2)

$$C = \frac{\epsilon_0 \epsilon_r A}{d} = \frac{Q}{V} \quad (\text{or}) \quad V = \frac{Qd}{\epsilon_0 \epsilon_r A}$$

$$= \frac{2.5 \times 10^{-10} \times 5 \times 10^{-3}}{8.85 \times 10^{-12} \times 3.5 \times 750 \times 10^{-6}}$$

$$= \frac{2.5 \times 5 \times 10^5}{8.85 \times 3.5 \times 750} \text{ V} = 53.8 \text{ V}$$

10. A monoatomic gas contains  $3 \times 10^{25}$  atoms/m<sup>3</sup> at 1 atmospheric pressure and at room temperature. The radius of gaseous atoms is 0.2 nm. Find the dipole moment per unit electric field, polarization, dielectric constant and polarizability.

**Sol:** Number of atoms per unit volume,  $N = 3 \times 10^{25}/\text{m}^3$

Radius of atoms,  $r = 0.2 \text{ nm} = 0.2 \times 10^{-9} \text{ m}$

Dipole moment  $p = ?$

Polarization,  $P = ?$

Dielectric constant,  $\epsilon_r = ?$

and Polarizability,  $\alpha_e = ?$

Dipole moment per unit electric field,  $p = 4\pi\epsilon_0 r^3$

$$= 4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times [0.2 \times 10^{-19}]^3 \\ = 8.9 \times 10^{-40} \text{ F-m}^2$$

Polarization,  $P = Np = 3 \times 10^{25} \times 8.9 \times 10^{-40} = 26.7 \times 10^{-15} \text{ C-m}$

To find dielectric constant,  $\epsilon_r$ :

$$\frac{P}{\epsilon_0 E} = \epsilon_r - 1$$

$$P = \epsilon_0 [\epsilon_r - 1] E$$

$$3 \times 10^{25} \times 4 \times \frac{22}{7} \times 8.85 \times 10^{-12} \times (0.2 \times 10^{-9})^3 = 8.85 \times 10^{-12} [\epsilon_r - 1] \times 1$$

$$\epsilon_r - 1 = 0.00302 \quad (\text{or}) \quad \epsilon_r = 1.00302$$

$$\text{Polarizability, } \alpha_e = \frac{\epsilon_0 (\epsilon_r - 1)}{N} = \frac{8.85 \times 10^{-12} \times 0.00302}{3 \times 10^{25}} \\ = 8.91 \times 10^{-40} \text{ F-m}^2$$

11. The relative permittivity of argon at 0° C and at 1 atmospheric pressure is 1.000435. Calculate the polarizability of the atom if the gas contains  $2.7 \times 10^{25}$  atoms/m<sup>3</sup>. Given  $\epsilon_0 = 8.85 \times 10^{-12} \text{ F/m}$

**Sol:** Relative permittivity,  $\epsilon_r = 1.000435$

Number density of atoms,  $N = 2.7 \times 10^{25}$  atoms/m<sup>3</sup>

Polarizability of the atom,  $\alpha_e = ?$

$$\alpha_e = \frac{\epsilon_0 (\epsilon_r - 1)}{N} \\ = \frac{8.85 \times 10^{-12} [1.000435 - 1]}{2.7 \times 10^{25}} = 1.426 \times 10^{-40} \text{ F-m}^2$$

12. If the relative permittivity of sulphur is 4.0, calculate its atomic polarizability. [given that sulphur in cubic form has a density of  $2.08 \times 10^3 \text{ kg/m}^3$  and its atomic weight is 32]

**Sol:** Relative permittivity of sulphur,  $\epsilon_r = 4.0$

Polarizability,  $\alpha_e = ?$

$$\alpha_e = \frac{\epsilon_0 (\epsilon_r - 1)}{N}$$

where  $N$  = number density of atoms

$$N = \frac{N_A \times D}{\text{atomic weight}} = \frac{6.02 \times 10^{26} \times 2.08 \times 10^3}{32}$$

$$= \frac{6.02 \times 2.08 \times 10^{29}}{32} = 0.3913 \times 10^{29}$$

$$\alpha_e = \frac{\varepsilon_0 (\varepsilon_r - 1)}{N}$$

$$= \frac{8.85 \times 10^{-12} \times [4 - 1] \times 32}{6.02 \times 2.08 \times 10^{29}} - \frac{8.85 \times 3 \times 32}{6.02 \times 2.08} \times 10^{-41}$$

$$= 6.785 \times 10^{-40} \text{ F-m}^2$$

## Multiple Choice Questions

1. Dielectrics are: ( )  
(a) metals (b) semiconductors  
(c) insulating materials (d) none

2. Local electric field is calculated by using the method suggested by: ( )  
(a) Lorentz (b) Weiss (c) Curie (d) Coulomb

3. If  $P$  is the polarization of a dielectric material of dielectric constant  $\epsilon_0$  and  $E$  is the macroscopic electric field, then internal field is: ( )  
(a)  $E + \frac{P}{\epsilon_0}$  (b)  $E + \frac{P}{3\epsilon_0}$   
(c)  $E + \frac{3P}{\epsilon_0}$  (d)  $3E + \frac{P}{\epsilon_0}$

4. A dielectric material can be polarized by applying \_\_\_\_\_ field on it. ( )  
(a) magnetic (b) gravitational  
(c) electric (d) meson

5. Polarization per unit applied electric field is called: ( )  
(a) electric susceptibility (b) magnetic susceptibility  
(c) electric polarization (d) dielectric constant

6. In the absence of an external electric field on a dipolar substance, the electric dipoles are: ( )  
(a) parallel (b) alternatively anti-parallel  
(c) randomly oriented (d) none

7. The total polarizability of a substance is equal to: ( )  
(a) orientational and ionic polarizabilities (b) ionic and electronic polarizabilities  
(c) both a and b (d) none

8. The dipolar polarizability for low applied electric fields, at temperature 'T' on a dipolar substance is [ $K_B$  = Boltzmann constant and  $p$  = dipole moment] ( )

(a)  $\frac{p^2}{3K_B T}$  (b)  $\frac{3p^2}{K_B T}$   
(c)  $\frac{p}{3K_B T^2}$  (d)  $\frac{3p}{K_B T^2}$

9. Dipolar polarization is actually applicable to: ( )

(a) gases (b) liquids (c) solids (d) both a and b

10. The observed ionic polarizability of NaCl molecule is: ( )

(a)  $1.3 \times 10^{-24} \text{ F}\cdot\text{m}^2$  (b)  $3.3 \times 10^{-24} \text{ F}\cdot\text{m}^2$   
(c)  $3.1 \times 10^{-24} \text{ F}\cdot\text{m}^2$  (d)  $5.3 \times 10^{-24} \text{ F}\cdot\text{m}^2$

11. The effective ionic charge in NaCl crystal is: ( )

(a)  $1e$  (b)  $1.3e$  (c)  $0.7e$  (d)  $0.5e$

12. If  $r$  is the radius of an atom and  $\epsilon_0$  is the permittivity of free space, then electronic polarizability is: ( )

(a)  $4\pi\epsilon_0 r^2$  (b)  $4\pi\epsilon_0 r^3$  (c)  $4\pi^2\epsilon_0 r^3$  (d)  $4\pi\epsilon_0^2 r^3$

13. Piezoelectric effect is shown by: ( )

(a) quartz (b) rochelle salt  
(c) barium titanate (d) all the above

14. Piezoelectric effect in quartz crystal is maximum along: ( )

(a) X-axis (b) Y-axis (c) Z-axis (d) optic axis

15. Piezoelectric effect is used: ( )

(a) to produce sound waves (b) to detect sound waves  
(c) as a pressure transducer (d) all

16. Quartz crystal is used: ( )

(a) to produce highly stable RF oscillations for broadcasting  
(b) in watches to maintain accurate time  
(c) both a and b  
(d) none

17. Ferroelectric materials are used: ( )

(a) to detect infrared radiation (b) to produce and detect sound waves  
(c) in the construction of memory devices (d) all

18. Ferroelectric materials are: ( )

(a) barium titanate and rochelle salt (b)  $\text{KH}_2\text{PO}_4$  and  $\text{NH}_4\text{H}_2\text{PO}_4$   
(c)  $\text{LiNbO}_3$  and  $\text{KNbO}_3$  (d) all the above

19. The ionic polarization ceases at \_\_\_\_\_ frequency of the applied electric field. ( )

(a)  $10^{11} \text{ Hz}$  (b)  $10^{13} \text{ Hz}$  (c)  $10^{14} \text{ Hz}$  (d)  $10^6 \text{ Hz}$

20. Insulating material used in capacitors should have: ( )  
(a) high permittivity and low loss factors  
(b) high resistivity and low frequency dependence of loss  
(c) good thermal stability and high dielectric strength  
(d) all
21. Chemically, an insulating material should be resistant to: ( )  
(a) oils and acids (b) alkalies and gas fumes  
(c) liquids (d) all the above
22. Dielectric material is used between the capacitor plates to: ( )  
(a) increase electric field (b) increase capacitance  
(c) decrease capacitance (d) decrease electric field
23. Dipole moment is defined as the \_\_\_\_\_ of one of the charge and separation between the charges. ( )  
(a) product (b) sum (c) ratio (d) none
24. The resultant electric field acting on the atoms or molecules of dielectric substance is known as \_\_\_\_\_ . ( )  
(a) local field (b) internal field (c) both a & b (d) none
25. Clausius-Mosotti relation makes relation between microscopic and macroscopic quantities of: ( )  
(a) electric field (b) capacitance  
(c) polarization (d) none
26. Dipole moment per unit volume of material is called: ( )  
(a) polarization (b) polarizability  
(c) both a & b (d) none
27. In the absence of an applied electric field on a dipolar substance, the polarization is: ( )  
(a) finite (b) zero  
(c) high (d) all the above
28. By applying electric field on a dipolar substance, it results in \_\_\_\_\_ polarization. ( )  
(a) electrical (b) ionic  
(c) orientational (d) all the above
29. The total polarizability of a substance, it is the sum of \_\_\_\_\_ polarizabilities: ( )  
(a) dipolar (b) ionic  
(c) electric (d) all the above
30. Orientational polarization is due to the \_\_\_\_\_ of polar molecules in dielectric substance. ( )  
(a) rotation (b) change in separation  
(c) both (d) none
31. In Greek, piezoelectricity means: ( )  
(a) pressure electricity (b) thermal electricity  
(c) friction electricity (d) hydroelectricity
32. Piezoelectric effect is shown by certain \_\_\_\_\_ symmetric crystals. ( )  
(a) centro (b) non-centro  
(c) mirror centro (d) none

33. Piezoelectric effect was discovered by \_\_\_\_\_ in 1880. ( )  
(a) Weiss (b) Thomson  
(c) Curie brothers (d) Alison

34. Crystals with centre of inversion \_\_\_\_\_ exhibit piezoelectric effect. ( )  
(a) do (b) do not  
(c) both a & b (d) none

35. Piezoelectric effect is a \_\_\_\_\_ effect. ( )  
(a) reversible (b) irreversible  
(c) both (d) none

36. Quartz crystal \_\_\_\_\_ piezoelectric effect along the optic axis. ( )  
(a) will show (b) will not show  
(c) both a & b (d) none

37. The natural frequency of quartz crystal \_\_\_\_\_ with temperature. ( )  
(a) do vary (b) do not vary  
(c) both a & b (d) none

38. Spontaneous polarization means, polarization of a material \_\_\_\_\_ external electric field. ( )  
(a) without applying (b) with applying  
(c) both (d) none

39. The dielectric constant of a ferroelectric material increases enormously as the temperature of the material reduces to its \_\_\_\_\_ temperature. ( )  
(a) Debye (b) de Broglie  
(c) Curie (d) Neel

40. Ferroelectrics show \_\_\_\_\_ under the action of alternating voltages. ( )  
(a) polarization (b) polarizability  
(c) hysteresis (d) none

41. The crystal structure of  $\text{BaTiO}_3$  above its curie temperature is \_\_\_\_\_. ( )  
(a) cubic (b) hexagonal  
(c) rhombohedral (d) triclinic

42. As the temperature of  $\text{BaTiO}_3$  is reduced to below curie temperature, the titanium and barium ions move up by 2.8% and oxygen ions move down by \_\_\_\_ %. ( )  
(a) 5 (b) 3 (c) 2 (d) 1

43. Ferroelectric materials are used in the manufacture of small-sized, \_\_\_\_\_ capacitance capacitors. ( )  
(a) small (b) large (c) medium (d) none

44. The fall in permittivity of dielectric material with increasing frequency of applied electric field is usually referred to as:  
(a) anomalous dispersion (b) optical dispersion  
(c) refraction (d) none ( )

45. The imaginary part of dielectric constant represent \_\_\_\_\_ of the material. ( )  
(a) dispersion (b) polarization  
(c) the dielectric loss (d) none

46. The dipolar polarization ceases at \_\_\_\_\_ frequency of applied electric field. ( )  
 (a)  $10^3$  Hz                    (b)  $10^6$  Hz                    (c)  $10^{11}$  Hz                    (d)  $10^{14}$  Hz
47. The electronic polarization exists up to a frequency of \_\_\_\_\_. ( )  
 (a)  $10^{15}$  Hz                    (b)  $10^{18}$  Hz                    (c)  $10^{20}$  Hz                    (d)  $10^{22}$  Hz
48. The real part of dielectric constant is strongly frequency-dependent and undergoes a change in sign called \_\_\_\_\_ dispersion. ( )  
 (a) optical                        (b) anomalous  
 (c) both a & b                    (d) none
49. High dielectric strength and high resistivity insulating materials are required to: ( )  
 (a) withstand high voltages                    (b) reduce leakage currents  
 (c) both a & b                                (d) none
50. An insulating material used in electric machine should have sufficient mechanical strength to withstand: ( )  
 (a) vibrations                        (b) shock                        (c) both a & b                        (d) none
51. The relation between polarizability and dielectric constant is given by: ( )  
 (a) Clausius-Mosotti relation                    (b) Thomson relation  
 (c) Curie-Weiss relation                        (d) none

## Answers

- |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1. c  | 2. a  | 3. b  | 4. c  | 5. a  | 6. c  | 7. c  | 8. a  | 9. d  | 10. b | 11. c |
| 12. b | 13. d | 14. b | 15. d | 16. c | 17. d | 18. d | 19. c | 20. d | 21. d | 22. b |
| 23. a | 24. c | 25. c | 26. a | 27. b | 28. d | 29. d | 30. a | 31. a | 32. b | 33. c |
| 34. b | 35. a | 36. b | 37. b | 38. a | 39. c | 40. c | 41. a | 42. d | 43. b | 44. a |
| 45. c | 46. b | 47. a | 48. b | 49. c | 50. c | 51. a |       |       |       |       |

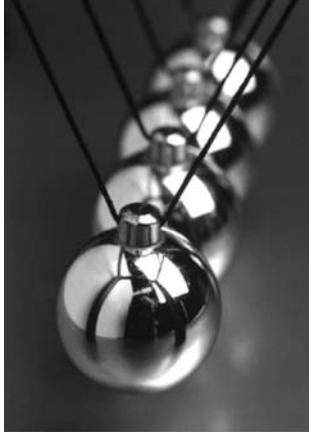
## Review Questions

- What is piezo electricity? (Set-1-Sept. 2007), (Set-2-May 2004), (Set-2-May 2003)
- With usual notations, show that  $P = \epsilon_0(\epsilon_r - 1)E$ . (Set-3-Sept. 2007), (Set-1-May 2004), (Set-4-Nov. 2004), (Set-1-May 2003)
- What is dipolar relaxation? Discuss the frequency dependence of orientational polarization. (Set-3-Sept. 2007), (Set-1-May 2004), (Set-4-Nov. 2004), (Set-1-May 2003)
- Explain electronic polarization in atoms and obtain an expression for electronic polarizability in terms of the radius of the atom. (Set-4-May 2007), (Set-4-May 2004), (Set-3-Nov. 2004), (Set-4-May 2003)
- Explain Clausius-Mosotti relation in dielectrics subjected to static fields. (Set-1-Sept. 2008), (Set-1-June 2005), (Set-3-June 2005), (Set-3-May 2003)
- What is orientational polarization? Derive an expression for the mean dipole moment when a polar material is subjected to an external field. (Set-1-June 2005), (Set-3-May 2004), (Set-3-May 2003)

7. Obtain an expression for the internal field seen by an atom in an infinite array of atoms subjected to an external field.  
(Set-1–Sept. 2007), (Set-2–May 2004), (Set-2–May 2003)
8. What are the important characteristics of ferroelectric materials?  
(Set-4–June 2005), (Set-2–Nov. 2004), (Set-4–Nov. 2004)
9. Describe the possible mechanisms of polarization in a dielectric material. (Set-4–June 2005), (Set-4–Nov. 2004)
10. Explain the polarization mechanism in dielectric materials. (Set-1–May 2007), (Set-1–Nov. 2003)
11. What are the important requirements of good insulating materials?  
(Set-1–May 2007), (Set-3–Sept. 2006), (Set-1–Nov. 2003), (Set-3–Nov. 2003)
12. Explain the concept of internal field in solids and hence obtain an expression for the static dielectric constant in elemental solid dielectric.  
(Set-3, Set-4–May 2006), (Set-2–Nov. 2003)
13. Discuss in detail the origin of ferroelectricity in barium titanate. (Set-3–Sept. 2006), (Set-3–Nov. 2003)
14. Explain the characteristics and function of transformer oil in transformers. (Set-2–Nov. 2004)
15. Explain briefly the classification of ferroelectric materials. (Set-2–June 2005)
16. What is meant by a local field in a solid dielectric? Derive an expression for the local field for structures possessing cubic symmetry.  
(Set-2–June 2005)
17. Give a schematic sketch of the variation of the total polarizability of a dielectric as a function of the frequency, explaining the physical origin of the various contributions and the relevant frequency ranges.  
(Set-2–Nov. 2004)
18. Discuss the variation of spontaneous polarization of roschelle salt with temperature.  
(Set-3–June 2005), (Set-1–May 2004)
19. Obtain an expression for the static dielectric constant of a monoatomic gas.  
(Set-3–June 2005), (Set-1–May 2004)
20. Explain the phenomenon of anomalous dielectric dispersion. (Set-1–May 2004)
21. What is intrinsic breakdown in dielectric materials?  
(Set-4–May 2007), (Set-4–May 2004), (Set-4–May 2003), (Set-3–Nov 2004)
22. Explain the electrochemical breakdown in dielectric materials. (Set-3, Set-4–May 2006)
23. Obtain a relation between electronic polarization and electric susceptibility of the dielectric medium.  
(Set-2–May 2007)
24. What is dielectric breakdown? Explain briefly the various factors contributing to breakdown in dielectrics.  
(Set-2–May 2007)
25. What is orientational polarization? Explain. Obtain an expression for the mean dipole moment when a polar material is subjected to an external electric field.  
(Set-2–Sept. 2007)
26. Describe the phenomenon of electronic polarization and obtain an expression for electronic polarization.  
(Set-3–May 2008)
27. Write notes on (i) Ferro electricity and (ii) Piezo electricity.  
(Set-1, Set-2, Set-3–May 2008)
28. Explain the following (i) Dielectric constant, (ii) Electric susceptibility, (iii) Electric polarization and (iv) Polarizability.  
(Set-1, Set-2–May 2008)

29. Explain the following: (i) Polarization vector and electric displacement. (Set-4–Sept. 2008)
30. Deduce an expression for Lorentz field relating to a dielectric material. (Set-4–Sept. 2008)
31. Explain the following: (i) Electric polarization and (ii) polarizability. (Set-1–Sept. 2008)
32. Describe the frequency dependence of dielectric constant.
33. Derive Clausius–Mosotti equation.
34. Explain the origin of different kinds of polarization.
35. Explain the ionic and orientation polarization.
36. Explain qualitatively frequency dependence of dielectric constant.
37. Explain the important requirements of insulators.
38. Explain the phenomenon of ferroelectricity with particular reference to barium titanate.
39. What is the frequency dependence of dielectric constant for a dielectric material?
40. Explain clearly the phenomenon of ferroelectricity.
41. Explain the theory of ferroelectricity and piezoelectricity.
42. State and explain the terms in Clausius–Mosotti relation.
43. Describe different types of polarization mechanisms.
44. What are important requirements of good insulating materials?
45. Write a note on piezoelectrics.
46. Write in detail various types of polarization in dielectrics and derive an expression for the orientational polarization at a specified temperature.
47. Derive an expression for the internal electric field in dielectrics exposed to a external electric field  $E$ .
48. Derive Clausius–Mosotti equation of dielectrics and explain the concept of complex dielectric constant.
49. Explain local field. Derive the expression for internal field for solids.
50. Arrive at the relation between the dielectric constant and atomic polarizability.
51. Obtain Clausius–Mosotti equation and explain how it can be used to determine the dipole moment of a polar molecule.
52. How does the total polarizability depend on frequency?
53. Explain piezoelectricity.
54. Derive the expression for dipolar polarizability.
55. Explain electronic polarization. Derive the expression for electronic polarizability.
56. Explain ferroelectricity. Mention its applications.

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## CHAPTER

# 7

## Magnetic Properties

### 7.1 Magnetic permeability

Magnetic permeability represents the ease with which a material allows magnetic force of lines to pass through it. The permeability of vacuum or free space is denoted by  $\mu_0$  and it is taken as the standard with respect to this the permeability of all materials is expressed. The permeability of the medium of a material is denoted as  $\mu$ ; it is the product of the permeability of free space ( $\mu_0$ ) and relative permeability ( $\mu_r$ ).

$$\therefore \mu = \mu_r \mu_0 \text{ H/M}$$

$\mu_r$  is purely a number; it has no units. The permeability of free space is:

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/M}$$

Let  $B$  be the magnetic flux density in a magnetic material by applying magnetic field of intensity  $H$  and  $B_0$  be the flux density at the same place if the material is removed [i.e., in air or vacuum]. Then,  $B_0 \propto H$

$$B_0 = \mu_0 H \quad \text{(7.1)}$$

$$\text{Similarly, } B = \mu H \quad \text{(7.2)}$$

Dividing Equation (7.2) by Equation (7.1)

$$\frac{B}{B_0} = \frac{\mu}{\mu_0} = \mu_r \quad \text{(7.3)}$$

Therefore, the relative magnetic permeability of a material is defined as the ratio of magnetic flux density [or magnetic induction] in a material to that in vacuum under the same applied magnetic field. The magnetic induction is the magnetic flux over unit area of a surface held normal to the flux. It is denoted by  $B$  and its SI unit is Tesla [Tesla = Wb/m<sup>2</sup>]. The SI unit of magnetic field strength  $H$  is A/m and that of  $\mu$  is wb/A-m or H/m. The Maxwell's equations exhibit that the speed of light in a medium ( $V$ ) =  $\frac{1}{\sqrt{\mu\varepsilon}}$

In vacuum,  $C = \frac{1}{\sqrt{\mu_0 \epsilon_0}}$ , where  $\epsilon_0$  and  $\epsilon$  are the permittivity of free space and permittivity in a material medium respectively

## 7.2 Magnetization ( $M$ )

A magnetic material acquires magnetism in an applied magnetic field. The magnetization is due to the rotation of magnetic dipoles of atoms or molecules of the substance in the direction of the applied magnetic field. The magnetic dipole moment per unit volume of the material is called intensity of magnetization or simply magnetization ( $M$ ).

$$\therefore \text{Magnetization } (M) = \frac{\text{Magnetic dipole moment of material}}{\text{Volume of the material}} \text{ A/m}$$

The magnetic flux density or magnetic induction ( $B$ ) inside the material is directly proportional to the applied magnetic field ( $H$ ) on the material.

$$\text{i.e., } B \propto H \quad (\text{or}) \quad B = \mu H = \mu_0 \mu_r H \quad (7.4)$$

where  $\mu$  = magnetic permeability of the material, Equation (7.4) can be written as:

$$B = \mu_0 \mu_r H + \mu_0 H - \mu_0 H = \mu_0 H + \mu_0 H [\mu_r - 1] \quad (7.5)$$

The magnetic induction inside the material is due to the applied field  $H$  and due to magnetization  $M$  of the material.

$$\text{So, } B = \mu_0 (H + M) = \mu_0 H + \mu_0 M \quad (7.6)$$

Comparing Equations (7.5) and (7.6), we have:

$$M = H [\mu_r - 1] \quad (7.7)$$

Equation (7.5) indicates that the magnetic flux density in a magnetic material by applied magnetic field is equal to the sum of the effect on vacuum and that on the material. The ratio of magnetization ( $M$ ) to the applied magnetic field strength ( $H$ ) is called the magnetic susceptibility ( $\chi$ ) of the material.

$$\therefore \chi = \frac{M}{H}$$

Using Equation (7.7),  $\chi = \mu_r - 1$

## 7.3 Origin of magnetic moment—Bohr magneton—electron spin

We know that electric current through a conductor develops magnetic field around it or current through a coil of wire will act as a magnet. This informs that there is an intimate relation between electric current and magnetic field. Flow of electrons along a path constitute electric current. In all atoms, electrons are revolving around the

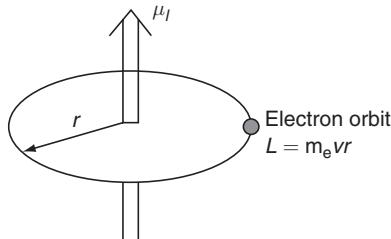
nucleus in different orbits. These revolving electrons constitute an electrical current in the orbits. These currents form magnetic dipoles. As electrons in an atom are revolving in different orbits that are randomly oriented, so the magnetic dipoles due to orbital motion of electrons are randomly oriented, results in zero magnetic dipole moment. The spin of orbital electrons and the spin of nucleus also contribute to the magnetic effects to an atom. Under an external applied magnetic field, these dipoles experience torque in the direction of the applied field and the atom acquires certain magnetism. Therefore, the magnetic dipole moment of an atom is due to the orbital motion of electrons, spin of electrons and spin of nucleus. We will study these contributions in detail separately.

### (i) Magnetic moment due to orbital motion of electrons and orbital angular momentum

As shown in Fig. 7.1, let an electron moving with a constant speed ' $v$ ' along a circular orbit of radius ' $r$ '. Let ' $T$ ' be the time taken to complete one revolution and  $-e$  be the charge on an electron. The charge that crosses any reference point in the orbit in unit time is  $\frac{-e}{T}$  and this is equal to current in the orbit. So, current in the orbit:

$$I = \frac{-e}{T} \quad \text{_____} \quad (7.8)$$

**Figure 7.1** Orbital angular momentum of an electron



The magnetic moment ( $\mu_l$ ) associated with the orbit due to orbital motion of electron is:

$$\mu_l = IA \quad \text{_____} \quad (7.9)$$

where  $A$  = area of the orbit =  $\pi r^2$

Equation (7.9) becomes:

$$\mu_l = \frac{-e\pi r^2}{T} \quad \text{_____} \quad (7.10)$$

$$\text{The angular velocity, } \omega = \frac{2\pi}{T} \quad (\text{or}) \quad T = \frac{2\pi}{\omega} \quad \text{_____} \quad (7.11)$$

Substituting Equation (7.11) in Equation (7.10), we have:

$$\mu_l = \frac{-e\pi r^2 \omega}{2\pi} = \frac{-er(r\omega)}{2} = \frac{-erv}{2} \quad \text{_____} \quad (7.12)$$

Since linear velocity ( $v$ ) =  $r\omega$

Multiplying and dividing Equation (7.12) with mass of electron,  $m_e$

$$\mu_l = \frac{-em_e vr}{2m_e} = \frac{-eL}{2m_e} \quad \text{_____ (7.13)}$$

where  $L$  = orbital angular momentum of the electron.

The negative sign in Equation (7.13) indicates that the angular momentum vector and magnetic momentum vector are in opposite direction. In quantum theory, the angular momentum is expressed as

$$L = l\hbar \quad \text{_____ (7.14)}$$

where  $l = 0, 1, 2, 3$ , etc. for s, p, d, f, etc. electrons and  $\hbar = \frac{\hbar}{2\pi}$ .

Substituting Equation (7.14) in Equation (7.13), we get:

$$\mu_l = \frac{-el\hbar}{2m_e} \quad \text{_____ (7.15)}$$

In the above equation, the quantity  $\frac{e\hbar}{2m_e}$  is an atomic unit called Bohr magneton represented as  $\mu_B$  and its value is equal to  $9.27 \times 10^{-24} \text{ A-m}^2$ .

$$\therefore \mu_l = -l\mu_B \quad \text{_____ (7.16)}$$

In many substances, the orbital magnetic moment of one electron in an atom gets cancelled by the orbital magnetic moment of other electron revolving in opposite direction in the same atom. Thus, the resultant magnetic dipole moment of an atom and in turn the substance is zero or very small.

## (ii) Magnetic moment due to spin of the electrons

In addition to orbital motion, the electrons spin around its own axis. The magnetic moment due to the spin of electrons is represented as  $\mu_s$ . This is analogous to Equation (7.13), in which orbital angular momentum is replaced by the spin angular momentum 'S' given by:

$$\mu_s = \gamma \left( \frac{e}{2m_e} \right) S \quad \text{_____ (7.17)}$$

where  $\gamma$  is called spin gyromagnetic ratio and it is defined as the ratio of the magnetic dipole moment to the angular momentum of an electron. The experimental value of  $\gamma$  for an electron is  $-2.0024$ . According to quantum theory, the spin angular momentum of an electron ( $S$ ) is  $S = \frac{1}{2}\hbar$ . The magnetic moment due to the spin of the electron is given by:

$$\mu_s = \gamma \left( \frac{e}{2m_e} \right) \frac{\hbar}{2} \quad \text{_____ (7.18)}$$

Substituting these values in the above equation:

$$\mu_s = 9.4 \times 10^{-24} \text{ A-m}^2$$

The magnetic moments due to the spin and the orbital motions of an electron are of the same order of magnitude.

If the atoms of a material consist of an even number of electrons, then the spin magnetic moments of pairs of electrons get cancelled due to the opposite spin. On the other hand, if the material consists of an odd number of electrons, then at least one electron remains unpaired and this leads to the magnetic moment of the atoms.

### (iii) Magnetic moment due to nuclear spin

Similar to electrons, the protons present in nucleus possess spin; the vectorial sum of all the protons spins is equal to the nuclear spin. The magnetic moment of a nucleus is expressed as nuclear magneton ( $\mu_n$ ) given as:

$$\mu_n = \left( \frac{e}{2m_p} \right) \hbar \quad \text{--- (7.19)}$$

where  $m_p$  = mass of a proton.

The value of  $\mu_n$  is equal to  $5.05 \times 10^{-27}$  A-m<sup>2</sup>. Since mass of a proton is nearly 2000 times heavier than an electron, so  $\mu_n$  is very small compared to  $\mu_B$  and it can be neglected. Therefore, the total magnetic moment of an atom will be mainly the vectorial sum of the orbital and spin magnetic moments of electrons.

## 7.4 Classification of magnetic materials

By the application of magnetic field, some materials will not show any effect that are called non-magnetic materials and those which show some effects are called magnetic materials. All magnetic materials magnetizes in an applied external magnetic field. Depending on the direction and magnitude of magnetization and also the effect of temperature on magnetic properties, all magnetic materials are classified into dia, para and ferromagnetic materials. Two more classes of materials have structure very close to ferromagnetic materials, but possess quite different magnetic properties. They are anti-ferromagnetic and ferrimagnetic materials. The properties of these materials are described below.

### (i) Diamagnetic material

Diamagnetic materials are repelled by the applied magnetic fields and they magnetize to a small extent in the opposite direction to that of an applied external magnetic field. The magnetic susceptibility is small and negative for these materials. Magnetic susceptibility represents the ease of magnetization of a substance and is equal to the ratio of magnetization of a material to the applied magnetic field. The relative permeability ( $\mu_r$ ) is less than 1 for these materials. Examples are gold, copper, silver, bismuth, lead, zinc and noble gases.

### (ii) Paramagnetic materials

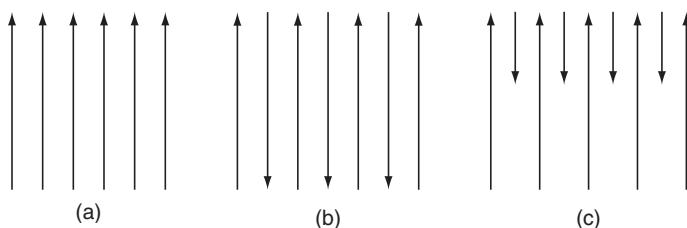
These materials are feebly attracted by external magnetic fields and they magnetize in the direction of the applied magnetic field. The magnetic susceptibility is small and positive. The relative permeability is greater than 1 for these materials. Paramagnetism is due to the spin and orbital motion of the electrons. Examples are aluminium, platinum, manganese chloride, salts of iron, nickel, tungsten and nitrogen.

### (iii) Ferromagnetic materials

These materials are strongly attracted by magnetic fields and they magnetize in the direction of the applied external magnetic field. The magnetic susceptibility is positive and large. The relative permeability is greater than 1 for these materials. The atoms or molecules of ferromagnetic materials have magnetic dipole moment due to the spin of the electrons. The permanent magnetic dipoles are all shown in Fig. 7.2(a). Examples are iron, cobalt, nickel and their alloys, Gadolinium and Dysprosium.

Figure 7.2

Magnetic dipole moments for adjacent atoms of (a) Ferro; (b) Antiferro and (c) Ferrimagnetic substances



### (iv) Anti-ferromagnetic materials

Antiferromagnetic materials show very little external magnetism. Magnetic susceptibility of these materials is positive and small. The atoms or molecules of anti-ferromagnetic materials possess magnetic dipole moment due to the spin of electrons. The magnetic dipole moments of adjacent atoms are anti-parallel as shown in Fig. 7.2(b). Due to the anti-parallel magnetic dipole moments, the magnetic effect of an anti-ferromagnetic material is zero, but possess magnetism due to temperature-dependent disruption of the magnetic moment alignment. Examples are copper chloride, oxides of manganese, cobalt and nickel.

### (v) Ferrimagnetic materials [Ferrites]

The magnetization of ferrimagnetic materials is intermediate to that of ferromagnetic and anti-ferromagnetic materials. The magnetic susceptibility is large and positive. The magnetic dipole moments of adjacent atoms or molecules of ferrimagnetic materials are anti-parallel and unequal in magnitude as shown in Fig. 7.2(c). This unequal magnetic dipole moments of adjacent atoms result in a net magnetization in the material. Examples are all ferrites have a general formula  $MOFe_2O_3$ , in which  $M$  stands for any divalent ion, for example copper, zinc, cadmium, iron, cobalt, nickel, etc.

## 7.5 Classical theory of diamagnetism [Langevin theory]

In this theory, we will obtain an expression for the change in magnetic moment of an orbiting electron in a diamagnetic atom and the induced magnetic moment per unit volume of diamagnetic material in the applied magnetic field  $B_0$ .

A revolving electron in an orbit constitutes electric current in the orbit. This electric current produces magnetic field perpendicular to the plane of the orbit. The electrons in an atom are revolving in different orbits, oriented in random directions. So, the sum of the magnetic moments produced by all these orbiting electrons in an atom is zero. Let the angular velocity of an electron in an orbit of radius ' $r$ ' is ' $\omega_0$ ' before applying magnetic field. The current in the orbit is  $I = (-e) \frac{\omega_0}{2\pi} = \frac{-e}{T} = \frac{-eV_0}{2\pi r} = \frac{-e\omega_0}{2\pi}$  [since  $V_0 = rw_0$ ].

The magnetic moment due to the orbiting electron

$$(\mu_i) = IA = \frac{-e\omega_0}{2\pi} (\pi r^2) = \frac{-e\omega_0 r^2}{2} \quad (7.20)$$

where  $A$  is the area inside the orbit. As shown in Figs. 7.3(a) and (b), the electrostatic force of attraction ( $F_e$ ) between a proton and an orbiting electron constitutes centripetal force on the electron and it is equal to

$$mr\omega_0^2 \left( = \frac{mv_0^2}{r} \right)$$

where  $v_0$  = linear velocity of the electron.

$$F_e = mr\omega_0^2 \quad (7.21)$$

After applying magnetic field  $B_0$ , an additional force  $F_B$  acts on the electron. Depending on the direction of the applied magnetic field and depending on the direction of rotation of electron, the force  $F_B$  either adds to  $F_e$  or reduces  $F_e$ . Let the centrifugal force after applying magnetic field be  $F (= mr\omega^2)$ , where  $\omega = \omega_0 \pm \Delta\omega$ ,  $\Delta\omega$  = change in the angular frequency of electron after applying magnetic field.

Then, we have:

$$F = F_e \pm F_B \quad (7.22)$$

The additional force is equal to:

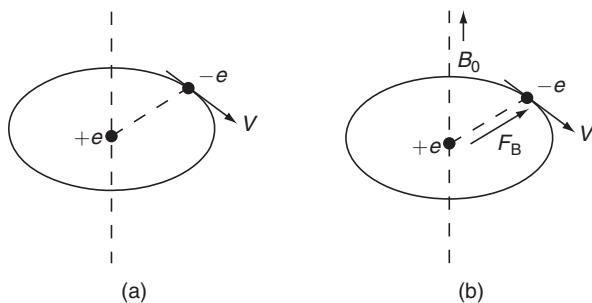
$$F_B = B_0 (-e) V = -B_0 er\omega \quad (7.23)$$

Equation (7.22) becomes:

$$mr\omega^2 = mr\omega_0^2 \pm B_0 er\omega$$

**Figure 7.3**

(a) Electron revolving in an orbit of radius ' $r$ ' around a proton in the absence of an external magnetic field; (b) Electron revolving in an orbit of radius ' $r$ ' around a proton in the presence of applied magnetic field  $B_0$



$$m\omega^2 = m\omega_0^2 \pm B_0 e\omega$$

or:

$$\omega^2 \pm \frac{B_0 e \omega}{m} - \omega_0^2 = 0 \quad \text{_____} \quad (7.24)$$

$$(\omega_0 + \Delta\omega)^2 \pm \frac{B_0 e}{m} (\omega_0 + \Delta\omega) - \omega_0^2 = 0 \quad [\text{taking } \omega \approx \omega_0 + \Delta\omega]$$

$$\omega_0^2 + \Delta\omega^2 + 2\omega_0\Delta\omega \pm \frac{B_0 e}{m} \omega_0 - \omega_0^2 = 0 \quad [\text{since } \Delta\omega \ll \omega_0]$$

Neglecting  $\Delta\omega^2$ , we have:

$$\Delta\omega = \pm \frac{B_0 e}{2m} \quad \text{_____} \quad (7.25)$$

The change in magnetic moment ( $\Delta\mu_i$ ) for the change in angular frequency ( $\Delta\omega$ ) is obtained using Equations (7.20) and (7.25)

$$\Delta\mu_i = \frac{-er^2}{2} \Delta\omega = \frac{-1}{2} er^2 \frac{B_0 e}{2m} = \frac{-e^2 r^2 B_0}{4m} \quad \text{_____} \quad (7.26)$$

The induced dipole moment has a direction opposite to the applied magnetic field. The magnetic moment induced when a pair of electrons have opposite rotation is:

$$(\mu_i - \Delta\mu_i) + (-\mu_i - \Delta\mu_i) = -2\Delta\mu_i \quad \text{_____} \quad (7.27)$$

This induced magnetic moment is in the opposite direction to  $B_0$ . This is the property of a diamagnetic material. Diamagnetic atoms have more than one electron and the orbits are also not circular. Suppose  $r_x$ ,  $r_y$  and  $r_z$  are the average values of radii of all electrons along three directions, then radius of the atom ( $r_0$ ) is:

$$r_0^2 = r_x^2 + r_y^2 + r_z^2 \quad \text{also if} \quad r_x^2 = r_y^2 = r_z^2 = \frac{r_0^2}{3}$$

The average radius of the orbit

$$r^2 = r_x^2 + r_y^2 = \frac{2}{3} r_0^2 \quad \text{_____} \quad (7.28)$$

Suppose the diamagnetic substance contains  $N$  atoms per unit volume and each atom has  $Z$  electrons, then the induced magnetic moment per unit volume ( $\mu_{\text{ind}}$ ) is:

$$\mu_{\text{ind}} = + NZ\Delta\mu_i = \frac{-NZe^2 \left(\frac{2}{3}\right) r_0^2 B_0}{4m} = \frac{-NZe^2 r_0^2 B_0}{6m} \quad \text{_____} \quad (7.29)$$

since  $B_0 = \mu_0 H$

$$\text{So, } \mu_{\text{ind}} = \frac{-NZ\mu_0 e^2 r_0^2 H}{6m} \quad (7.30)$$

$$\text{The atomic susceptibility, } \chi = \frac{\mu_{\text{ind}}}{H} = \frac{-NZ\mu_0 e^2 r_0^2}{6m} \quad (7.31)$$

The value of  $\chi$  is of the order of  $10^{-6}$ .

## 7.6 Theory of paramagnetism

The atoms of paramagnetic material possess permanent magnetic moment. In the absence of an applied external magnetic field, the magnetic dipoles of paramagnetic atoms are oriented in random directions, so that there is no resultant magnetism of the material. By applying an external magnetic field on a paramagnetic material, the dipoles are rotated by different extents proportional to the strength of field in the direction of the applied magnetic field, so that the material acquires magnetism.

To calculate magnetic susceptibility, we consider  $N$  number of magnetic dipoles per unit volume of material of which  $N_p$  dipoles are parallel to the applied field and  $N_a$  dipoles are anti-parallel when a magnetic field  $H$  applied at temperature  $TK$ .

$$\begin{aligned} \text{The net magnetization of the material, } M &= N_p \mu_B - N_a \mu_B \\ &= (N_p - N_a) \mu_B \end{aligned} \quad (7.32)$$

$$\text{where } \mu_B = \text{Bohr magneton} = \frac{e\hbar}{2m}$$

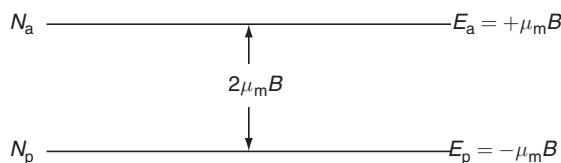
$$\text{Also the magnetic susceptibility } \chi = (\mu_r - 1) = \frac{M}{H} \quad (7.33)$$

The torque ( $\tau$ ) experienced in the applied magnetic field is:

$$\tau = \mu_m B = \mu_0 \mu_m H \quad (7.34)$$

where  $\mu_m$  is the moment of magnetic dipole. Figure (7.4) shows the energy difference between parallel and anti-parallel spin dipoles.

**Figure 7.4 Energy difference between parallel and anti-parallel magnetic dipoles**



Consider the energy  $\theta$  of a dipole is zero when it is perpendicular to the field. The energy of dipole when it makes an angle  $\theta$  to the field is:

$$E = \int_{90^\circ}^{\theta} \mu_0 \mu_m H \sin \theta d\theta = -H \mu_0 \mu_m \cos \theta$$

Energy of anti-parallel dipole is obtained by putting  $\theta = 180^\circ$

$$\text{i.e., } E_a = \mu_0 \mu_m H$$

Similarly, energy of parallel dipole is obtained by putting  $\theta = 0^\circ$

$$\text{i.e., } E_p = -\mu_0 \mu_m H$$

$$E_a - E_p = 2\mu_0 \mu_m H \quad \dots \quad (7.35)$$

For a single spin moment,  $\mu_m = \mu_B$

$$\text{So, } E_a - E_p = 2\mu_0 \mu_B H \quad \dots \quad (7.36)$$

Using Boltzmann statistics, the ratio  $\frac{N_a}{N_p}$  is given by:

$$\frac{N_a}{N_p} = \exp \left[ (E_p - E_a) / K_B T \right]$$

Using Equation (7.36)

$$\begin{aligned} \frac{N_a}{N_p} &= \exp \left[ -2\mu_0 \mu_B H / K_B T \right] \\ &= \exp(-2\alpha), \quad \text{where} \quad \alpha = \mu_0 \mu_B H / K_B T \end{aligned}$$

To obtain  $N_a$  and  $N_p$  separately in terms of  $N$ , consider:

$$1 + \frac{N_a}{N_p} = \frac{N_a + N_p}{N_p} = \frac{N}{N_p}$$

$$\text{Hence, } \frac{N}{N_p} = 1 + \exp(-2\alpha)$$

$$\text{or } N_p = \frac{N}{1 + \exp(-2\alpha)} = \frac{N \exp(\alpha)}{\exp(\alpha) + \exp(-\alpha)} \quad \dots \quad (7.37)$$

Similarly,

$$N_a = \frac{N \exp(-\alpha)}{\exp(\alpha) + \exp(-\alpha)} \quad \dots \quad (7.38)$$

Hence,

$$N_p - N_a = N \frac{\exp(\alpha) - \exp(-\alpha)}{\exp(\alpha) + \exp(-\alpha)} = N \tan h(\alpha) \quad (7.39)$$

Substituting the above equation in Equation (7.32), we have:

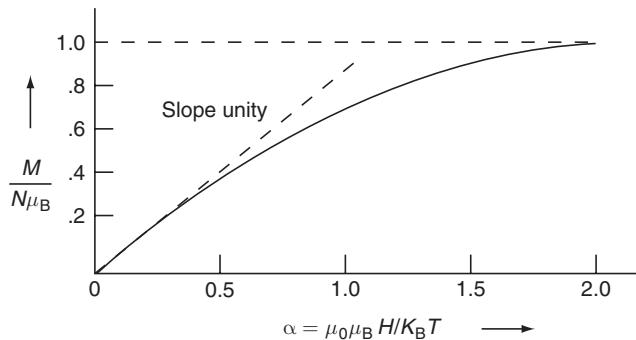
$$\text{The net magnetization } M = (N_p - N_a) \mu_B = N \mu_B \tan h \alpha \quad (7.40)$$

where  $\alpha = \mu_0 \mu_B H / K_B T$

In Fig. 7.5,  $\frac{M}{N \mu_B}$  is plotted against the variable,  $\alpha$

**Figure 7.5**

**The solid curve represents  $M/N \mu_B$  as a function of  $\alpha = \mu_0 \mu_B H / K_B T$ . A dotted line through the origin of slope unity corresponds to  $\alpha \ll 1$ ,  $\tan h(\alpha) \cong \alpha$**



$\alpha = \mu_0 \mu_B H / K_B T$  for  $\alpha \ll 1$ ,  $\tan h(\alpha) \cong \alpha$  and for  $\alpha \gg 1$ ,  $\tan h(\alpha)$  approaches unity. So, for strong fields at low temperatures, the magnetization approaches  $N \mu_B$  i.e., the dipoles are aligned parallel to the applied field. For low field at normal temperatures,  $\mu_0 \mu_B H \ll K_B T$ , under these conditions  $\alpha \ll 1$  so  $\tan h(\alpha) \cong \alpha$ .

$$\text{Hence, } M \cong N \mu_0 \mu_B^2 H / K_B T \quad \text{for} \quad \mu_0 \mu_B H \ll K_B T \quad (7.41)$$

$$\chi = \frac{M}{H} = (\mu_r - 1) = \frac{N \mu_0 \mu_B^2}{K_B T} = \frac{C}{T} \quad (7.42)$$

where  $C = \frac{N \mu_0 \mu_B^2}{K_B}$  = Curie constant

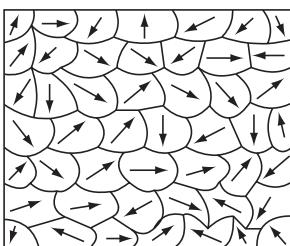
Hence, we find that the susceptibility varies as  $\frac{1}{T}$ .

The above equation is known as Curie law of paramagnetism.

## 7.7 Domain theory of ferromagnetism

In 1907, Weiss proposed domain theory to explain ferromagnetism. According to this theory, a single crystal of ferromagnetic solid compresses a large number of small regions, and each region is spontaneously magnetized to saturation extent called a domain as shown in Fig. 7.6. The domain size may vary from  $10^{-6}$  to the entire volume of the crystal. The spin magnetic moments of all the atoms in a domain are oriented in a particular direction. The magnetization directions of different domains of the specimen are random so that the resultant magnetization of the material is zero in the absence of an external magnetic field. These domains arise because the energy is not minimum when a large specimen has a uniform magnetization.

**Figure 7.6 Ferromagnetic domains**



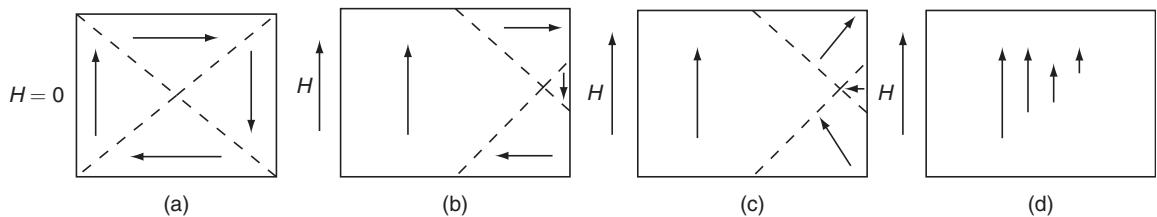
A ferromagnetic material magnetizes when an external magnetic field is applied. The individual domains contribute to the total magnetization,  $M$ , of the specimen. Becker suggested two independent processes by which magnetization of the specimen takes place. They are: (i) the domains that are parallel or nearly parallel to the direction of applied magnetic field will grow in size at the cost of other domains and (ii) the magnetic moments of the domains can rotate in the direction of applied field. A symbolic representation of the response of the domains to the magnetic field is shown in Fig. 7.7.

By the applied magnetic field, either domain wall moments or rotation of domains magnetic moments or both depending on the strength of the applied magnetic field takes place.

If weak magnetic field is applied on a ferromagnetic material, then the domains of the material whose magnetic moments are parallel or nearly parallel to the direction of applied field will expand in size whereas the domains in which magnetic moments are unfavourably oriented to the applied field will diminish in size as shown in Fig. 7.7(b). This change produces large magnetization for the bulk material.

**Figure 7.7**

**(a) Domain orientation in the absence of magnetic field; (b) Domain enhancement shrinkage due to weak fields; (c) Domain rotation due to strong fields; (d) Saturation due to very high fields**



Application of higher magnetic fields rotates [twists] partially the domain's magnetic moments in the direction of the magnetic field as shown in Fig. 7.7(c). This results in further increase in the magnetization of the bulk material.

Application of very strong magnetic fields on a ferromagnetic material results in required amount of rotation of magnetic moments so as to align parallel to the applied field as shown in Fig. 7.7(d). This is the highest magnetization of the material called saturated magnetization.

## Effect of temperature

The Curie-Weiss law for magnetic susceptibility for ferromagnetic substance is:

$$\chi = \frac{C}{T - \theta}$$

where  $C$  = Curie constant,  $\theta$  = Curie temperature and  $T$  is the temperature of the ferromagnetic material. Here, ' $\theta$ ' represents the tendency towards alignment of the dipole moments and on the other hand  $T$  represents the tendency of random orientation of dipoles due to thermal agitation. For  $T > \theta$ , the thermal agitation is predominant; so, the substance is paramagnetic. As the temperature ( $T$ ) is lowered and if comparable to  $\theta$ , the spin-exchange interaction begins. The temperature at which the spontaneous magnetization sets in is called the Curie temperature.

For all temperatures,  $T < \theta$ , the material behaves as ferromagnetic.

## Experimental evidences for domain structure

One experimental evidence for the existence of magnetic domains was given by Bitter from magnetic powder pattern microphotographs of domain boundaries. In this method, a drop of colloidal solution of ethyl acetate containing a fine powder of magnetic material such as magnetite is put on a carefully prepared [clean and plane] surface of ferromagnetic material. This drop spreads on the surface. When this is observed under the microscope, it is found that the magnetite particles in the suspension are moved and highly concentrated along certain well-defined lines. The ethyl acetate evaporates leaving the particles alone. The magnetite particles are attracted to the lines due to the local inhomogeneity of magnetic field, and the lines indicate change in the magnetic field direction of material. The non-uniformity of magnetite particles on the surface indicates that the material is magnetized in different directions at different regions; such a type of each region is called a domain. This can be photographed. If there are no such domains or the complete material is a single domain, then the magnetization would be uniform all over the surface and no concentration of particles would occur.

Fowler and Fryer described another technique for the existence of magnetic domains. This is described in the following way. The surface of a ferromagnetic material is illuminated with polarized light and viewed through an analyser. The surface appears with areas of different intensity, due to the existence of domains. This can be explained with Kerr magneto-optical effect.

When plane polarized light [electromagnetic waves] incident on the surface of ferromagnetic material, they interact with the magnetic field present at different regions on the surface of material and the plane of polarization is rotated on reflection by different extents at different regions on the surface. Due to the differences in the intensity and direction of magnetic field at different regions, the reflected light appears non-uniform. This confirms the existence of domains.

## Origin of [Ferromagnetic] domains

In free state, all physical systems attain minimum energy and that is the condition for stability. On this basis, one can conclude that domains exist in ferromagnetic materials to minimize the total energy of the substance. The total energy of a ferromagnetic solid consists of exchange energy, magnetic field energy, anisotropy energy, domain wall energy and magnetostrictive energy. These energies are described below:

### (a) Exchange energy

This is represented as  $E_{\text{ex}} = -2J_e \sum S_i S_j$ , where  $J_e$  = total angular momentum quantum number of an electron,  $S_i$  and  $S_j$  are the spin quantum number of  $i$ th and  $j$ th electrons. This energy is minimum when the spins are parallel.

### (b) Magnetic field energy

The magnetic poles formed at the ends of the magnetized specimen produces an external magnetic field. If  $H$  is the intensity of magnetic field in a small volume  $dV$ , then the magnetic field energy in that volume is  $\frac{1}{8\pi} H^2 dV$ . Around the specimen, the intensity of field will be different at different regions. The complete field energy is represented by integration as  $\frac{1}{8\pi} \int H^2 dV$ .

### (c) Anisotropy energy

It was experimentally found that much higher fields are required to produce saturated magnetization along certain directions than some other directions in ferromagnetic crystals. They are called hard and easy directions of magnetizations in the crystal. The excess of magnetic field energy required to saturate magnetize the specimen in a direction over that of an easy direction of magnetization is called anisotropy energy in that direction of magnetization. For example, in BCC iron, much higher fields are required to twist the domains to produce saturation magnetization along [111] direction than that of [100] direction. So, [100] direction is the easy direction and that of [111] direction is the hard direction of magnetization in BCC iron. The anisotropy energy is of the order of  $10^5$  erg/cm<sup>3</sup>. In nickel, [111] direction is the easy and [100] direction is the hard direction of magnetization. The anisotropy energy is of  $10^4$  erg/cm<sup>3</sup>. In cobalt, hexagonal crystal axis is the easy direction and [100] is the hard direction of magnetization, and its anisotropy energy is  $10^6$  erg/cm<sup>3</sup>.

### (d) Domain wall [or Bloch wall] energy

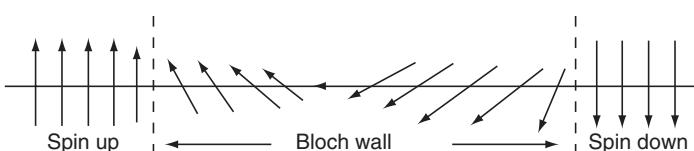
We know that different domains of a ferromagnetic material magnetizes in different directions. As we go from one domain to its neighbouring domain, the spin [or magnetization] direction does not change abruptly but changes gradually over many atomic planes as shown in Fig. (7.8). So, the spin-exchange energy is lower than when a change occurs abruptly to the same extent. Usually, the domain wall thickness varies from 200 to 300 lattice constants.

### (e) Magnetostrictive energy

The change in dimensions of a material on magnetization is called magetostriction. The work done by the magnetic field to produce magnetostriction is stored as energy in the material called energy of magnetostriction or magnetoelastic energy. If the lattice is not strained, then this energy will be zero.

**Figure 7.8**

Shows the change in spin magnetic moment in the domain wall between two domains

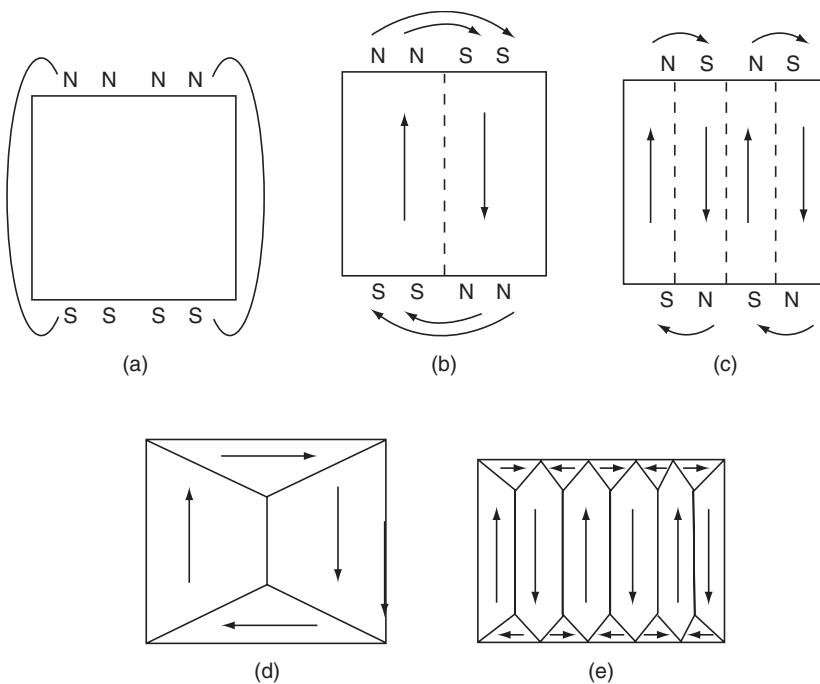


## Explanation for origin of domains

Explanation for the origin of domains is given based on minimization of all the above energies. Suppose the material is magnetized in an easy direction of magnetization so that the anisotropic energy is minimum and let the spin magnetic moments of atoms are parallel so that the exchange energy is minimum and the material compresses as a single domain shown in Fig. 7.9(a). Magnetic poles will be developed at the free ends of the specimen and produce external magnetic fields so that magnetic field energy will be high. To reduce this field energy, let the domain will be sub-divided into two equal domains such that opposite poles at the same end as shown in Fig. 7.9(b), so that field is confined only to a small region near the sample end and magnetic field energy would be reduced to one-half of its previous value. This configuration is at lower energy state than the previous one as shown in Fig. 7.9(c). This process of division leads to lowering of field energy. When the sub-division increases, then the domain wall area and hence the domain wall energy increases. The process of sub-division will be continued [up to  $n$ -domains so that the magnetic field energy is reduced to  $(1/n)^{th}$  of its initial value] up to a stage at which the decreases in magnetic field energy are equal to the increase in domain wall energy. This is the minimum energy state. With further sub-division, the increase in domain wall energy exceeds the decrease in magnetic field energy. This will not happen because this violates minimum energy configuration. Although the magnetic field energy is reduced considerably by the sub-division, but it is not equal to zero.

There is an arrangement shown in Fig. 7.9(d) for which the magnetic field energy is zero. In this configuration, the magnetization is continuous inside the material so that no free poles are formed anywhere in the material. There is no external magnetic field associated with the magnetization and the magnetic field energy

**Figure 7.9 Shows the origin of magnetic domains**



is zero in this case. During the formation of this configuration, the dimensions of the material are changed and this is associated with magnetostrictive strain energy. For example, iron on magnetization, expands in the direction of magnetization and contracts laterally so that the volume remains constant.

The magnetostrictive strain energy can be reduced by reducing the size of strain-producing horizontal domains as shown in Fig. 7.9(e). In this configuration, the number of vertical domains increases and also subdivision will be continued until the decrease in magnetostrictive strain energy is compensated by the increase in domain wall energy.

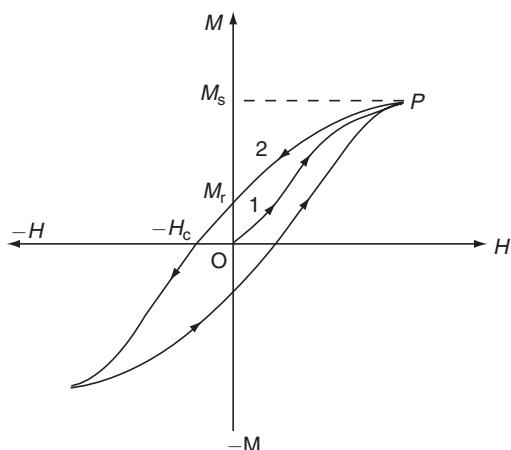
## 7.8 Hysteresis curve

Hysteresis means retardation or lagging of an effect behind the cause of the effect. In magnetism, hysteresis has been used between the applied magnetic field ( $H$ ) and magnetization ( $M$ ) of a magnetic material. Here, the effect is magnetization of a material and the cause of magnetization is the applied magnetic field. Usually, in magnetic materials, the magnetization of a material lags behind the applied magnetic field. This can be explained in detail, in the following way:

We start with an unmagnetized ( $M = 0$ ) ferromagnetic specimen. With an increasing applied magnetic field on it, the magnetization of the specimen increases from zero to high values. The increase is non-linear. With small applied fields, the domains pointing approximately in the field direction increase at the expense of those that are not. In other words, their boundaries move so as to expand the favourable domains. This gives rise to a small magnetization corresponding to the initial portion of the hysteresis curve shown in Fig. 7.10.

With somewhat higher fields, the magnetization increases rapidly with  $H$ . At these field strengths, the boundary moments are often large and irreversible. i.e., the boundaries do not go back into their original position on reducing  $H$ . Application of still higher fields, rotates (twists) the magnetization vectors in to the field direction. i.e., all the domains point in the direction of  $H$ , then the specimen is said to be saturated magnetized ( $M = M_s$ ). The saturated magnetization is represented as point 'P' in Fig. 7.10. If the field is decreased, then the magnetization decreases below the value  $M_s$ , but this decrease of  $M$  does not occur along the same

**Figure 7.10** Hysteresis curve



path (curve 1), because the domains do not easily return to the original random arrangement. As  $H$  is reduced to zero,  $M$  does not decrease in phase but lags behind  $H$ . The value of  $M$  that remains in the material when  $H$  is reduced to zero is called residual magnetization or remanence magnetism ( $M_r$ ).

To remove the residual magnetism in the material, magnetic field is applied in the opposite direction and gradually increased from zero. The magnetization in the material becomes zero for an applied magnetic field of  $-H_c$ , called coercive field for the material. Further increase of the applied magnetic field in the opposite direction results in the material magnetization in the opposite direction. Again decreasing the magnetic field in the opposite direction to zero results in the residual magnetism in opposite direction. Again increasing magnetic field in the forward direction, we will get a curve that completes a closed loop called hysteresis loop. This loop includes some area. This area indicates the amount of energy wasted in one cycle of operation.

## 7.9 Anti-ferromagnetic substances

Anti-ferromagnetism arises when the spin magnetic moments of neighbouring atoms of the crystal are anti-parallel so that the spin magnetic moments of alternate atoms are parallel. Because of opposite spin moments, we consider an anti-ferromagnetic crystal consists of two different types of atoms i.e., say A-type atoms and B-type atoms. The crystal structure consists of interpenetration of two cubic sublattices, one of with A atoms and the other with B atoms. One sub-lattice spontaneously magnetized in one direction and the other in opposite direction. One may therefore suggests the BCC structure for an anti-ferromagnetic crystal with A atoms occupying the corner points and B atoms at the centre of the cubes as shown in Fig. 7.11. Examples are MnO, NiO, FeO, CoO, MnS, etc.

In the absence of an external applied magnetic field, the magnetization of anti-ferro magnetic specimen will be zero, because of anti-parallel and equal spin magnetic moments. By the application of the external magnetic field, a small magnetization in the direction of the applied magnetic field takes place. This magnetization varies with temperature as shown in Fig. 7.12. The susceptibility increases with an increase of temperature up to  $T_N$ , called the Neel temperature, at Neel temperature the magnetization (or susceptibility) is maximum and above it the magnetization decreases with an increasing temperature, confirming the relation  $\chi = \frac{C}{T + \theta}$ , where  $C$  = Curie constant and  $\theta$  is paramagnetic Curie temperature. The decrease of

Figure 7.11

Opposite magnetic moments of A-type and B-type atoms in the unit cell of antiferromagnetic substance

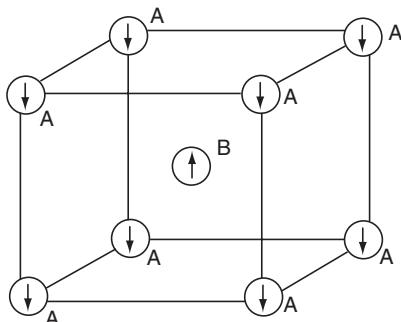
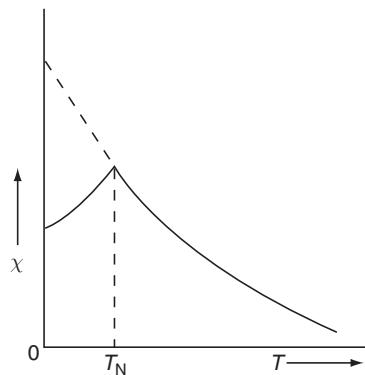


Figure 7.12

Shows the variation of magnetic susceptibility ( $\chi$ ) of antiferromagnetic substance with temperature



magnetization with an increase of temperature is a property of the paramagnetic substances; therefore, the specimen becomes paramagnetic above  $T_N$ .

The variation of magnetic susceptibility with temperature for para, ferro and anti-ferro magnetic materials is shown in Fig. 7.13. In this diagram, a graph has been plotted between  $\frac{1}{\chi}$  versus temperature. For the above materials, the susceptibilities can be expressed as:

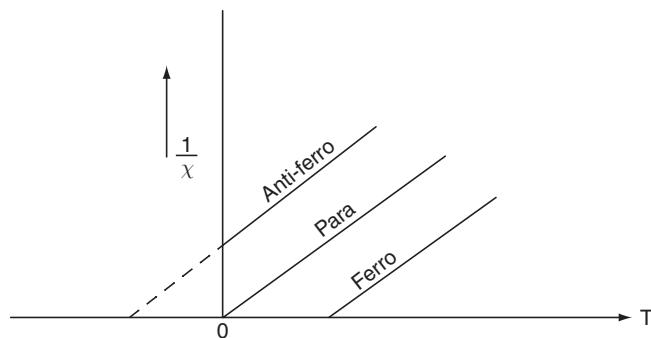
$$\chi = \frac{C}{T} \text{ for paramagnetic}$$

$$\chi = \frac{C}{T - \theta} \text{ for ferromagnetic}$$

and  $\chi = \frac{C}{T + \theta}$  for anti-ferromagnetic materials.

Figure 7.13

Shows the variation of susceptibility with temperature for para, ferro and antiferromagnetic materials



## 7.10 Ferrimagnetic substances [Ferrites]

In ferrimagnetic crystals, the magnetization of two sublattices occurs as the one in anti-ferromagnetic crystals but of unequal magnitudes, which results a non-zero value. The ferrimagnetic crystals consist of two or more different kinds of atoms. Chemically, they are expressed as  $M_e^{++} Fe_2^{+++} O_4^{-}$ , where  $M_e^{++}$  stands for a suitable divalent metal ion such as  $Fe^{++}$ ,  $Co^{++}$ ,  $Ni^{++}$ ,  $Mg^{++}$ ,  $Mn^{++}$ ,  $Zn^{++}$ ,  $Cd^{++}$ , etc. The  $Fe_2^{+++}$  is a trivalent ferric ion. If we insert  $Ni^{++}$  for  $Me^{++}$ , then the compound would be called as nickel ferrite, if  $Fe^{++}$  is inserted for  $Me^{++}$ , then the compound is ferrous ferrite, written as  $Fe^{++} Fe_2^{+++} O_4^{-}$  or in more familiar form as  $Fe_3 O_4$ .

X-ray crystallography reveals that usually ferrite oxygens have FCC structure with tetrahedral and octahedral interstitial spaces. The tetrahedral space is surrounded by four oxygens and octahedral space is surrounded by six oxygens. These sites are denoted as A-sites and B-sites, respectively. The divalent and trivalent metal ions occupy these spaces. The arrangement of cations in these spaces shows the magnetic properties of these materials.

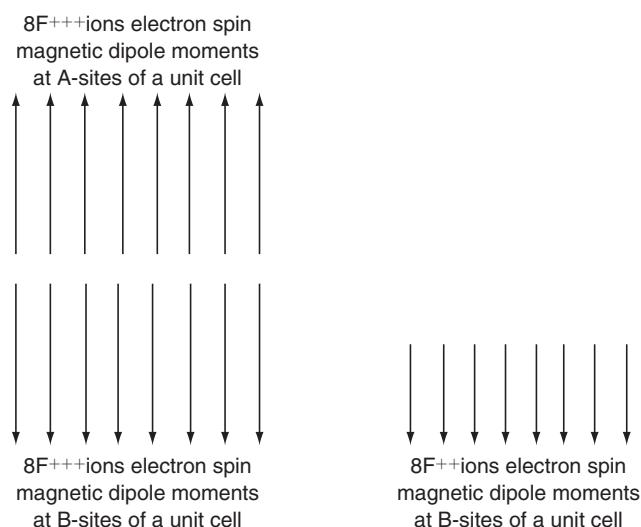
The magnetization of ferrimagnetic materials can be understood by taking one of the material as an example say, ferrous ferrite  $[Fe^{++} Fe_2^{+++} O_4^{-}]$ . This is a natural ferrite called magnetite.

The saturated magnetization of a ferrous ferrite molecule is explained as follows: saturated magnetization can be calculated from the number of unpaired electron spins of the  $Fe^{++}$  and  $Fe^{+++}$  ions.  $Fe^{++}$  ion has six 3d electrons, of which four have unpaired spins and  $Fe^{+++}$  ion has five unpaired electron spins. Assuming all the spins are parallel, we expect a saturated magnetic moment of  $[4 + 2 \times 5] \mu_B = 14 \mu_B$  per molecule of magnetite. Whereas experimental value is  $4.08 \mu_B$  per molecule, so we rule out the parallelism of all the electron spins in a molecule. We may conclude that half of the  $Fe^{+++}$  ion electron spins are in one direction and the remaining  $Fe^{+++}$  and  $Fe^{++}$  ion electron spins are in the opposite direction so that the magnetic moment per molecule of ferrous ferrite is  $4\mu_B$ . This is in agreement with the experimental value.

The magnetization in the unit cell of ferrous ferrite is explained in the following way: The unit cell contains 8 molecules of ferrous ferrite or 32 divalent oxygens, 16 trivalent iron ions and 8 divalent iron ions. There are 8 tetrahedral voids called A-sites and 16 octahedral voids called B-sites. In magnetite, 8  $Fe^{+++}$  ions occupy all the A-sites and the remaining 8  $Fe^{+++}$  and 8  $Fe^{++}$  ions occupy B-sites. Figure 7.14 represents the magnetic

Figure 7.14

Shows the magnetic dipole moments of ferric and ferrous ions in the unit cell of ferrous ferrite



dipole moments of ferric and ferrous ions in the unit cell. Each arrow represents the magnetic dipole moment of a ion. With this arrangement, the  $\text{Fe}^{+++}$  ion contribution to the magnetic moment vanishes completely and the net magnetic moment is due to  $\text{Fe}^{++}$  ions only and equal to  $4\mu_B$  per molecule.

## 7.11 Soft and hard magnetic materials

During the process of magnetization, the domain wall moment takes place so that the favourably oriented domains increase in size and unfavourably oriented domains shrink.

Based on the resistance to the moment of domain walls by the applied magnetic field, the area inside the hysteresis loop and on some other properties, the magnetic materials are divided into soft and hard magnetic materials. Now, we shall discuss these materials separately.

### (a) Soft magnetic materials

The resistance to the moment of domain walls is less and it is easy to magnetize. The soft magnetic materials are characterized by: (i) low remanent magnetization, (ii) low coercivity, (iii) low hysteresis losses, (iv) high magnetic permeability and (v) high susceptibility so that they can be magnetized and demagnetized easily.

The most widely used soft magnetic materials are: (1) pure iron, (2) alloys of iron-silicon, (3) iron-cobalt, (4) iron-nickel (permalloy) often other alloying elements are added. Some other substances are: (5) mumetal (alloy of Ni, Cu, Cr & Fe) and (6) amorphous ferrous alloys (alloys of Fe, Si & B).

Now, we see the applications of various soft magnetic materials:

- (1) pure iron is frequently used as the magnetic core for direct current (DC) applications.
- (2) iron-silicon alloys containing up to 5% silica possess high electrical resistivity and high magnetic permeability and are used as core materials for AC current machinery. Eddy current losses could be minimized using iron-silicon alloys. They are used for low-frequency and high-power applications.
- (3) Iron-nickel alloys are used for audio frequency applications. In iron-nickel alloys, nickel composition may vary from 35 to nearly 100%. Generally, the permeability increases with an increase of nickel content. Maximum permeability is obtained for 79% of nickel and the rest iron. The alloy containing 79% Ni, 15% Fe, 5% Mo and 0.5% Mn is known as supermalloy that possesses very high permeability.
- (4) Iron-cobalt alloys have very high magnetic saturation than either iron or cobalt; maximum saturation is obtained for a composition of about 35 to 50% of cobalt.
- (5) Soft magnetic materials are also used in magnetic amplifiers, magnetic switching circuits and the other applications under alternate magnetic fields.

### (b) Hard magnetic materials

The resistance to the moment of the magnetic domain walls is large. The causes for such a nature are also due to the presence of impurities of non-magnetic materials or the lattice imperfections. The presence of defects increases the mechanical hardness to the material and an increase the electrical resistivity and reduces eddy current losses. Hard magnetic materials are characterized by: (i) high remanent magnetization, (ii) high coercivity, (iii) high saturation flux density, (iv) low permeability and (v) high hysteresis loss.

Most widely used permanent magnetic materials are low alloy steels containing 0.6% to 1% carbon. Other materials are: (1) alnico [alloy of Al, Ni, Co, Cu and Fe], (2) tungsten steel alloy, (3) platinum-cobalt alloy and (4) invar, etc.

Hard magnetic materials are used to prepare permanent magnets. Most of them are manufactured from alloys of steel with tungsten and chromium. The permanent magnets are used in magnetic separators, magnetic detectors, in speakers used in audio systems and microphones. Hard magnets made of carbon steel find application in the making of magnets for toys and certain types of measuring meters because of its low cost.

## Comparison between soft and hard magnetic materials

Soft Magnetic Materials	Hard Magnetic Materials
1. Small amount of magnetic field is sufficient to saturately magnetise the material. Since the resistance for the moment of domains is less	1. Large amount of magnetic field is required for saturated magnetization. Since the resistance for the moment of domain is large.
2. Hysteresis loss is less so the area inside the hysteresis loop is less for soft magnetic materials.	2. Hysteresis loss is large so the area inside the hysteresis loop is more for hard magnetic materials.
3. Coercivity and retentivity is less so, the material can be magnetized and demagnetized easily.	3. Coercivity and retentivity is large so, the material can not be easily magnetized and demagnetized.
4. In these materials the magnetic permeability and magnetic susceptibility is large.	4. These materials possess low values of magnetic permeability and magnetic susceptibility.
5. Soft magnetic materials are used in the preparation of magnetic core materials used in transformers, electric motors, magnetic amplifiers, magnetic switching circuits, etc.	5. Hard magnetic materials are used in the preparation of permanent magnets. They are used in loud speakers, toys, in measuring meters, microphones, magnetic detectors, magnetic separators, etc.,

## 7.12 Applications of ferrites

The various applications are described below:

- (1) Ferrites are used in thermal sensing switches used in refrigerators, air conditioners, electronic ovens, etc.
- (2) The magnetostrictive property of ferrites is utilized in producing ultrasonic waves from a ferrite rod by the application of an alternating magnetic field.
- (3) The insulating property of ferrites finds their use in electric motors; they are also used as flat rings for loud speakers, wind screen wiper motors and correction magnets for TV.
- (4) Some ferrites possess high rectangular hysteresis loop, so they are useful in the construction of computer memory system for rapid storage and retrieval of digital information.
- (5) Mixed ferrites possess high resistivity and good magnetic properties, so they can be used to prepare cores used in inductors and transformers.
- (6) Mn-Zn ferrites are used in television deflection yokes, cores for television line output transformers and standard power supplies. These materials are used in induction cores, antennas for medium and long wave broadcasting, transductors [variable inductors], automatic control systems, frequency modulation, switching, filters, etc.

- (7) Ni-Zn ferrites are useful in wide band transformers, antennas for medium and long wave broadcasting, power transformer cores, inductor cores and antennas for short wave broadcasting.
- (8) Oxides of  $\gamma\text{-Fe}_2\text{O}_3$ ,  $\text{Fe}_3\text{O}_4$  and  $\text{CrO}_2$  are used in magnetic recording of audio, visual and digital information because of their high remanence magnetization. The most widely used material is cobalt modified  $\gamma\text{-Fe}_2\text{O}_3$  and  $\text{CrO}_2$ .
- (9) The non-reciprocity of some ferrites, such as garnets, are used in a variety of devices like isolators, calculators, switches, etc. An isolator is a device in which the incident electromagnetic wave can propagate forward, so that there is no reverse wave.

## Formulae

$$\begin{array}{lll} 1. \quad \mu = \mu_r \mu_0 H/m & \text{where} & \mu_0 = 4\pi \times 10^{-7} \text{H/m} \\ 2. \quad B_0 = \mu_0 H & \text{and} & B = \mu H \text{ so } \frac{B}{B_0} = \mu_r \\ 3. \quad B = \mu_0 (H + M) & & 4. \quad M = H [\mu_r - 1] \\ 5. \quad \chi = \frac{M}{H} & & 6. \quad \mu_l = IA = \frac{-e\pi r^2}{T} = \frac{-erv}{2} = \frac{-eL}{2m_e} = \frac{-el\hbar}{2m_e} = l\mu_B \\ & & \text{where } \mu_B = 9.27 \times 10^{-24} \text{ A-m}^2 \\ 7. \quad \mu_s = \gamma \left( \frac{e}{2m_e} \right) \frac{\hbar}{2} = 9.4 \times 10^{-24} \text{ A-m}^2 & & 8. \quad \mu_n = \left( \frac{e}{2m_p} \right) \hbar = 5.05 \times 10^{-27} \text{ A-m}^2 \\ 9. \quad \chi = \frac{C}{T - \theta} & \text{for ferromagnetic} & 10. \quad \chi = \frac{C}{T + \theta} & \text{for anti-ferromagnetic} \\ 11. \quad \chi = \frac{C}{T} & \text{for para magnetic} & & \end{array}$$

## Solved Problems

1. The magnetic susceptibility of silicon is  $-0.4 \times 10^{-5}$ . Calculate the flux density and magnetic moment per unit volume when magnetic field of intensity  $5 \times 10^5 \text{ A/m}$  is applied.

**Sol:** Given:  $\chi = -0.4 \times 10^{-5}$

$$H = 5 \times 10^5 \text{ A/m}$$

$$B = ? \quad \text{and} \quad M = ?$$

$$B = \mu_0(H + M) = \mu_0 H(1 + \chi)$$

$$= 4\pi \times 10^{-7} \times 5 \times 10^5 [1 - 0.4 \times 10^{-5}] = 4\pi \times 5 \times 10^{-2} \times 0.9996 = 0.62 \text{ Wb/m}^2$$

$$M = \chi H = -0.4 \times 10^{-5} \times 5 \times 10^5 = -2.0 \text{ A/m.}$$

2. The magnetic field strength in silicon is  $1000 \text{ A/m}$ . If the magnetic susceptibility is  $-0.25 \times 10^{-5}$ , calculate the magnetization and flux density in silicon.

**Sol:** Magnetic field strength ( $H$ ) =  $1000 \text{ A/m}$

$$\text{Magnetic susceptibility } (\chi) = -0.25 \times 10^{-5}$$

$$\text{Magnetization } (M) = \chi H = -0.25 \times 10^{-5} \times 1000 = -0.25 \times 10^{-2} \text{ A/m.}$$

$$\begin{aligned}\text{Magnetic flux density } (B) &= \mu_0(H + M) = 4\pi \times 10^{-7} (1000 - 0.25 \times 10^{-2}) \\ &= 1.25 \times 10^{-3} \text{ Wb/m}^2.\end{aligned}$$

3. When a magnetic material is subjected to a magnetic field of intensity 250 A/m. Its relative permeability is 15. Calculate its magnetization and magnetic flux density.

**Sol:** Given data are:

Intensity of applied magnetic field ( $H$ ) = 250 A/m

Relative permeability ( $\mu_r$ ) = 15

Magnetization ( $M$ ) = ?

Magnetic flux density ( $B$ ) = ?

$$M = H[\mu_r - 1] = 250 [15 - 1] \text{ A/m} = 250 \times 14 = 3500 \text{ A/m}$$

$$B = \mu_0 [H + M] = 4\pi \times 10^{-7} [250 + 3500] \text{ Wb/m}^2 = 4.71 \times 10^{-3} \text{ Wb/m}^2$$

4. Calculate magnetic dipole moment per unit volume and flux density of a material placed in magnetic field of intensity 1000 A/m. The magnetic susceptibility is  $-0.42 \times 10^{-3}$ .

**Sol:** The given data are:

The intensity of magnetic field ( $H$ ) = 1000 A/m

Magnetic susceptibility ( $\chi$ ) =  $-0.42 \times 10^{-3}$

Magnetic moment per unit volume or Magnetization ( $M$ ) =  $\chi H$

$$= -0.42 \times 10^{-3} \times 1000 = -0.42 \text{ A/m}$$

Flux density or magnetic induction ( $B$ ) =  $\mu_0(H + M)$

$$= 4\pi \times 10^{-7} \times [1000 - 0.42] = 1.257 \times 10^{-3} \text{ Wb/m}^2$$

5. A circular loop of copper having a diameter of 10 cm carries a current of 500 mA. Calculate the magnetic moment associated with the loop.

(Set-2–Nov. 2004), (Set-1–Nov. 2003)

**Sol:** Magnetic moment,  $\mu = \text{area} \times \text{current}$

Diameter of the loop,  $2r = 10 \text{ cm} = 0.1 \text{ m}$

or radius of the loop,  $r = 5 \text{ cm} = 0.05 \text{ m}$

Current in the loop,  $i = 500 \text{ mA} = 0.5 \text{ A}$

$$\therefore \mu = \pi r^2 i = \frac{22}{7} \times (0.05)^2 \times 0.5 = 3.93 \times 10^{-3} \text{ A} \cdot \text{m}^2$$

6. A magnetic material has a magnetization of 3300 A/m and flux density of 0.0044 Wb/m<sup>2</sup>. Calculate the magnetizing force and the relative permeability of the material.

(Set-4–Nov. 2003)

**Sol:** Magnetization,  $M = 3300 \text{ A/m}$

Flux density,  $B = 0.0044 \text{ Wb/m}^2$

Magnetizing force,  $H = ?$

Relative permeability,  $\mu_r = ?$

$$B = \mu_0 [H + M]$$

$$\frac{B}{\mu_0} - M = H$$

$$H = \frac{0.0044 \times 7}{4 \times 22 \times 10^{-7}} - 3300 = 3500 - 3300 = 200 \text{ A/m}$$

$$M = H[\mu_r - 1]$$

$$\mu_r = 1 + \frac{M}{H} = 1 + \frac{3300}{200} = 1 + 16.5 = 17.5$$

7. An electron in a hydrogen atom circulates with a radius 0.052 nm. Calculate the change in its magnetic moment if a magnetic induction ( $B$ ) = 3 Wb/m<sup>2</sup> acts at right angles to the plane of orbit.

(Set-3–Nov. 2004), (Set-2–Nov. 2003)

**Sol:** Radius of hydrogen atom,  $r = 0.052 \text{ nm} = 0.52 \times 10^{-10} \text{ m}$

Magnetic induction that acts perpendicular to orbit,  $B = 3 \text{ Wb/m}^2$

Change in magnetic moment,  $\Delta\mu = ?$

$$\begin{aligned}\Delta\mu &= \frac{er^2}{2} \frac{eB}{2m} = \frac{e^2 r^2 B}{4m} \frac{[1.6 \times 10^{-19}]^2 \times [0.52 \times 10^{-10}]^2 \times 3}{4 \times 9.1 \times 10^{-31}} \text{ A-m}^2 \\ &= 5.715 \text{ A-m}^2.\end{aligned}$$

8. Calculate the change in magnetic moment of a circulating electron in an applied field of 2 tesla acting perpendicular to the plane of the orbit. Given  $r = 5.29 \times 10^{-11} \text{ m}$  for the radius of the orbit.

(Set-3–May 2004)

**Sol:** Applied magnetic field perpendicular to orbit,  $B = 2 \text{ Tesla}$

Radius of the orbit,  $r = 5.29 \times 10^{-11} \text{ m}$

Change in magnetic moment,  $d\mu = ?$

$$\begin{aligned}d\mu &= \frac{er^2}{2} \frac{eB}{2m} = \frac{e^2 r^2 B}{4m} = \frac{(1.6 \times 10^{-19})^2 \times (5.29 \times 10^{-11})^2 \times 2}{4 \times 9.1 \times 10^{-31}} \text{ A-m}^2 \\ &= 3.936 \times 10^{-29} \text{ A-m}^2\end{aligned}$$

9. A paramagnetic material has  $10^{28}$  atoms per m<sup>3</sup>. Its susceptibility at 350 K is  $2.8 \times 10^{-4}$ . Calculate the susceptibility at 300 K.

(Set-4–Nov. 2004)

**Sol:** Number of atoms,  $N = 10^{28}/\text{m}^3$

Susceptibility at 350 K,  $\chi_1 = 2.8 \times 10^{-4}$

Temperature,  $T_1 = 350 \text{ K}$

Susceptibility at 300 K,  $\chi_2 = ?$

Temperature,  $T_2 = 300 \text{ K}$

For paramagnetic substance  $\chi = \frac{C}{T}$  or  $C = \chi T$

$$\therefore \chi_1 T_1 = \chi_2 T_2$$

$$\chi_2 = \frac{\chi_1 T_1}{T_2} = \frac{2.8 \times 10^{-4} \times 350}{300} = 3.267 \times 10^{-4}$$

10. The magnetic field in the interior of a certain solenoid has the value of  $6.5 \times 10^{-4}$  T when the solenoid is empty. When it is filled with iron, the field becomes 1.4 T. Find the relative permeability of iron.

(Set-3–June 2005)

**Sol:** Magnetic field without iron material,  $B_0 = 6.5 \times 10^{-4}$  Tesla

Magnetic field with iron material,  $B = 1.4$  Tesla

$$\text{The relative permeability of iron, } \mu_r = \frac{B}{B_0} = \frac{1.4}{6.5 \times 10^{-4}} = \frac{14000}{6.5} = 2153.85$$

## Multiple Choice Questions

1. The magnetic susceptibility of a diamagnetic substance is: ( )  
(a) negative (b) zero  
(c) positive and low value (d) positive and high value

2. Ferrites show: ( )  
(a) diamagnetism (b) paramagnetism  
(c) ferromagnetism (d) ferrimagnetism

3. A Bohr magneton is equal to: ( )  
(a)  $9.27 \times 10^{-14} \text{ A-m}^2$  (b)  $9.27 \times 10^{-24} \text{ A-m}^2$   
(c)  $6.27 \times 10^{-14} \text{ A-m}^2$  (d)  $6.27 \times 10^{-24} \text{ A-m}^2$ .

4. If the applied magnetic field will not show any effect on a material, then the material is a: ( )  
(a) diamagnetic material (b) ferromagnetic material  
(c) anti-ferromagnetic material (d) non-magnetic material

5. A material which magnetizes to a small extent in the opposite direction to the applied external magnetic field is: ( )  
(a) ferrimagnetic material (b) anti-ferromagnetic material  
(c) diamagnetic material (d) paramagnetic material

6. Examples for diamagnetic materials are: ( )  
(a) gold and copper (b) bismuth and lead  
(c) zinc and noble gases (d) all the above

7. The materials which are feebly attracted by external magnetic fields are \_\_\_\_\_ magnetic materials. ( )  
(a) para (b) ferro  
(c) ferri (d) anti-ferro

8. Examples for paramagnetic materials are: ( )  
(a) aluminium and platinum (b) manganese chloride  
(c) salts of iron and nickel (d) all

9. The magnetic susceptibility is positive and large for \_\_\_\_\_ magnetic materials. ( )  
(a) ferro (b) para (c) ferri (d) anti-ferro

10. The magnetic dipole moments of neighbouring atoms are anti-parallel and unequal for \_\_\_\_\_ magnetic material. ( )  
(a) anti-ferro (b) ferri  
(c) dia (d) para

11. The domain theory of ferromagnetism was proposed by: ( )
  - (a) Curie
  - (b) Ronald
  - (c) Weiss
  - (d) Einstein
12. The polarized light reflected on the surface of a ferromagnetic substance appears as: ( )
  - (a) non-uniform intensity at different regions on the surface
  - (b) uniform intensity at different regions on the surface
  - (c) very low intensity at different regions on the surface
  - (d) none of the above
13. If ' $H$ ' is the intensity of magnetic field in a volume  $dV$ , then the field energy in that volume is: ( )
  - (a)  $\frac{1}{8\pi} H^2 dV$
  - (b)  $\frac{1}{8\pi} H dV$
  - (c)  $8\pi H dV$
  - (d) none
14. The anisotropy energy in BCC iron along [111] direction over that of [100] direction is: ( )
  - (a)  $10^5$  erg/cm<sup>3</sup>
  - (b)  $10^4$  erg/cm<sup>3</sup>
  - (c)  $10^6$  erg/cm<sup>3</sup>
  - (d)  $10^3$  erg/cm<sup>3</sup>
15. If ' $I$ ' is the current due to the orbital motion of an electron, then the magnetic moment associated with that orbit of area ' $A$ ' is: ( )
  - (a)  $I/A$
  - (b)  $A/I$
  - (c)  $I + A$
  - (d)  $IA$
16. Magnetic dipole moment per unit volume of material is called: ( )
  - (a) polarization
  - (b) permeability
  - (c) magnetization
  - (d) magnetic induction
17. Magnetic flux over a unit area of a surface held normal to the flux is: ( )
  - (a) magnetic induction
  - (b) magnetic permeability
  - (c) magnetization
  - (d) relative magnetic permeability
18. The neighbouring atomic magnetic moments of anti-ferromagnetic substance is: ( )
  - (a) equal and parallel
  - (b) equal and anti-parallel
  - (c) unequal and parallel
  - (d) unequal and anti-parallel
19. The magnetic moment of atom is due to: ( )
  - (a) the spin of electrons
  - (b) the angular momentum of the electrons
  - (c) by the applied magnetic field
  - (d) all the above
20. The spin magnetic moments of neighbouring atoms of a ferromagnetic substance are: ( )
  - (a) parallel
  - (b) anti-parallel
  - (c) random
  - (d) perpendicular
21. If an electron of mass,  $m_e$  revolving in an orbit with an angular momentum ' $L$ ', then it is associated with magnetic moment of: ( )
  - (a)  $\frac{eL}{m_e}$
  - (b)  $\frac{eL}{2m_e}$
  - (c)  $\frac{2eL}{m_e}$
  - (d)  $\frac{m_e}{2eL}$
22. The SI unit of magnetic moment is: ( )
  - (a) Wb
  - (b) Wb/m<sup>2</sup>
  - (c) A-m<sup>2</sup>
  - (d) A/m<sup>2</sup>
23. The magnetostrictive strain energy can be reduced by: ( )
  - (a) increasing the size of strain-producing horizontal domains
  - (b) decreasing the size of strain-producing horizontal domains
  - (c) decreasing the size of strain-producing vertical domains
  - (d) increasing the size of strain-producing vertical domains

24. If  $C$  and  $\theta$  are the Curie constant and paramagnetic Curie temperature of a paramagnetic substance at a temperature  $T$ K, the magnetic susceptibility is: ( )
- (a)  $\frac{C}{T - \theta}$       (b)  $\frac{C}{T + \theta}$       (c)  $\frac{C}{T}$       (d) none of the above
25. Soft magnetic materials possess: ( )
- (a) low remanent magnetization  
 (b) low coercivity and hysteresis losses  
 (c) high magnetic permeability and susceptibility  
 (d) all the above
26. Hard magnetic materials possess: ( )
- (a) high remanent magnetization and coercivity  
 (b) low permeability  
 (c) high hysteresis loss  
 (d) all the above
27. Hard magnetic materials are used in: ( )
- (a) magnetic separators and detectors  
 (b) speakers used in audio systems and microphones  
 (c) in toys and measuring meters  
 (d) all the above
28. Ferrites are used in: ( )
- (a) thermal-sensing switches used in refrigerators and air conditioners  
 (b) to produce ultrasonic waves  
 (c) in electric motors  
 (d) all the above
29. The ratio of magnetic flux density in a material to that in vacuum under the same applied magnetic field is called: ( )
- (a) relative magnetic permeability  
 (b) relative permeability  
 (c) magnetic induction  
 (d) none of the above
30. The ratio of magnetization to the applied magnetic field strength of a material is called: ( )
- (a) magnetic susceptibility      (b) magnetic permeability  
 (c) magnetic induction      (d) none of the above
31. A material which is repelled by an external magnetic field is \_\_\_\_\_ magnetic material. ( )
- (a) para      (b) ferro      (c) anti-ferro      (d) dia
32. A material which is strongly attracted by magnetic fields is \_\_\_\_\_ magnetic material. ( )
- (a) para      (b) ferro      (c) anti-ferro      (d) dia
33. Examples for ferromagnetic materials are: ( )
- (a) iron      (b) cobalt      (c) nickel      (d) all the above
34. If  $M$  stands for a divalent ion, a general formula for ferrites is: ( )
- (a)  $\text{MoFe}_2\text{O}_3$       (b)  $\text{MoFeO}_3$       (c)  $\text{MoFe}_2\text{O}$       (d)  $\text{MFe}_2\text{O}_3$

35. The change in dimensions of a material on magnetization is called: ( )  
(a) piezoelectricity (b) ferroelectricity  
(c) magnetostriction (d) none

36. Hysteresis means \_\_\_\_\_ of an effect behind the cause of effect. ( )  
(a) lagging (b) advancing (c) both a & b (d) none

37. For an anti-ferromagnetic substance, the magnetic susceptibility is maximum at \_\_\_\_\_ temperature. ( )  
(a) Fermi (b) Debye (c) Neel (d) Curie

38. The magnetic dipole moment per molecule of ferrous ferrite is equal to: ( )  
(a)  $2\mu_B$  (b)  $8\mu_B$  (c)  $4\mu_B$  (d)  $16\mu_B$

39. The hysteresis loss is less for \_\_\_\_\_ magnetic materials. ( )  
(a) dia (b) para (c) hard (d) soft

40. The alloy containing 79% Ni, 15% Fe, 5% Mo and 0.5% Mn is known as superm alloy possess: ( )  
(a) very low permeability (b) very high permeability  
(c) very low magnetic induction (d) none of the above

41. \_\_\_\_\_ magnetic materials are used in magnetic amplifiers and in magnetic switching circuits. ( )  
(a) dia (b) para (c) soft (d) hard

42. Some ferrites possess rectangular hysteresis loop, so they are used in the construction of \_\_\_\_\_ devices. ( )  
(a) memory (b) transformer core  
(c) permanent magnets (d) none of the above

43. Ni-Zn ferrites are used in: ( )  
(a) power transformer cores (b) inductor cores  
(c) antenna's for short wave broadcasting (d) all the above

44. The unit of magnetic permeability of a diamagnetic substance is independent of: ( )  
(a) temperature (b) pressure (c) humidity (d) none

45. The magnetic permeability of a diamagnetic substance is independent of: ( )  
(a) temperature (b) pressure (c) humidity (d) none

46. The ratio of magnetic moment ( $M$ ) to the angular momentum ( $L$ ) of an electron is called \_\_\_\_\_ ratio. ( )  
(a) gyromagnetic ratio (b) magnetic susceptibility  
(c) permeability (d) none of the above

47. Below curie temperature, a ferromagnetic substance possess \_\_\_\_\_ magnetization. ( )  
(a) dia (b) para (c) spontaneous (d) none

48. The area enclosed by hysteresis loop of a ferromagnetic substance represents \_\_\_\_\_ loss per cycle. ( )  
(a) magnetization (b) dielectric (c) energy (d) power

49. Every domain of a ferromagnetic substance is \_\_\_\_\_ magnetized. ( )  
(a) dia (b) spontaneously (c) para (d) none

50. The boundary between domains is called \_\_\_\_\_ ( )  
(a) Bloch wall (b) potential wall (c) both a & b (d) none

51. Paramagnetic atoms possess \_\_\_\_\_ number of electrons. ( )  
 (a) even                    (b) odd                    (c) both a & b            (d) none
52. A current loop behaves as a \_\_\_\_\_. ( )  
 (a) electric motor                    (b) magnetic shell  
 (c) electric shell                    (d) none of the above
53. Magnetic permeability represents the \_\_\_\_\_ with which a material allows magnetic force of lines to pass through it. ( )  
 (a) difficult                    (b) easy                    (c) both a & b            (d) none

## Answers

1. a	2. d	3. b	4. d	5. c	6. d	7. a	8. d	9. a	10. b	11. c	12. a
13. a	14. a	15. d	16. c	17. a	18. b	19. d	20. a	21. b	22. c	23. b	24. c
25. d	26. d	27. d	28. d	29. a	30. a	31. d	32. b	33. d	34. a	35. c	36. a
37. c	38. c	39. d	40. b	41. c	42. a	43. d	44. a	45. a	46. a	47. c	48. c
49. b	50. a	51. b	52. b	53. b							

## Review Questions

- What are paramagnetic and diamagnetic materials? Explain. (Set-4–Sept. 2006), (Set-1, Set-4–June 2005), (Set-4–Nov. 2004)
- Explain the properties of paramagnetic materials. (Set-3–Nov. 2003)
- Define the terms permeability ( $\mu$ ) susceptibility, magnetic induction ( $B$ ), magnetic field ( $H$ ) and magnetization ( $M$ ) with reference to magnetism. Obtain a relation between magnetic susceptibility, magnetization and magnetic field. (Set-2–Nov. 2004), (Set-1–Nov. 2003)
- Explain how the magnetic materials are classified from the atomic point of view. (Set-4–Nov. 2003)
- What are the differences between hard and soft magnetic materials? (Set-4–Nov. 2003)
- Explain the origin of diamagnetism. Obtain an expression for the diamagnetic susceptibility of a magnetic material. (Set-3–Nov. 2004), (Set-2–Nov. 2003)
- Distinguish between ferromagnetic, anti-ferromagnetic and ferrimagnetic materials. (Set-3–Nov. 2003)
- Obtain an expression for paramagnetic susceptibility ( $\chi$ ). How does the magnetic susceptibility of a material vary with temperature? (Set-4–Nov. 2004)
- Draw the  $B$ - $H$  curve for a ferromagnetic material and identify the retentivity and the coercive field on the curve. (Set-4–Sept. 2006), (Set-1, Set-4–June 2005)
- Explain clearly the differences between hard and soft magnetic materials. What are mixed ferrites? Mention their uses. (Set-2–June 2005)
- How ferrites are superior to ferromagnetic materials? (Set-2–June 2005)
- Give an account of ferromagnetic materials. (Set-3–May 2004)
- Explain the important properties of ferrites. (Set-2–May 2003), (Set-4–May 2004)

14. What are the characteristics of soft magnetic materials? (Set-3–June 2005)
15. Define magnetization and show that.  $B = \mu_0 (H + M)$ . (Set-3–May 2004)
16. What is ferromagnetic curie temperature? Discuss the behaviour of a ferromagnetic material below the curie temperature. (Set-3–June 2005)
17. In a hydrogen atom, an electron having charge  $e$  revolves around the nucleus at a distance of  $r$  metre with an angular velocity ' $\omega$ ' rad/sec. Obtain an expression for magnetic moment associated with it due to its orbital motion. (Set-1–Nov. 2004)
18. What are the sources of permanent dipole moment in magnetic materials? (Set-2–Sept. 2008), (Set-4–May 2004), (Set-2–May 2003)
19. Define the terms magnetic susceptibility, magnetic permeability, magnetic induction and magnetization. (Set-4–May 2004), (Set-2–May 2003)
20. Explain hysteresis of a ferromagnetic material. (Set-1–May 2004), (Set-3–May 2003)
21. Explain ferrimagnetism and anti-ferromagnetism. (Set-1–May 2004), (Set-3–May 2003)
22. How materials are classified as dia or para or ferromagnetism? Explain. (Set-1–May 2004), (Set-3–May 2003)
23. What are ferrites? Explain the magnetic properties of ferrites and mention their industrial applications. (Set-3–May 2007), (Set-2–May 2004), (Set-4–May 2003)
24. What is ferromagnetism? What are the distinguishing features of ferromagnetism? (Set-3–May 2007), (Set-2–May 2004), (Set-4–May 2003)
25. In hydrogen atom, an electron ' $e$ ' revolves around the nucleus at a distance of ' $r$ ' metre with an angular velocity  $\omega$  rad/sec. Obtain an expression for magnetic moment associated with it due to its orbital motion. (Set-1–May 2003)
26. Define magnetic moment. Explain the origin of magnetic moment at the atomic level. What is a Bohr magneton? (Set-1–Nov. 2004), (Set-1–May 2003)
27. Explain clearly difference between hard and soft magnetic materials. (Set-4–May 2008)
28. Explain the hysteresis loop observed in ferromagnetic materials. (Set-4–May 2008)
29. Define the terms magnetic susceptibility, magnetic induction and permeability. (Set-1–May 2006)
30. How is magnetic susceptibility of a material is measured? (Set-1–May 2006)
31. Explain the salient features of anti-ferromagnetic materials. (Set-1–May 2006)
32. What is meant by ferromagnetic materials? Give example. (Set-2–May 2006)
33. Explain the hysteresis properties of ferromagnetic materials. (Set-2–May 2006), (Set-2–Sept. 2008)
34. Mention the various properties of paramagnetic materials. (Set-2–May 2006)
35. What are the properties of antiferromagnetic materials? (Set-1–Sept. 2006)
36. Explain how antiferromagnetic materials are different from diamagnetic and paramagnetic materials. (Set-1–Sept. 2006)
37. State the properties of diamagnetic materials. (Set-4–Sept. 2007), (Set-2–Sept. 2006)
38. Explain the terms (i) Magnetic flux density, (ii) Magnetic field strength, (iii) Magnetization and (iv) Magnetic susceptibility. How they are related to each other. (Set-3–Sept. 2008)

39. What are hard and soft magnetic materials? Write their characteristic properties and applications.  
(Set-3–Sept. 2008)
40. What is meant by Neel temperature?  
(Set-1–Sept. 2006)
41. Write notes on ferroelectricity.  
(Set-2–Sept. 2008)
42. Draw and explain B–H curve for a ferromagnetic material placed in a magnetic field.  
(Set-4–Sept. 2007), (Set-2–Sept. 2006)
43. Discuss the theory of paramagnetism.  
(Set-4–Sept. 2007), (Set-2–Sept. 2006)
44. Write short notes on hysteresis curve.
45. Explain ferromagnetism and B–H curve.
46. Write the importance of hard magnetic materials in engineering applications.
47. Explain in detail the classification of magnetic materials on the basis of electron spin.
48. What is Bohr magneton? How is it related to magnetic moment of electron?
49. Explain in detail domain theory of ferromagnetism.
50. Explain the origin of magnetic moment. Find the magnetic dipole moments due to orbital and spin motions of an electron.
51. Show the nature of magnetic dipole moments in ferro, ferri and anti-ferro magnetic materials.
52. Describe hysteresis loop. How is it used to classify magnets?
53. Give an account of the uses of ferrites.
54. Describe the experimental evidence to demonstrate the existence of ferromagnetic domains.
55. Explain in detail the concept of ferromagnetic domains and explain how it was experimentally established.
56. What are ferromagnetic domains? Explain their existence.
57. Explain the different contributions for the formation of domains in a ferromagnetic material.
58. Write on Bohr magneton.
59. Write briefly on hysteresis in ferromagnets.
60. Write the necessary theory to relate electron momentum to the origin of magnetism and write the brief classification of magnetism in materials based on the temperature dependence of susceptibility.
61. Explain hysteresis in soft and hard magnetic materials and their specific applications.
62. Explain Weiss theory of ferromagnetic materials.
63. Give the qualitative explanation of quantum theory for paramagnetic materials.
64. Explain hysteresis using domain structure.
65. Explain the properties of ferrimagnetic materials.
66. Explain ferromagnetism based on domain structure.
67. Explain the formation of domains based on exchange interaction.
68. Explain the formation of Bloch wall with a neat diagram.

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## CHAPTER

# 8

# Semiconductors and Physics of Semiconductor Devices

## 8.1 Introduction

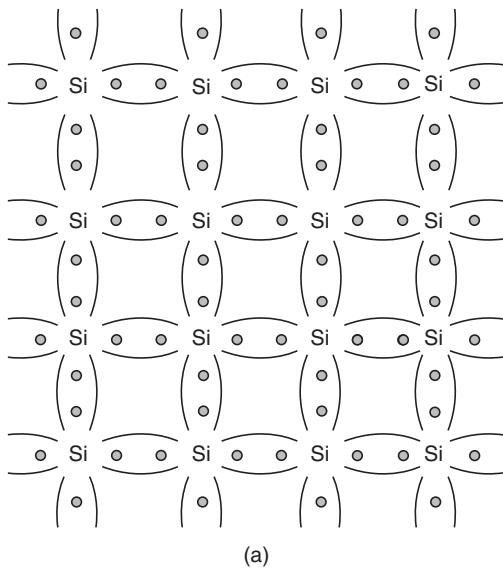
Based on electrical conductivity, materials are divided into conductors, insulators and semiconductors. Usually, metals are good conductors of electricity and all dielectrics are insulators. The electrical conductivity of semiconductors lie in between metals and dielectrics. Good examples for semiconductor are germanium and silicon. These elements belong to IV group in the periodic table. At 0K, these elements are insulators, whereas at room temperatures they possess certain amount of conductivity. Pure germanium and silicon are called intrinsic semiconductors. By adding a small quantity of either III group or V group element atoms as impurity into pure Ge or Si, the electrical conductivity of the material increases. This impure semiconductor is called an extrinsic semiconductor.

## 8.2 Intrinsic semiconductors—carrier concentration

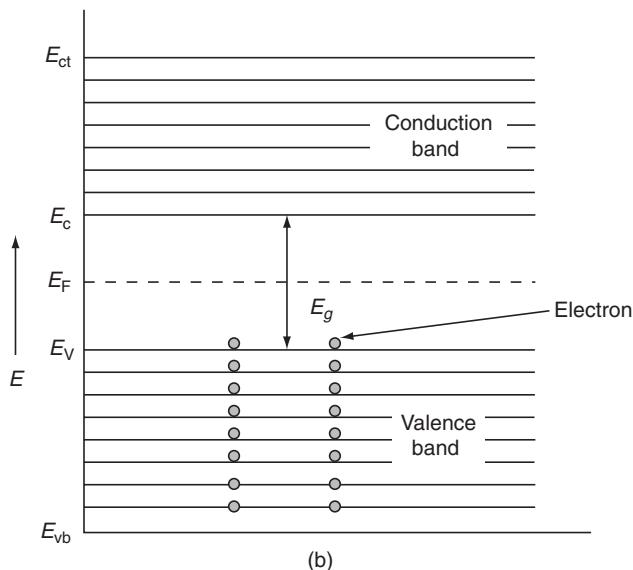
Pure germanium or silicon crystal is called an intrinsic semiconductor. Each semiconductor atom possesses four valence electrons in the outermost orbit. To get stability, each of these atoms has to get eight electrons in the outermost orbit, so that each atom makes four covalent bonds with the surrounding four other atoms in the crystal. A two-dimensional representation of the crystal structure of silicon (or germanium) at 0K is shown in Fig. 8.1(a). The band diagram of this material is shown in Fig. 8.1(b).

At 0K, all the valence electrons of Si atoms are participating in covalent bonds and their energies constitute a band of energies called valence band. So, at 0K, valence band is completely filled and conduction band is empty of electrons. The allowed band of energies above valence band is called conduction band. Suppose, if we raise the temperature of the semiconductor to some room temperature  $T$ K, at this temperature some of the electrons which are participating in covalent bonds and present in the top energy levels of valence band will take thermal energies. If the increase in thermal energy of electrons present in top energy levels of valence band is equal to or greater than energy gap of the semiconductor, then electrons come away from bonding and move freely inside the crystal as shown in Fig. 8.2(a). Now these electrons possess energies equal to the lower energy levels of conduction band. These free electrons participate in electrical conduction, hence the band in which these electrons present is named

Figure 8.1 (a) Crystal structure of Si at 0 K; (b) Band diagram of Si at 0 K



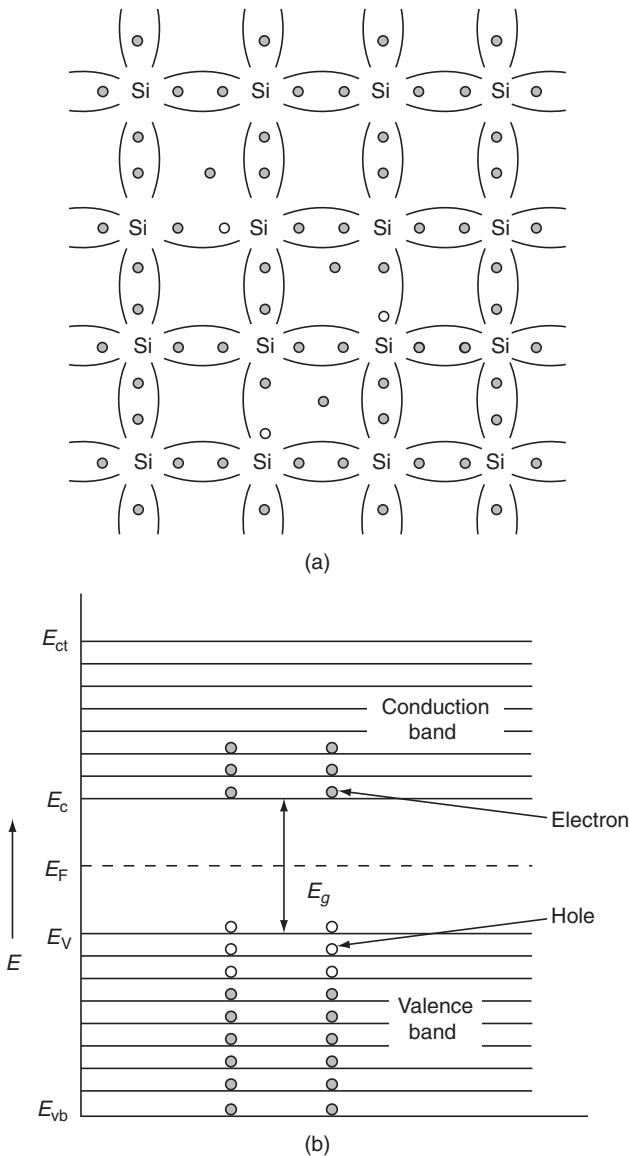
(a)



(b)

as conduction band. If an electron comes away from bonding, then that atom acquires one unit positive charge, then it participates in electrical conduction. This electron vacancy or electron deficiency of an intrinsic semiconductor is called hole. The electron vacancies in valence band will exist as holes in the valence band as shown in Fig. 8.2(b).

Thus, at temperature  $T_K$ , in an intrinsic semiconductor, if  $n$  covalent bonds are broken per unit volume of the material, then there will be  $n$  electrons in the conduction band and the same number of holes in the valence

Figure 8.2 (a) Crystal structure of Si at  $T\text{K}$ ; (b) Band diagram of Si at  $T\text{K}$ 

band. Usually, the number of free (or conduction) electrons present per unit volume of material, whose energies lie in the conduction band is called electron concentration and is represented as ' $n$ '. Similarly, the number of holes present per unit volume of the semiconductor and in the valence band is called hole concentration represented as ' $p$ '. Both the free electrons and holes present in the material participate in electrical conduction. The free electrons and holes present per unit volume of the material is called carrier concentration.

At some temperature  $T\text{K}$ , the free electron and hole concentration in an intrinsic semiconductor can be extracted in the following way:

## Electron concentration

The number of free electrons per unit volume of semiconductor having energies in between  $E$  and  $E + dE$  is represented as  $N(E) dE$  [i.e., in a width of  $dE$ ].  $N(E) dE$  can be obtained by multiplying the number of available electron states between  $E$  and  $E + dE$  per unit volume of the material,  $g_e(E) dE$  with the probability that an electron occupies an electron state at energy  $E$  [i.e.,  $f_e(E)$ ].

Therefore, we have:

$$N(E) dE = g_e(E) dE f_e(E) \quad (8.1)$$

The number of electrons present in the conduction band per unit volume of material ' $n$ ' is obtained by integrating  $N(E) dE$  between the limits  $E_c$  and  $E_{ct}$  where  $E_c$  and  $E_{ct}$  are the bottom and top energy levels of conduction band, respectively.

$$\text{i.e.,} \quad n = \int_{E_c}^{E_{ct}} N(E) dE = \int_{E_c}^{E_{ct}} g_e(E) f_e(E) dE \quad (8.2)$$

Equation (8.2) can be represented as:

$$n = \int_{E_c}^{\infty} g_e(E) f_e(E) dE - \int_{E_{ct}}^{\infty} g_e(E) f_e(E) dE \quad (8.3)$$

Above  $E_{ct}$ , electrons will not be present. Hence, Equation (8.3) becomes:

$$n = \int_{E_c}^{\infty} g_e(E) f_e(E) dE \quad (8.4)$$

The Fermi-Dirac distribution function  $f_e(E)$  can be represented as:

$$f_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} \quad (8.5)$$

Compared to the exponential value, the '1' in the denominator is negligible.

$$\text{i.e.,} \quad \exp\left(\frac{E - E_F}{K_B T}\right) \gg 1$$

$$\text{Hence,} \quad f_e(E) = \frac{1}{\exp\left(\frac{E - E_F}{K_B T}\right)} = \exp\left(\frac{E_F - E}{K_B T}\right) \quad (8.6)$$

The density of electron states  $g_e(E)$  in the energy space from  $E = 0$  to  $E$  can be written as:

$$g_e(E) = \frac{\pi}{2} \left( \frac{8m_e^*}{\hbar^2} \right)^{\frac{3}{2}} (E - 0)^{\frac{1}{2}} \quad (8.7)$$

where  $m_e^*$  is the effective mass of an electron and  $\hbar$  is Planck's constant.

$$g_e(E) dE = \frac{\pi}{2} \left( \frac{8m_e^*}{\hbar^2} \right)^{\frac{3}{2}} (E - 0)^{\frac{1}{2}} dE \quad (8.8)$$

To evaluate  $n$ , the density of states is counted from  $E_c$ , since the minimum energy state in conduction band is  $E_c$ . So Equation (8.8) becomes:

$$g_e(E)dE = \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} (E - E_c)^{1/2} dE \quad (8.9)$$

Substituting Equations (8.6) and (8.9) in (8.4) gives:

$$\begin{aligned} n &= \int_{E_c}^{\infty} \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} (E - E_c)^{1/2} \exp\left(\frac{E_F - E}{K_B T}\right) dE \\ &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} \int_{E_c}^{\infty} (E - E_c)^{1/2} \exp\left(\frac{E_F - E}{K_B T}\right) dE \end{aligned} \quad (8.10)$$

The above equation can be simplified by the following substitution:

$$\text{Put } \varepsilon = E - E_c \quad (8.11)$$

$$\text{So, } d\varepsilon = dE$$

In Equation (8.11),  $E_c$  is constant, as we change the variable  $E$  to  $\varepsilon$  in Equation (8.10), the integral limits also change.

In Equation (8.11), as  $E \rightarrow E_c$  then  $\varepsilon \rightarrow 0$  and  $E \rightarrow \infty$ , then  $\varepsilon$  also  $\rightarrow \infty$ . With reference to Fig. 8.2(b), the exponential term in Equation (8.10) becomes:

$$\begin{aligned} \exp\left(\frac{E_F - E}{K_B T}\right) &= \exp\left(\frac{(E_F - E_c) + (E_c - E)}{K_B T}\right) = \exp\left(\frac{(E_F - E_c) - \varepsilon}{K_B T}\right) \\ &= \exp\left(\frac{(E_F - E_c)}{K_B T}\right) \exp\left(\frac{-\varepsilon}{K_B T}\right) \end{aligned} \quad (8.12)$$

Substituting Equations (8.11) and (8.12) in (8.10), we get:

$$\begin{aligned} n &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} \int_0^{\infty} \varepsilon^{1/2} \exp\left(\frac{E_F - E_c}{K_B T}\right) \exp\left(\frac{-\varepsilon}{K_B T}\right) d\varepsilon \\ &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} \exp\left(\frac{E_F - E_c}{K_B T}\right) \int_0^{\infty} \varepsilon^{1/2} \exp\left(\frac{-\varepsilon}{K_B T}\right) d\varepsilon \end{aligned} \quad (8.13)$$

The integral (I) in the above equation can be simplified by substitution. Put  $\varepsilon = x^2$

$$\text{so that } d\varepsilon = 2x dx$$

$$\begin{aligned} \text{Then } I &= \int_0^{\infty} x \exp\left(\frac{-x^2}{K_B T}\right) 2x dx \\ &= \int_0^{\infty} 2x^2 \exp\left(\frac{-x^2}{K_B T}\right) dx \end{aligned}$$

$$= \frac{\sqrt{\pi}}{2(1/K_B T)^{3/2}} = \frac{\sqrt{\pi}}{2} (K_B T)^{3/2} \quad (8.14)$$

Substituting Equation (8.14) in (8.13) gives:

$$\begin{aligned} n &= \frac{\pi}{2} \left( \frac{8m_e^*}{h^2} \right)^{3/2} \exp \left( \frac{E_F - E_C}{K_B T} \right) \frac{\sqrt{\pi}}{2} (K_B T)^{3/2} \\ &= \frac{1}{4} \left( \frac{8m_e^* \pi K_B T}{h^2} \right)^{3/2} \exp \left( \frac{E_F - E_C}{K_B T} \right) \\ n &= \frac{8}{4} \left[ \frac{2m_e^* \pi K_B T}{h^2} \right]^{3/2} \exp \left( \frac{E_F - E_C}{K_B T} \right) \\ n &= 2 \left[ \frac{2m_e^* \pi K_B T}{h^2} \right]^{3/2} \exp \left[ -\left( \frac{E_C - E_F}{K_B T} \right) \right] \end{aligned} \quad (8.15)$$

The term  $2 \left[ \frac{2m_e^* \pi K_B T}{h^2} \right]^{3/2}$  is almost a constant compared with the exponential term as the temperature changes. So, it is a pseudo constant and is given by the symbol  $N_c$ . So, we have:

$$n = N_c \exp \left[ -\frac{(E_C - E_F)}{K_B T} \right] \quad (8.16)$$

## For hole concentration

The number of holes per unit volume of semiconductor in the energy range  $E$  and  $E + dE$  in valence band is represented as  $P(E) dE$ .  $P(E) dE$  can be obtained by multiplying the number of available hole states between  $E$  and  $E + dE$  per unit volume of the material [i.e.,  $g_h(E) dE$ ] with the hole probability in a hole state at energy  $E$  [i.e.,  $f_h(E)$ ].

$$\text{Therefore, } P(E) dE = g_h(E) f_h(E) dE \quad (8.17)$$

The number of holes present in the valence band per unit volume of material ' $p$ ' is obtained by integrating  $P(E) dE$  between the limits  $E_{vb}$  and  $E_v$  where  $E_v$  and  $E_{vb}$  are the top and bottom energy levels of valence band, respectively.

i.e.,

$$p = \int_{E_{vb}}^{E_v} P(E) dE = \int_{E_{vb}}^{E_v} g_h(E) f_h(E) dE \quad (8.18)$$

Equation (8.18) can be represented as:

$$p = \int_{-\infty}^{E_v} g_h(E) f_h(E) dE - \int_{-\infty}^{E_{vb}} g_h(E) f_h(E) dE \quad (8.19)$$

below  $E_{vb}$  holes will not exist. Hence, Equation (8.19) becomes:

$$p = \int_{-\infty}^{E_v} g_h(E) f_h(E) dE \quad (8.20)$$

The presence of a hole can be represented as the absence of an electron. Hence, the Fermi-Dirac function of holes  $f_h(E)$  in the valence band is:

$$\begin{aligned} f_h(E) &= 1 - f_e(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} \\ &= \frac{\exp\left(\frac{E - E_F}{K_B T}\right)}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)} = \frac{1}{1 + \frac{1}{\exp\left(\frac{E - E_F}{K_B T}\right)}} = \frac{1}{1 + \exp\left(\frac{E_F - E}{K_B T}\right)} \end{aligned}$$

Compared to exponential, the '1' in the denominator is negligible, i.e.,  $\exp\left(\frac{E_F - E}{K_B T}\right) \gg 1$

$$\text{Hence, } f_h(E) = \exp\left(\frac{E - E_F}{K_B T}\right) \quad \text{_____ (8.21)}$$

The density of hole states between  $E$  and  $E + dE$  in valence band can be written similar to Equation (8.9) for electrons.

$$g_h(E) dE = \frac{\pi}{2} \left[ \frac{8m_h^*}{h^2} \right]^{3/2} (E_V - E)^{1/2} dE \quad \text{_____ (8.22)}$$

where  $m_h^*$  is the effective mass of hole.

Substituting Equations (8.21) and (8.22) in (8.20),

$$\begin{aligned} \text{we get } p &= \int_{-\infty}^{E_V} \frac{\pi}{2} \left[ \frac{8m_h^*}{h^2} \right]^{3/2} (E_V - E)^{1/2} \exp\left(\frac{E - E_F}{K_B T}\right) dE \\ &= \frac{\pi}{2} \left[ \frac{8m_h^*}{h^2} \right]^{3/2} \int_{-\infty}^{E_V} (E_V - E)^{1/2} \exp\left(\frac{E - E_F}{K_B T}\right) dE \quad \text{_____ (8.23)} \end{aligned}$$

The above equation can be simplified by the substitution:

$$\text{Put } \varepsilon = E_V - E \quad \text{_____ (8.24)}$$

$$\text{so } d\varepsilon = -dE$$

In Equation (8.24),  $E_V$  is constant, as we change the variable  $E$  to  $\varepsilon$  in Equation (8.23), the integral limits also change.

In Equation (8.24), as  $E \rightarrow E_V$  then  $\varepsilon \rightarrow 0$  and  $E \rightarrow -\infty$ , then  $\varepsilon \rightarrow \infty$  with reference to Fig. 8.2(b), the exponential term in Equation (8.23) becomes:

$$\exp\left(\frac{E - E_F}{K_B T}\right) = \exp\left(\frac{(E - E_V) + (E_V - E_F)}{K_B T}\right)$$

$$= \exp\left[\frac{-\varepsilon + E_V - E_F}{K_B T}\right] = \exp\left[\frac{-\varepsilon}{K_B T}\right] \exp\left[\frac{E_V - E_F}{K_B T}\right] \quad (8.25)$$

Substituting Equations (8.24) and (8.25) in (8.23), we get:

$$p = \frac{\pi}{2} \left[ \frac{8m_h^*}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{E_V - E_F}{K_B T}\right] \int_0^\infty \varepsilon^{\frac{1}{2}} \exp\left(\frac{-\varepsilon}{K_B T}\right) d\varepsilon \quad (8.26)$$

From Equation (8.14), we know the integral value:

$$\begin{aligned} \text{So, } p &= \frac{\pi}{2} \left[ \frac{8m_h^*}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{E_V - E_F}{K_B T}\right] \frac{\sqrt{\pi}}{2} (K_B T)^{\frac{3}{2}} \\ &= \frac{1}{4} \left[ \frac{8m_h^* \pi K_B T}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{E_V - E_F}{K_B T}\right] \\ &= 2 \left[ \frac{2m_h^* \pi K_B T}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{-(E_F - E_V)}{K_B T}\right] \end{aligned} \quad (8.27)$$

The term  $2 \left[ \frac{2m_h^* \pi K_B T}{h^2} \right]^{\frac{3}{2}}$  is almost constant compared with the exponential term as the temperature changes. So, it is a pseudo constant and is given by the symbol  $N_v$ . So, we have:

$$p = N_v \exp\left[\frac{-(E_F - E_V)}{K_B T}\right] \quad (8.28)$$

## To evaluate Fermi energy

At temperature  $T$ K, the electron concentration ' $n$ ' is equal to hole concentration ' $p$ ' in an intrinsic semiconductor i.e.,  $n = p$ .

Equating Equations (8.15) and (8.27), we get:

$$\begin{aligned} 2 \left[ \frac{2\pi m_e^* K_B T}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{-(E_C - E_F)}{K_B T}\right] &= 2 \left[ \frac{2\pi m_h^* K_B T}{h^2} \right]^{\frac{3}{2}} \exp\left[\frac{-(E_F - E_V)}{K_B T}\right] \\ \left( m_e^* \right)^{\frac{3}{2}} \exp\left[\frac{-(E_C - E_F)}{K_B T}\right] &= \left( m_h^* \right)^{\frac{3}{2}} \exp\left[\frac{-(E_F - E_V)}{K_B T}\right] \\ \exp\left[\frac{E_F - E_V}{K_B T}\right] \times \exp\left[\frac{-(E_C - E_F)}{K_B T}\right] &= \left[ \frac{m_h^*}{m_e^*} \right]^{\frac{3}{2}} \\ \exp\left[\frac{E_F - E_V - E_C + E_F}{K_B T}\right] &= \left[ \frac{m_h^*}{m_e^*} \right]^{\frac{3}{2}} \\ \exp\left[\frac{2E_F - (E_C + E_V)}{K_B T}\right] &= \left( \frac{m_h^*}{m_e^*} \right)^{\frac{3}{2}} \end{aligned}$$

Taking logarithms on both sides, we get:

$$\begin{aligned}
 \frac{2E_F - (E_C + E_V)}{K_B T} &= \frac{3}{2} \ln \left[ \frac{m_h^*}{m_e^*} \right] \\
 2E_F - (E_C + E_V) &= \frac{3}{2} K_B T \ln \left( \frac{m_h^*}{m_e^*} \right) \\
 2E_F &= E_C + E_V + \frac{3}{2} K_B T \ln \left( \frac{m_h^*}{m_e^*} \right) \\
 \therefore E_F &= \frac{E_C + E_V}{2} + \frac{3}{4} K_B T \ln \left( \frac{m_h^*}{m_e^*} \right) \quad (8.29)
 \end{aligned}$$

Normally,  $m_h^*$  is greater than  $m_e^*$ , since  $\ln \left( \frac{m_h^*}{m_e^*} \right)$  is very small so that  $E_F$  is just above the middle of energy gap and slightly rises with increase of temperature. In case of Si and Ge,  $m_h^* \approx m_e^*$ , hence the Fermi level lies at the middle of energy gap.

### To find intrinsic concentration ( $n_i$ )

Inside a semiconductor, electrons and holes will be lost due to electron-hole recombinations and electron-hole pairs will be created due to thermal energies. The electron concentration and hole concentration remain constant as long as the temperature remains constant. At temperature  $TK$ , in an intrinsic semiconductor  $n = p = n_i$ , where  $n_i$  is called intrinsic concentration.

$$\text{Also the product } np = n_i^2 \quad (8.30)$$

Substituting Equations (8.16) and (8.28) in (8.30) gives:

$$\begin{aligned}
 n_i^2 &= (N_V N_C) \exp \left[ \frac{-(E_C - E_F)}{K_B T} \right] \exp \left[ \frac{-(E_F - E_V)}{K_B T} \right] \\
 &= N_V N_C \exp \left[ \frac{-E_C + E_F - E_F + E_V}{K_B T} \right] \\
 &= (N_V N_C) \exp \left[ \frac{-(E_C - E_V)}{K_B T} \right] \\
 &= (N_V N_C) \exp \left( \frac{-E_g}{K_B T} \right) \quad (\text{Since } E_g = E_c - E_v) \\
 \therefore n_i &= (N_V N_C)^{1/2} \exp \left( \frac{-E_g}{2K_B T} \right) \quad (8.31)
 \end{aligned}$$

Also substituting Equations (8.15) and (8.27) in (8.30) gives:

$$np = n_i^2 = 4 \left[ \frac{2\pi K_B T}{h^2} \right]^3 (m_e^* m_h^*)^{3/2} \exp \left( \frac{-E_g}{K_B T} \right)$$

$$n_i = 2 \left[ \frac{2\pi K_B T}{h^2} \right]^{3/2} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2K_B T}\right) \quad (8.32)$$

If  $m_e^* = m_h^* = m$ , where  $m$  is the rest mass of an electron, then Equation (8.32) becomes:

$$\begin{aligned} n_i &= 2 \left( \frac{2\pi m K_B T}{h^2} \right)^{3/2} \exp\left(\frac{-E_g}{2K_B T}\right) \\ &= 2 \left( \frac{2\pi m K_B}{h^2} \right)^{3/2} T^{3/2} \exp\left(\frac{-E_g}{2K_B T}\right) \\ &= CT^{3/2} \exp\left(\frac{-E_g}{2K_B T}\right) \quad (8.33) \end{aligned}$$

where

$$C = 2 \left[ \frac{2\pi m K_B}{h^2} \right]^{3/2} = 4.83 \times 10^{21}$$

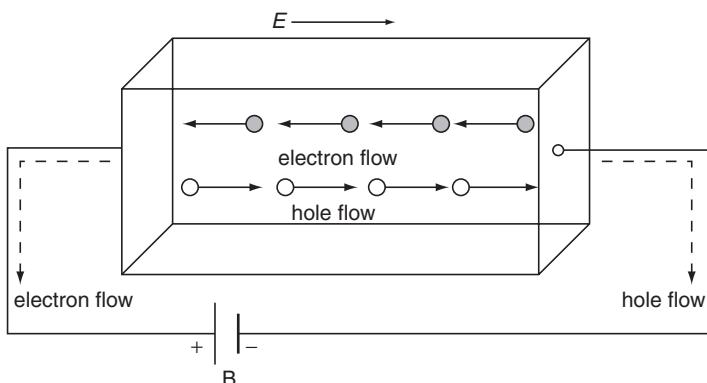
At 300 K, for a semiconductor having  $E_g \approx 1$  eV,  $n_i \approx 10^{17}/\text{m}^3$ .

## 8.3 Electrical conductivity of a semiconductor

In a semiconductor, the conduction band electrons and valence band holes will participate in electrical conduction. To obtain an expression for electrical conductivity, we consider a rectangular bar of intrinsic semiconductor connected to a battery as shown in Fig. 8.3. Then, electric field exists along X-direction. This field accelerates the free (or conduction band) electrons along negative X-direction and holes along X- direction. So, the velocity of electrons along negative X-direction increases and attains some constant resultant velocity. This constant velocity is called drift velocity, represented as  $v_d$ . This drift velocity is superimposed on their random thermal motion. The total electrical current through the semiconductor is the sum of electron current  $I_e$  and hole current  $I_h$ .

The total current ( $I$ ) =  $I_e + I_h$ .

**Figure 8.3** Shows the electric current in intrinsic semiconductor



To find an expression for electrical conductivity, first we shall consider electron flow in the semiconductor. Let  $A$  be the area of cross section of the bar,  $v_{de}$  be the drift velocity of electrons and 'n' be the number of conduction band electrons per unit volume of the semiconductor. Then, the free electrons present in a volume  $A v_{de}$  will cross an imaginary plane assumed to be perpendicular to the bar in 1 second.

$$\text{The number of electrons crossing the imaginary plane in 1 s} = n A v_{de} \quad (8.34)$$

$$\therefore \text{The electron charge which crosses the plane in 1 s} = I_e = n e A v_{de} \quad (8.35)$$

$$\text{The electron current density, } J_e = \frac{I_e}{A} = n e v_{de} \quad (8.36)$$

From Ohm's law, the current density ( $J_e$ ) due to electrons is given as:

$$J_e = \sigma_e E \quad (8.37)$$

where  $\sigma_e$  is the electrical conductivity of electrons.

From Equations (8.36) and (8.37), we have:

$$\sigma_e E = n e v_{de} \quad (8.38)$$

The drift velocity produced per unit applied electric field is called the mobility of electrons represented as:

$$\mu_e = \frac{v_{de}}{E} \quad (\text{or}) \quad v_{de} = \mu_e E \quad (8.39)$$

Substituting Equation (8.39) in (8.38) gives:

$$\sigma_e E = n e \mu_e E \quad (\text{or}) \quad \sigma_e = n e \mu_e \quad (8.40)$$

Equation (8.40) represents electrical conductivity due to electrons.

Similarly, the electrical conductivity of holes ( $\sigma_h$ ) can be obtained. Let  $p$  be the number of holes per unit volume of the material,  $\mu_h$  is the mobility of holes and the charge on a hole is  $e$ , then:

$$\sigma_h = p e \mu_h \quad (8.41)$$

The total conductivity of a semiconductor is given by the sum of Equations (8.40) and (8.41).

$$\begin{aligned} \text{i.e.,} \quad \sigma &= \sigma_e + \sigma_h = n e \mu_e + p e \mu_h \\ &= e [n \mu_e + p \mu_h] \end{aligned} \quad (8.42)$$

For an intrinsic semiconductor,  $n = p = n_i$ , where  $n_i$  is called intrinsic density. So, Equation (8.42) can be represented as

$$\sigma_i = n_i e [\mu_e + \mu_h] \quad (8.43)$$

The mobilities of carriers depend on temperature in the following way  $\mu \propto \frac{1}{T^{3/2}}$

For electrons,  $\mu_e = \alpha T^{-3/2}$  and for holes  $\mu_h = \beta T^{-3/2}$  (8.44)

where  $\alpha$  and  $\beta$  are proportionality constants.

$$\begin{aligned} \text{So,} \quad \mu_e + \mu_h &= (\alpha + \beta) T^{-3/2} \\ &= \gamma T^{-3/2} \quad (8.45) \quad \text{where } \gamma = \alpha + \beta \end{aligned}$$

Substituting Equation (8.45) in (8.43), we get:

$$\sigma_i = n_i e \gamma T^{-3/2} \quad \text{--- (8.46)}$$

The intrinsic concentration  $n_i$  is given as:

$$n_i = CT^{3/2} \exp\left[\frac{-E_g}{2K_B T}\right] \quad \text{--- (8.47)} \quad \text{where} \quad C = 2 \left[\frac{2\pi m K_B}{h^2}\right]^{3/2}$$

Substituting Equation (8.47) in (8.46) gives:

$$\begin{aligned} \sigma_i &= CT^{3/2} \exp[-E_g/2K_B T] e \gamma T^{-3/2} \\ &= \gamma C e \exp[-E_g/2K_B T] \\ &= B \exp[-E_g/2K_B T] \quad \text{--- (8.48)} \quad \text{where} \quad B = \gamma C e = \text{constant} \end{aligned}$$

This is the expression for electrical conductivity of an intrinsic semiconductor. The resistivity ( $\rho_i$ ) can be written as:

$$\rho_i = \frac{1}{\sigma_i} = \frac{1}{B} \exp\left(\frac{E_g}{2K_B T}\right) = A \exp\left(\frac{E_g}{2K_B T}\right) \quad \text{--- (8.49)}$$

where  $A = \frac{1}{B} = \text{constant}$

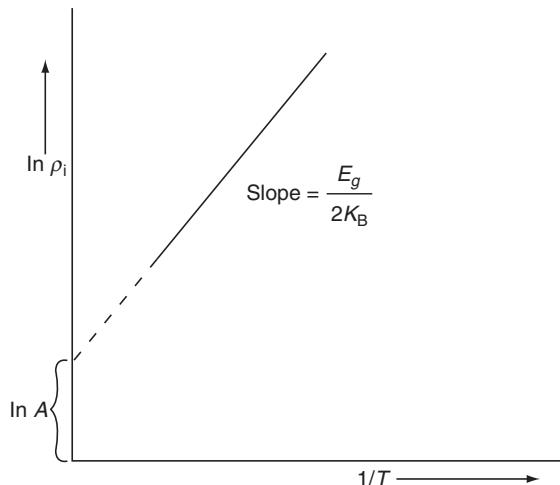
## To find energy gap of a semiconductor

Taking logarithms on both sides of Equation (8.49), we have:

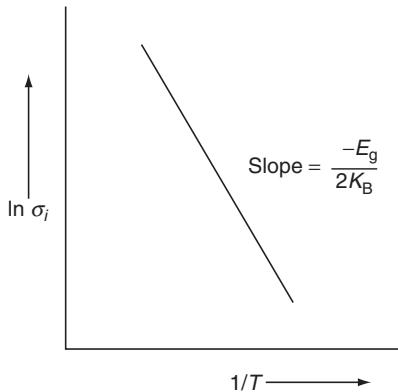
$$\ln \rho_i = \frac{E_g}{2K_B T} + \ln A \quad \text{--- (8.50)}$$

This equation represents a straight line.

**Figure 8.4** A graph between  $\ln \rho_i$  versus  $1/T$  for an intrinsic semiconductor



**Figure 8.5** A graph between  $\ln \sigma_i$  versus  $1/T$  for an intrinsic semiconductor



At different temperatures, the resistivity ( $\rho_i$ ) of an intrinsic semiconductor has been determined. A graph has been plotted between  $\ln \rho_i$  versus  $1/T$  as shown in Fig. 8.4.

The graph is a straight line, and the slope of the line is equal to  $E_g/2K_B$ . Equating the slope of the graph to  $E_g/2K_B$ ,  $E_g$  can be determined.

The intercept on  $\ln \rho_i$  axis is equal to  $\ln A$ . We can also obtain energy gap using Equation (8.48). A graph can be drawn between  $\ln \sigma_i$  versus  $1/T$ , the resulting graph is a straight line as shown in Fig. 8.5. This graph has a negative slope, which is equal to  $-E_g/2K_B$ , from this,  $E_g$  can be obtained. The energy gap of Ge and Si are 0.72 eV and 1.12 eV respectively.

### Increase of temperature to double the conductivity

From Equation (8.46), we know doubling the conductivity is equal to doubling the intrinsic concentration by raising the temperature. The intrinsic concentration is:

$$n_i = (N_V N_C)^{1/2} \exp\left[\frac{-E_g}{2K_B T}\right] \quad (8.51)$$

To double  $n_i$ , the increase in temperature is (say)  $\Delta T$ , then, we have:

$$2n_i = (N_V N_C)^{1/2} \exp\left[\frac{-E_g}{2K_B(T + \Delta T)}\right] \quad (8.52)$$

Dividing Equation (8.52) by (8.51), we have:

$$2 = \exp\left[\frac{-E_g}{2K_B(T + \Delta T)}\right] \exp\left[\frac{E_g}{2K_B T}\right] \Rightarrow 2 = \exp\left[\frac{E_g}{2K_B} \left(\frac{1}{T} - \frac{1}{T + \Delta T}\right)\right]$$

$$2 = \exp\left[\frac{E_g}{2K_B} \frac{\Delta T}{T(T + \Delta T)}\right] \Rightarrow 2 = \exp\left[\frac{E_g}{2K_B} \frac{\Delta T}{T^2}\right]$$

$$\text{since} \quad T(T + \Delta T) \approx T^2$$

Taking logarithms on both sides, we get:

$$\ln 2 = \frac{E_g}{2K_B T} \left( \frac{\Delta T}{T} \right) \quad (\text{or}) \quad \frac{\Delta T}{T} = \frac{2K_B T}{E_g} \ln 2 \quad (8.53)$$

In Equation (8.53),  $\Delta T$  represents the increase in temperature to double the electrical conductivity of an intrinsic semiconductor. At room temperature, the conductivities of Si and Ge doubles for every  $10^\circ\text{C}$  and  $15^\circ\text{C}$  increase in temperature, respectively. Therefore, we conclude that semiconductors are very sensitive to the temperature changes.

## 8.4 Extrinsic semiconductors

The conductivity of an intrinsic semiconductor can be increased enormously by adding small amounts of impurity atoms [such as III or V group atoms]. For example, the conductivity of silica is increased by 1000 times on adding 10 parts of boron per million part of Si. The process of adding impurities is called doping and the impurity added is called dopant. The doping is done during crystallization process [i.e., when the substance is in molten state]. On crystallization, the impurity atoms replace some of the intrinsic atoms.

When some pentavalent [Group V] impurity atoms such as P [or As, Sb, Bi, etc.] are added to an intrinsic semiconductor Si (or Ge), then the impurity atoms interlock in the crystal lattice because the size of impurity atoms is not greatly different from that of silica atoms. As shown in Fig. 8.6(a), four of the five valence electrons of phosphorous will make covalent bonds with the surrounding silica atoms and the fifth electron is feebly attached with the phosphorous atom at 0 K. The ground state energy of this fifth electron lies just below the conduction band of silica. The phosphorous atoms create an energy level that lies at 0.045 eV below the conduction band of silica as shown in Fig. 8.6(b). The number of electron states in this level is equal to the number of phosphorous atoms present per unit volume of the material. Each electron state is represented by a dash in this energy level. At 0 K, the fifth electron of phosphorous atoms occupy these electron states. If we slightly rise the temperature of the material such that the increase in the energy of fifth electron of phosphorous is equal to or greater than 0.045 eV, then that electron enters into the conduction band of silica. In the crystal, that electron moves away from the binding forces of phosphorous atom and moves freely in the crystal. Now, this electron will participate in electrical conduction.

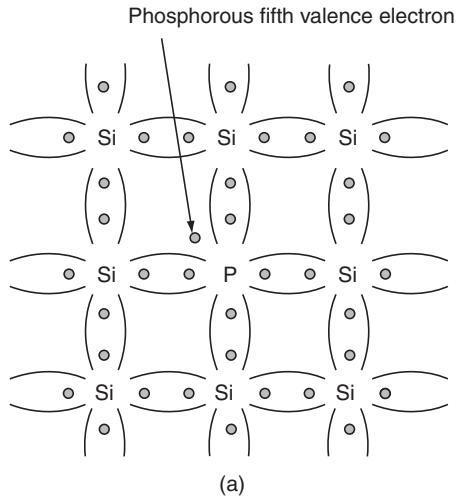
The increase in temperature to free the fifth electron of phosphorous is very much less compared to the increase in temperature to break a covalent bond in the crystal. This means the phosphorous atoms readily give electrons for conduction, and also the energy level created by phosphorous atoms in the energy gap is called donor energy level ( $E_D$ ). Even at low temperatures, the donor level donates electrons to the conduction band as shown in Fig. 8.6(c).

When an electron leaves a phosphorous atom, then it remains as a positive ion, but holes will not be created. So, we have large number of electrons in the conduction band than the holes in the valence band. At room temperature  $TK$ , the number of electrons in the conduction band is equal to the number of phosphorous atoms per unit volume and the number of covalent bonds broken per unit volume of the material, whereas the number of holes in the valence band is equal to the number of covalent bonds ruptured per unit volume of the material. The free electrons are very large in number compared to the holes in the material. Electrons are the majority carriers and holes are the minority carriers, so this material is called n-type semiconductor.

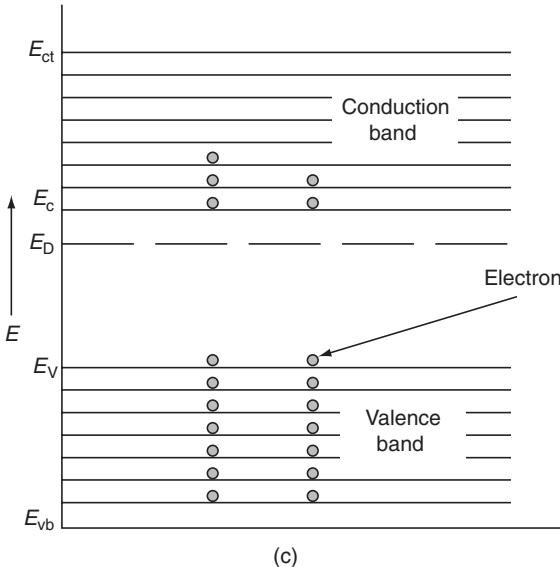
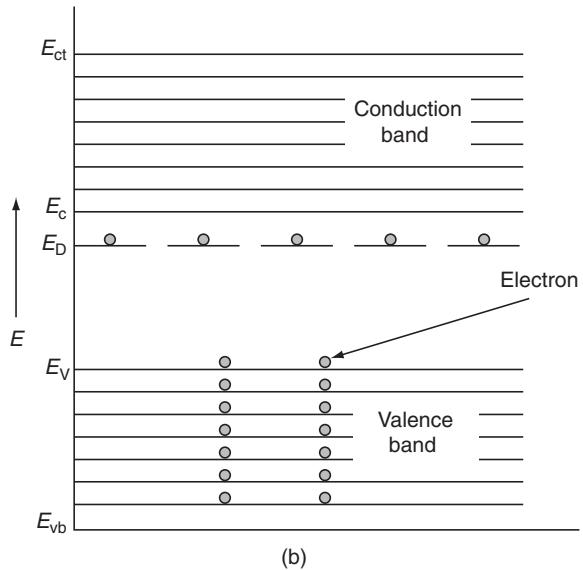
Instead of adding pentavalent impurity atoms, if trivalent [Group III] impurity atoms such as B [or Al, Ga, In, etc.] atoms are doped in an intrinsic semiconductor, Si (or Ge), then the impurity atoms occupy some of the silica atom sites because the size of impurity atoms and Si atoms is almost the same. As shown in Fig. 8.7(a), with three valence electrons each boron atom makes three covalent bonds with the surrounding three silica atoms. To attain stability, it completes fourth covalent bond by accepting a stray electron in its vicinity. Since this stray electron belongs to a silica atom, silica atom acquires a hole. The boron atoms introduce an energy level just above the valence band in the energy gap of silica crystal. The number

Figure 8.6

(a) Two dimensional crystal structure of silica doped with phosphorous atoms; (b) Energy band diagram of n-type material at 0 K; (c) Energy band diagram of n-type material at TK

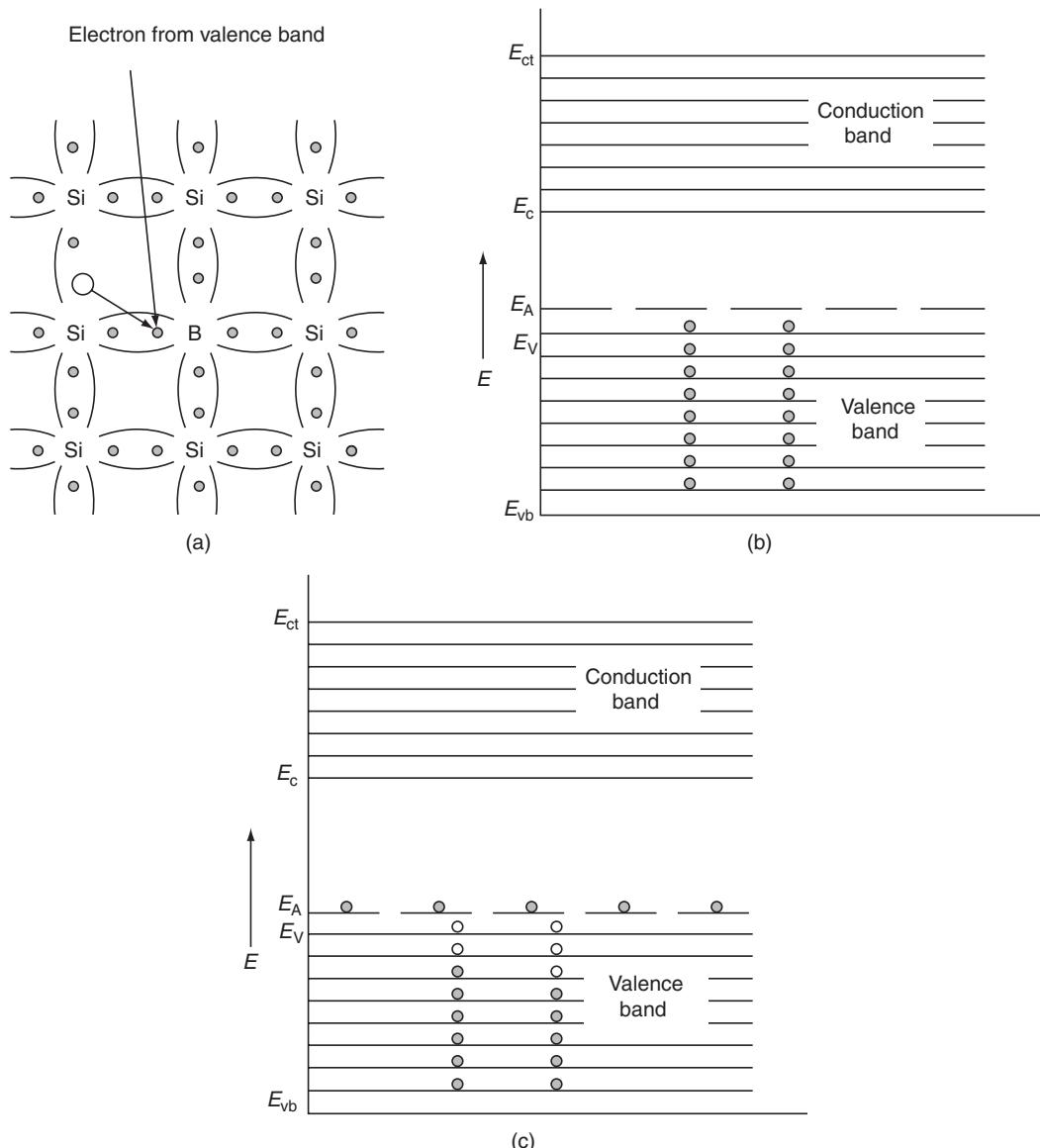


(a)



of electron states in this energy level is equal to the number of boron atoms present per unit volume of silica crystal. Each electron state of this energy level is represented by a dash in the band diagram as shown in Fig. 8.7(b). This energy level is called acceptor energy level because the electron states in this energy level readily receive electrons from the valence band. The number of holes formed in the valence band is equal to the number of electrons transferred to acceptor states. Since the energy difference between acceptor level and valence band energy levels is very small, so even at very low temperatures the valence band electrons gain sufficient thermal energy to occupy the acceptor energy level states as shown in Fig. 8.7(c).

**Figure 8.7** (a) Crystal structure of a p-type material; (b) Energy band diagram of p-type material at 0 K; (c) Energy band diagram of p-type material at  $T_K$



After receiving an electron, the boron atom becomes a negative ion. At room temperature  $T_K$ , the number of holes present per unit volume of the material is equal to the number of boron ions and number of covalent bonds ruptured. In this material, holes are large compared to conduction electrons. Holes are majority carriers and electrons are minority carriers, so this type of material is called a p-type semiconductor.

In a semiconductor at  $T_K$ , the rate of electron hole recombination is proportional to electron concentration and hole concentration. In general, the recombination rate is proportional to the product  $np$ . In an intrinsic

semiconductor,  $n = p = n_i$ , so that  $np = n_i^2$ . In case of n-type semiconductor,  $n$  is large and correspondingly  $p$  is less so that the product remains constant. Similarly, in case of p-type semiconductor, holes are large; so correspondingly conduction electrons reduces so that the product  $np$  remains constant.

## 8.5 Carrier concentration in extrinsic semiconductors

The number of charge carriers present per unit volume of a semiconductor material is called carrier concentration. Suppose donor and acceptor atoms are doped in a semiconductor, then at some room temperature  $TK$ , the material contains  $n, p, N_A^-$  and  $N_D^+$ , which denote number of conduction electrons, holes, acceptor ions and donor ions per unit volume of material, respectively. The material will be electrically neutral if,

$$n + N_A^- = p + N_D^+ \quad (8.54)$$

That is the total negative charge due to conduction electrons and acceptor ions is equal to holes and donor ions in unit volume of material. Equation (8.54) is called charge neutrality equation. In the above equation,

$$n = N_C \exp\left[\frac{-(E_C - E_F)}{K_B T}\right] \quad \text{and} \quad p = N_V \exp\left[\frac{-(E_F - E_V)}{K_B T}\right] \quad (8.55)$$

And the product of acceptor concentration and the probability of finding an electron in acceptor level gives the concentration of acceptor ions [i.e.,  $N_A^-$ ].

$$\therefore N_A^- = \frac{N_A}{1 + \exp\left[\frac{E_A - E_F}{K_B T}\right]} \quad (8.56)$$

Similarly, the donor ions concentration is:

$$\begin{aligned} N_D^+ &= N_D \left[ 1 - \frac{1}{1 + \exp\left[\frac{(E_D - E_F)}{K_B T}\right]} \right] = N_D \left[ \frac{\exp\left[\frac{E_D - E_F}{K_B T}\right]}{1 + \exp\left[\frac{E_D - E_F}{K_B T}\right]} \right] \\ &= N_D \left[ \frac{1}{1 + \exp\left(\frac{E_F - E_D}{K_B T}\right)} \right] \end{aligned} \quad (8.57)$$

In n-type material, there are no acceptor atoms [and hence the acceptor ions], so  $N_A^- = 0$ . At 0 K, all the electron states in donor level are occupied by electrons. As the temperature is increased from 0 K, some of the electrons jump from these donor states into the conduction band, leaving these states empty of electrons. Also the concentration of holes is extremely less compared with the concentration of conduction electrons [i.e.,  $p \ll n$ ]. From Equation (8.54), we have:

$$n = p + N_D^+$$

$$(\text{or}) \quad n \approx N_D^+ \quad (\text{since } p \ll N_D^+) \quad [\text{since } p \ll N_D^+]$$

At some room temperature  $T$ K, almost all the donor atoms donate electrons to conduction band. So, in n-type material, the free electron concentration is almost equal to the donor atoms. Then, Equation (8.58) can be written as:

$$n_n \approx N_D \quad \text{_____} \quad (8.59)$$

where  $n_n$  represents electrons in n-type material

The hole concentration in n-type material can be obtained by applying law of mass action [i.e.,  $np = n_i^2$ ] as  $n_n p_n = n_i^2$

$$\text{(or)} \quad p_n = \frac{n_i^2}{n_n} \approx \frac{n_i^2}{N_D} \quad \text{_____} \quad (8.60)$$

where  $p_n$  represents holes concentration in n-type material. In n-type material at 0 K, the Fermi energy level lies in the middle of  $E_C$  and  $E_D$  as shown in Fig. 8.8(a).

$$\text{i.e.,} \quad E_F = \frac{E_C + E_D}{2}$$

As the temperature increases from 0 K, the Fermi level shifts upwards according to Equation (8.61) slightly due to ionization of donor atoms. With further increase of temperature, electron-hole pairs are generated due to the breaking of covalent bonds, hence Fermi level shifts downwards.

$$E_F = \frac{E_C + E_D}{2} + \frac{1}{2} K_B T \ln \left( \frac{N_D}{N_C} \right) \quad \text{_____} \quad (8.61)$$

In p-type semiconductor, there are no donor atoms [and hence no  $N_D^+$  ions], so  $N_D^+ = 0$ . At 0 K, all the acceptor levels are not occupied by electrons. As the temperature is increased from 0 K, some electrons jump from top valence band energy levels to the acceptor states, leaving holes in the valence band and acceptor ions  $N_A^-$  are formed. At some room temperature  $T$ K, concentration of conduction electrons is extremely less compared with hole concentration.

$$\therefore \text{From Equation (8.54), we have:} \quad n + N_A^- = p \quad \text{_____} \quad (8.62)$$

$$\text{(or)} \quad N_A^- \approx p \quad \text{_____} \quad (8.63) \quad [\text{since } n \ll N_A^-]$$

At some room temperature  $T$ K, in p-type material, the hole concentration is almost equal to the acceptor atoms in unit volume of the material. So, Equation (8.63) can be written as:

$$p_p \approx N_A \quad \text{_____} \quad (8.64)$$

where  $p_p$  represents holes in p-type material

The electron concentration in p-type material can be obtained by applying law of mass action [i.e.,  $pn = n_i^2$ ] as  $n_p p_p = n_i^2$

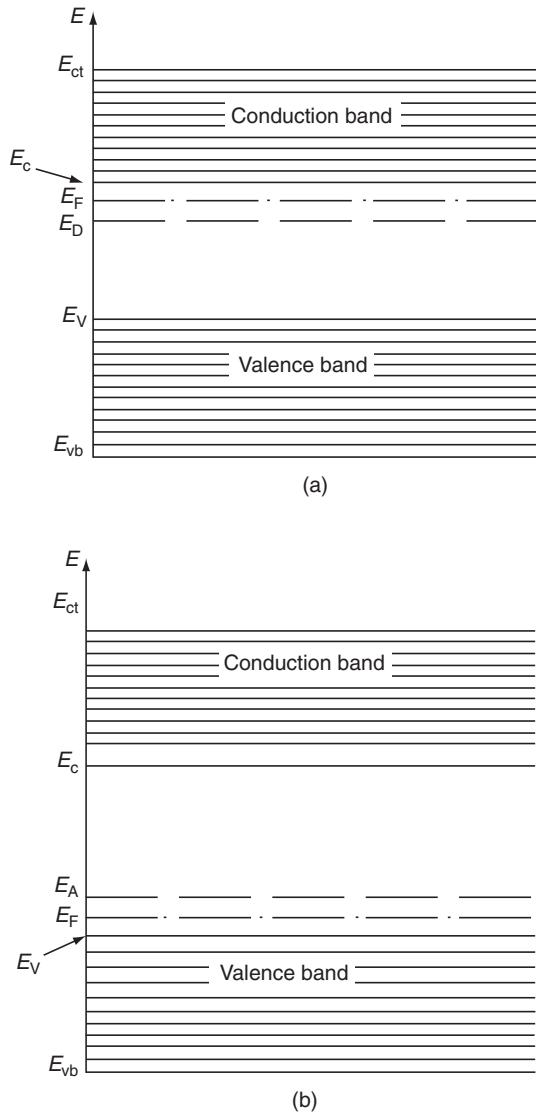
$$\text{(or)} \quad n_p = \frac{n_i^2}{p_p} \approx \frac{n_i^2}{N_A} \quad \text{_____} \quad (8.65)$$

where  $n_p$  represent free electron concentration in p-type material. In p-type material, the Fermi level lies in between  $E_V$  and  $E_A$  at 0 K, as shown in Fig. 8.8(b). As the temperature is increased from 0 K, the Fermi level shifts downwards slightly as per Equation (8.66) due to ionization of acceptor atoms. And with further increase of temperature, electron-hole pairs are generated due to the rupture of covalent bonds, so Fermi level shifts upwards.

$$E_F = \frac{E_V + E_A}{2} - \frac{K_B T}{2} \ln \left( \frac{N_A}{N_V} \right) \quad \text{_____} \quad (8.66)$$

Figure 8.8

(a) Band diagram of n-type material at 0 K; (b) Band diagram of p-type material at 0 K



## 8.6 Minority carrier life time

In this topic, we will study the life time of minority carriers in an extrinsic semiconductor. In n-type semiconductor, hole carrier life time and in p-type semiconductor electron carrier life time are called the minority carrier life times. This can be explained in the following way.

In a semiconductor, the conduction electrons and holes are moving in random directions. So, for every second, some free electrons may come across holes or some holes may come across free electrons and recombination takes place. For every recombination, a pair of electron-hole will be lost in the material. The number of recombinations take place in 1 second per unit volume of the material is called recombination rate and is represented by ' $R$ '. The recombination rate is proportional to electron concentration and hole concentration in the material. In general, recombination rate is proportional to the product of electron and hole concentrations.

$$\text{i.e., } R \propto np$$

$$R = rnp \quad \dots \quad (8.67)$$

where ' $r$ ' is the proportionality constant called recombination coefficient. Suppose a semiconductor is in thermal equilibrium at some (room) temperature  $T$ K. At this temperature, due to recombination, the carrier concentration should decrease, but actually carrier concentration remains constant as long as the temperature remains constant. So, equal number of electrons and holes is generated due to thermal energy. The number of electron-hole pairs created in 1 second per unit volume of the material is called carrier generation rate and is represented as ' $g$ '. In the semiconductor on an average, a hole exists for a time  $\tau_p$  and an electron exists for a time  $\tau_n$  before recombination. In n-type material,  $\tau_p$  is called minority carrier life time and in p-type material  $\tau_n$  is called minority carrier life time. The rate of change of hole concentration in n-type material is:

$$\frac{dp}{dt} = g_T - rnp \quad \dots \quad (8.68)$$

where  $g_T$  is thermal generation rate of electrons and holes.

$$\text{At thermal equilibrium, } \frac{dp}{dt} = 0$$

$$\therefore g_T = rm_0 p_0 \quad \dots \quad (8.69)$$

where  $n_0$  and  $p_0$  are equilibrium concentrations of electrons and holes, respectively.

Let an n-type semiconductor is slightly disturbed from equilibrium by thermal or by optical excitation, then few excess of holes ( $\Delta p$ ) and equal number of electrons ( $\Delta n$ ) are created in unit volume. Then, the percentage increase of holes [minority carriers] is much larger than percentage increase of electrons. Hence, we are interested in hole (minority) carrier life time in n-type material. The excess of hole recombination rate (or loss) at a time ' $t$ ' is given by:

$$\begin{aligned} -\frac{d}{dt}(\Delta p) &= r(n_0 + \Delta n)(p_0 + \Delta p) - rm_0 p_0 \\ &= r(n_0 p_0 + n_0 \Delta p + \Delta n p_0 + \Delta n \Delta p - n_0 p_0) \\ &\approx r[n_0 \Delta p + \Delta n p_0] \end{aligned}$$

$$(\text{or}) \quad \frac{d\Delta p}{dt} = -r \Delta p [n_0 + p_0] \quad \dots \quad (8.70) \quad [\text{Since } \Delta n = \Delta p]$$

In the above equation, the quantity  $r(n_0 + p_0)$  has the dimensions of time inverse.

$$\text{So, } \frac{1}{r(n_0 + p_0)} = \tau = \text{minority carrier life time.}$$

$$\text{Equation (8.70) can be written as: } -\frac{d}{dt} \Delta p = \frac{\Delta p}{\tau} \quad \dots \quad (8.71)$$

Equation (8.71) is integrated by variable separation method.  $\frac{d(\Delta p)}{(\Delta p)} = \frac{-dt}{\tau}$

(or)  $\ln(\Delta p) = \frac{-t}{\tau} + \ln C$  where  $\ln C$  is integration constant

$$\ln\left(\frac{\Delta p}{C}\right) = \frac{-t}{\tau}$$

Taking exponential on both sides,  $(\Delta p) = C e^{-t/\tau}$  (8.72)

'C' can be found by applying initial conditions.

At  $t = 0$ ,  $\Delta p$  is equal to  $(\Delta p)_0 = C$

Equation (8.72) becomes  $\Delta p = (\Delta p)_0 e^{-t/\tau}$  (8.73)

After time  $\tau$  from excitation of semiconductor [i.e., at  $t = \tau$ ]

$$\Delta p = (\Delta p)_0 e^{-\tau/\tau} = \frac{(\Delta p)_0}{e} = \frac{(\Delta p)_0}{2.718} = 37\% \text{ of } (\Delta p)_0$$

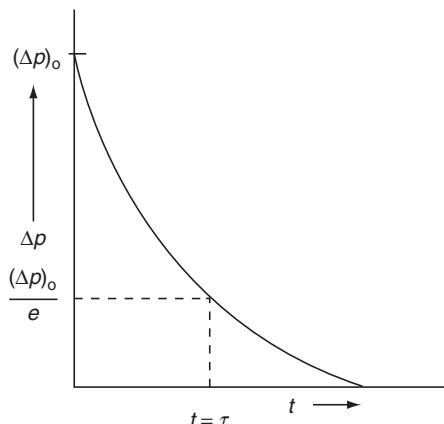
So, minority carrier life time ( $\tau$ ) is defined as the time in which the excess carrier concentration reduces to  $1/e$  or 37% of its initial value. The life time in a pure semiconductor free from defects range from 2000 to 3000 micro seconds.

A graph plotted between  $\Delta p$  versus 't' is shown in Fig. 8.9.

The carrier life time depends on the bulk of the material, i.e., life time measured in an infinite crystal and on the surface, i.e., the life time measured due to the condition on sample surface.

$$\begin{aligned} \text{Then, } \Delta p &= (\Delta p)_0 \exp\left(\frac{-t}{\tau_B}\right) \exp\left(\frac{-t}{\tau_S}\right) = (\Delta p)_0 \exp\left[-t\left(\frac{1}{\tau_B} + \frac{1}{\tau_S}\right)\right] \\ &= (\Delta p)_0 \exp\left(\frac{-t}{\tau}\right) \end{aligned}$$

**Figure 8.9 Excess hole [minority] carrier concentration decay with respect to time**



$$\therefore \frac{1}{\tau} = \frac{1}{\tau_B} + \frac{1}{\tau_S}$$

where  $\tau$  = observed life time

$\tau_B$  = bulk life time and  $\tau_s$  = surface life time

$\tau_B$  is measured by observing  $\tau$  for a variety of surface treatments.

## 8.7 Drift and diffusion currents

Often, we come across drift and diffusion currents in semiconductors. The drift current occurs due to an applied electric field on a semiconductor and the diffusion current occurs whenever carrier concentration gradient exists in the material. In a semiconductor, both currents are explained separately in the following way.

### (a) Drift current

Let us consider a semiconductor material of length ' $l$ ' at some (room) temperature  $T_K$ . At this temperature, the free electron and hole concentrations are  $n$  and  $p$ , respectively. The free electrons and holes possess random motions so that they do not possess any resultant velocity in any direction inside the crystal. When a voltage ' $V$ ' is applied across the semiconductor, then the intensity of electric field ( $E$ ) in the material is equal to  $V/l$ . This electric field ( $E$ ) exerts a force  $eE$  on each carrier, so that an acceleration  $eE/m$  acts on the carriers, the velocities of electrons and holes are increased in opposite directions up to certain constant value called drift velocity of carriers. These velocities will not increase to large values because of electrical resistance due to thermal vibrations of ions (or atoms) at that temperature. The drift velocities of electrons and holes produce drift current in the material. The drift current density of electrons is:

$$J_{n,\text{drift}} = nev_{de} \quad (8.74)$$

where  $v_{de}$  is the drift velocity of electrons and ' $n$ ' is the number of conduction (free) electrons per unit volume of material. The current density of electrons can also be represented using Ohm's law as:

$$J_{n,\text{drift}} = \sigma_n E \quad (8.75)$$

where  $\sigma_n$  is the electrical conductivity of free electrons.

From Equations (8.74) and (8.75) we have:

$$\sigma_n E = nev_{de} \quad (8.76)$$

The drift velocity of an electron can be found in the following way:

The moment at which we apply electric field [ $E$ ] on the semiconductor ( $t = 0$ ), the drift velocity is zero [ $v_{de} = 0$ ]. The electric field exerts a force  $eE$  on each electron, so that each electron acquires constant drift velocity  $v_{de}$  after time  $\tau$ , called collision time.  $v_{de}$  can be obtained from equations of motion [ $v = u + at$ , as in dynamics].

$$v_{de} = 0 + \left( \frac{eE}{m} \right) \tau = \left( \frac{e\tau}{m} \right) E \quad (8.77)$$

In Equation (8.77)  $e\tau/m$  is constant and it can be represented as  $\mu_n$  [ $= e\tau/m$ ], called mobility of electrons. Therefore, Equation (8.77) can be represented as:

$$v_{de} = \mu_n E \quad (8.78)$$

Substituting Equation (8.78) in (8.76) we have:

$$\sigma_n E = ne\mu_n E \quad (\text{or}) \quad \sigma_n = ne\mu_n \quad (8.79)$$

Similarly, the conductivity of holes can be written as:

$$\sigma_p = pe\mu_p \quad (8.80)$$

The total drift conductivity of the semiconductor is:

$$\sigma = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p \quad (8.81)$$

In an intrinsic semiconductor,  $n = p = n_i$

$$\text{so } \sigma_i = n_i e(\mu_n + \mu_p) \quad (8.82)$$

The resistivity ( $\rho$ ) of the semiconductor is:

$$\rho = \frac{1}{\sigma} = \frac{1}{ne\mu_n + pe\mu_p} \quad (8.83)$$

Using Equation (8.81), we can write the drift current densities of electrons and holes as:

$$J_{n,\text{drift}} = ne\mu_n E \quad (8.84) \quad \text{and} \quad J_{p,\text{drift}} = pe\mu_p E \quad (8.85)$$

The total drift current density is equal to sum of electron and hole drift current densities.

$$J_{\text{drift}} = ne\mu_n E + pe\mu_p E \quad (8.86)$$

The variation of conductivity with temperature can be described as follows: At 0 K, there are no carriers in the semiconductor. As the temperature of a semiconductor is increased from 0 K to some low temperature, then the electrons present in donor level will go to conduction band in n-type semiconductor or electrons present in valence band will go to acceptor level to produce holes in valence band of p-type semiconductor. By increasing temperature from 0 K to some low temperature ( $T_K$ ), the carrier concentration increases in the extrinsic semiconductor. Also the thermal vibrations of ions and hence electrical resistivity increases. The increase in conductivity depends on the relative values of the above two quantities, so conductivity increases. Afterwards as the temperature of extrinsic semiconductor is increased near to room temperature, the carrier concentration would not increase and resistivity increases. So, the material possesses positive temperature coefficient of resistivity. Above room temperature, the intrinsic carrier concentration and hence the conductivity increases with rise of temperature compared to the increase of resistivity. So, the material possesses negative temperature coefficient of resistivity at and above room temperatures. At higher temperatures, the material exhibits its intrinsic behaviour [i.e., the covalent bonds are ruptured with an increase of temperature and forms equal conduction electrons and holes in the semiconductor].

## (b) Diffusion current

Non-uniform concentration of charge carriers produces diffusion current. Non-uniform concentration of charge carriers can be formed by thermal or radiation excitation of a part of the material or by injecting carriers into the material through surface.

Suppose the concentration of electrons and holes increases by  $\Delta n$  and  $\Delta p$  at a point in the material due to excitation. These excess carriers diffuse to low concentrated place; the rate of diffusion according to Fick's law is proportional to concentration gradient  $\frac{\partial \Delta n}{\partial x}$  along X-direction for excess electrons. As the flow takes place from high concentration region to low concentration region, so the rate of flow of electrons

is proportional to  $-\frac{\partial}{\partial x} \Delta n$ , and the rate of flow of electrons through unit area is equal to  $-D_n \frac{\partial(\Delta n)}{\partial x}$ . Here,  $D_n$  is the proportionality constant called diffusion coefficient of electrons. This electron charge flow constitutes electron diffusion current density represented as  $J_{n, \text{diff}}$

$$J_{n, \text{diff}} = (-e) \times \left[ -D_n \frac{\partial(\Delta n)}{\partial x} \right] = D_n e \frac{\partial(\Delta n)}{\partial x} \quad (8.87)$$

Similarly for holes,

$$J_{p, \text{diff}} = (e) \times \left[ -D_p \frac{\partial(\Delta p)}{\partial x} \right] = -D_p e \frac{\partial(\Delta p)}{\partial x} \quad (8.88)$$

where  $D_p$  is called diffusion coefficient of holes. Even though the excess electrons and holes diffuses in the same direction, their current densities are in opposite direction because of opposite charge on electron and hole. The total diffusion current is:

$$\begin{aligned} J_{\text{diff}} &= J_{n, \text{diff}} + J_{p, \text{diff}} \\ &= D_n e \frac{\partial(\Delta n)}{\partial x} - D_p e \frac{\partial(\Delta p)}{\partial x} \end{aligned} \quad (8.89)$$

If there is concentration gradient along X-direction and if we apply an electric field  $E$  on it, then the total current in the semiconductor is the sum of drift and diffusion currents. The total current due to electrons and holes are:

$$\begin{aligned} J_n &= J_{n, \text{drift}} + J_{n, \text{diff}} \\ &= ne\mu_n E + D_n e \frac{\partial(\Delta n)}{\partial x} \end{aligned} \quad (8.90)$$

$$\begin{aligned} J_p &= J_{p, \text{drift}} + J_{p, \text{diff}} \\ &= pe\mu_p E - D_p e \frac{\partial(\Delta p)}{\partial x} \end{aligned} \quad (8.91) \quad \text{and} \quad J = J_n + J_p$$

$$J_{\text{total}} = ne\mu_n E + D_n e \frac{\partial(\Delta n)}{\partial x} + pe\mu_p E - D_p e \frac{\partial(\Delta p)}{\partial x} \quad (8.92)$$

## 8.8 Einstein's relations

Einstein showed the direct relation between the mobility ( $\mu$ ) and diffusion coefficient ( $D$ ) of a semiconductor. Suppose a semiconductor is in equilibrium at some temperature  $TK$  with no applied electric field. The free electrons and holes distribution is uniform and there is no net current flow in any direction. Any disturbance in the carrier concentration leads to diffusion current in the material. As the material is at some temperature  $TK$ , it possesses electrical resistance due to thermal vibrations of ions. The product of resistance and diffusion current results in voltage and hence electric field in the material. Therefore, in equilibrium, the drift and diffusion currents due to excess concentration are equal. So, for electrons, we can write:

$$(\Delta n)e\mu_n E = D_n e \frac{\partial(\Delta n)}{\partial x} \quad (8.93)$$

The force ( $F$ ) on excess electrons ( $\Delta n$ ) to restore equilibrium is given by the product of  $\Delta n$  and electric force  $eE$  on each electron. Thus, we have:

$$F = (\Delta n) eE \quad \text{_____} \quad (8.94)$$

Equation (8.93) can be written as:

$$(\Delta n) eE = \frac{D_n}{\mu_n} e \frac{\partial(\Delta n)}{\partial x} = F \quad \text{_____} \quad (8.95)$$

At temperature  $T$ K, the force on excess electrons to maintain equilibrium depends on thermal energy of excess electrons [equal to  $K_B T$ ] times the concentration gradient  $\frac{\partial(\Delta n)}{\partial x}$ .

$$\text{Thus, } F = K_B T \frac{\partial(\Delta n)}{\partial x} \quad \text{_____} \quad (8.96)$$

Equations (8.95) and (8.96) are equal.

$$\frac{D_n}{\mu_n} e \frac{\partial(\Delta n)}{\partial x} = K_B T \frac{\partial(\Delta n)}{\partial x} \quad (\text{or}) \quad \frac{D_n}{\mu_n} = \frac{K_B T}{e} \quad \text{_____} \quad (8.97)$$

$$(\text{or}) \quad D_n = \mu_n \frac{K_B T}{e} \quad \text{_____} \quad (8.98)$$

Similarly, for holes,

$$\frac{D_p}{\mu_p} = \frac{K_B T}{e} \quad \text{_____} \quad (8.99) \quad (\text{or}) \quad D_p = \mu_p \frac{K_B T}{e} \quad \text{_____} \quad (8.100)$$

From Equations (8.97) and (8.99), we have:

$$\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} \quad \text{_____} \quad (8.101) \quad (\text{or}) \quad \frac{D_n}{D_p} = \frac{\mu_n}{\mu_p} \quad \text{_____} \quad (8.102)$$

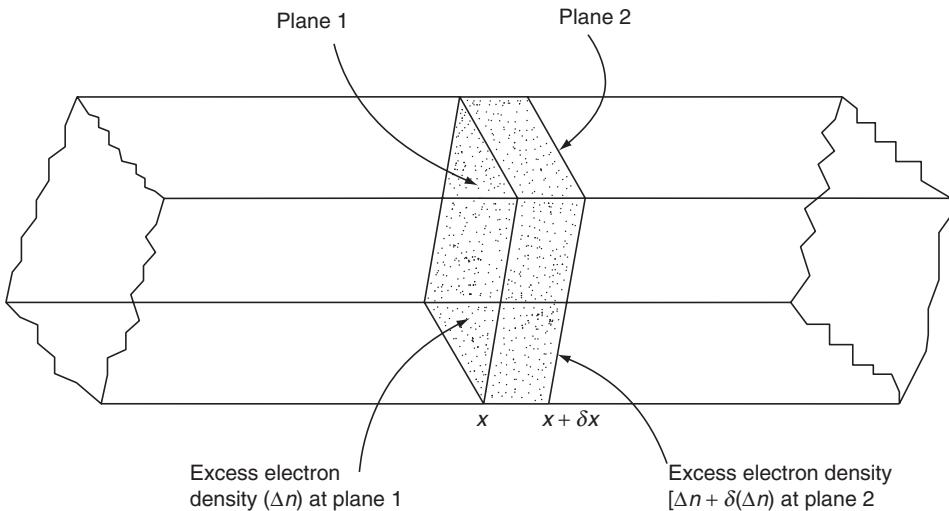
Equations (8.97) to (8.102) are called Einstein's equations. Using the above equations, the diffusion coefficients of electrons and holes can be determined. At 300 K,  $\frac{K_B T}{e} = 26$  mV. The diffusion coefficients for Si are  $D_n = 3.6 \times 10^{-3}$  m<sup>2</sup>/s and  $D_p = 1.3 \times 10^{-3}$  m<sup>2</sup>/s and for Ge,  $D_n = 10 \times 10^{-3}$  m<sup>2</sup>/s and  $D_p = 5 \times 10^{-3}$  m<sup>2</sup>/s.

## 8.9 Continuity equation

The mathematical relations formed from the excess carriers in unit volume of semiconductor due to generation, recombination, drift and diffusion are called continuity equations. The continuity equation can be derived with reference to an elemental volume  $A \delta x$  at  $x$  in a rectangular bar of semiconductor is shown in Fig. 8.10.

Let the number of excess electrons in the element due to generation, recombination, drift and diffusion is  $\Delta n$  ( $A \delta x$ ) and the rate of increase of this number in the element is:

Figure 8.10 A rectangular bar of semiconductor



$$\frac{\partial}{\partial t}(\Delta n) A \delta x \quad \text{_____ (8.103)}$$

This value can be extracted separately in the following way:

- (a) Rate of increase of an excess electron concentration due to generation and recombination: At thermal equilibrium, the rate of generation is equal to rate of recombination represented as  $r n_0 p_0$ , where  $r$  is recombination coefficient,  $n_0$  and  $p_0$  are equilibrium concentration of free electrons and holes. Due to thermal or optical excitation, carriers are generated and the concentration of electrons and holes becomes  $n_0 + \Delta n$  and  $p_0 + \Delta p$ . Now, the recombination rate is equal to  $r(n_0 + \Delta n)(p_0 + \Delta p)$ . The rate of increase of carriers per unit volume is equal to the difference between the two rates of recombination.

$$\text{i.e., } -\frac{\partial(\Delta n)}{\partial t} = r(n_0 + \Delta n)(p_0 + \Delta p) - r n_0 p_0$$

$$\begin{aligned} -\frac{\partial(\Delta n)}{\partial t} &= r[n_0 p_0 + n_0 \Delta p + p_0 \Delta n + \Delta n \Delta p - n_0 p_0] \\ &\approx r[n_0 \Delta p + p_0 \Delta n] \quad [\text{since } \Delta p \Delta n \text{ is negligible}] \\ &\approx r \Delta n (n_0 + p_0) \quad [\text{since } \Delta n = \Delta p] \end{aligned}$$

$$\approx \frac{\Delta n}{\tau_n} \quad [\text{since } \tau_n = \frac{1}{r(n_0 + p_0)} = \text{carrier life time of the electrons}]$$

$$\therefore \frac{\partial(\Delta n)}{\partial t} = \frac{-\Delta n}{\tau_n} \text{ per unit volume of the material}$$

In the element of volume  $A\delta x$ ,

$$\frac{\partial(\Delta n)}{\partial t} A\delta x \Big|_{\text{gen and recomb}} = \frac{-\Delta n}{\tau_n} A\delta x \quad \dots \quad (8.104)$$

(b) Rate of increase of excess electron concentration due to drift: Due to the applied electric field ' $E$ ', electrons drift into the element at plane 2 and leave at plane 1. Let the excess electron concentration at plane 1 is  $\Delta n$ , so the electron current at plane 1 i.e., the electron current leaving the element is  $\Delta n (e\mu_n E)A$ , where  $A$  is the cross-sectional area of the element. Similarly, let the excess electron concentration at plane 2 be  $[\Delta n + \delta(\Delta n)]$ , so the electron current at plane 2 i.e., current entering the element is  $[\Delta n + \delta(\Delta n)] (e\mu_n E)A$ . The net rate of increase of the electron charge in the element is equal to  $[\Delta n + \delta(\Delta n)] e\mu_n E A - \Delta n e\mu_n E A$ . The rate of increase of the number of excess electrons in the element due to drift is represented as  $\frac{\partial(\Delta n)}{\partial t} A\delta x|_{\text{drift}}$  and is equal to:

$$\frac{\partial(\Delta n)}{\partial t} A\delta x \Big|_{\text{drift}} = \frac{[\Delta n + \delta(\Delta n)][e\mu_n E]A - [\Delta n e\mu_n E]A}{e} = \delta(\Delta n) \mu_n E A$$

$$\text{But } \delta(\Delta n) = \frac{\partial}{\partial x}(\Delta n) \delta x$$

$$\text{So } \frac{\partial(\Delta n)}{\partial t} A\delta x \Big|_{\text{drift}} = \frac{\partial(\Delta n)}{\partial x} \mu_n E A \delta x \quad \dots \quad (8.105)$$

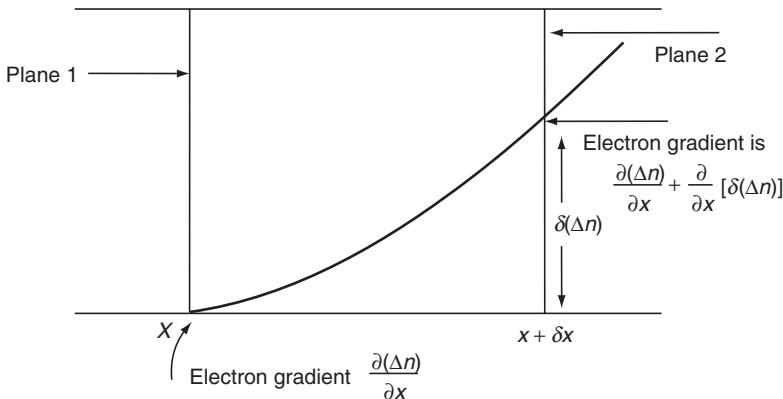
(c) Rate of increase of excess electron concentration due to diffusion: Diffusion is due to the concentration gradient of carriers. Let the excess electron concentration gradient at  $x$  is  $\frac{\partial(\Delta n)}{\partial x}$  and at  $x + \delta x$  is  $\frac{\partial}{\partial x}[\Delta n + \delta(\Delta n)]$  as shown in Fig. 8.11.

The rate of diffusion of electrons into the element at plane 2 is greater than the rate of diffusion out of the element at plane 1. The number of electrons diffuses into the element in unit time is:

$$D_n A \left[ \frac{\partial}{\partial x} (\Delta n + \delta(\Delta n)) \right] = D_n A \left[ \frac{\partial}{\partial x} (\Delta n) + \frac{\partial^2}{\partial x^2} (\Delta n) \delta x \right] \left[ \text{because } \delta(\Delta n) = \frac{\partial(\Delta n)}{\partial x} \delta x \right]$$

**Figure 8.11**

**Electron diffusion in the elemental volume of semiconductor due to nonuniform electron density**



$$= D_n A \left[ \frac{\partial(\Delta n)}{\partial x} + \frac{\partial^2(\Delta n)}{\partial x^2} \delta x \right]$$

And the number of electrons diffuses out of the element in unit time is  $= D_n A \frac{\partial(\Delta n)}{\partial x}$

The rate of increase of number of electrons in the element is represented as  $\frac{\partial(\Delta n)}{\partial t} A \delta x|_{\text{diff}}$  and is equal to

$$\begin{aligned} \frac{\partial(\Delta n)}{\partial t} A \delta x|_{\text{diff}} &= D_n A \left[ \frac{\partial(\Delta n)}{\partial x} + \frac{\partial^2(\Delta n)}{\partial x^2} \delta x \right] - D_n A \frac{\partial(\Delta n)}{\partial x} \\ &= D_n \frac{\partial^2(\Delta n)}{\partial x^2} A \delta x \quad \text{_____ (8.106)} \end{aligned}$$

The rate of increase of excess electrons in the element is equal to sum of Equations (8.104), (8.105) and (8.106) and is equal to Equation (8.103).

$$\therefore \frac{\partial(\Delta n)}{\partial t} A \delta x = -\frac{\Delta n}{\tau_n} A \delta x + \frac{\partial(\Delta n)}{\partial x} \mu_n E A \delta x + D_n \frac{\partial^2(\Delta n)}{\partial x^2} A \delta x$$

$$(\text{or}) \quad \therefore \frac{\partial(\Delta n)}{\partial t} = -\frac{\Delta n}{\tau_n} + \frac{\partial(\Delta n)}{\partial x} \mu_n E + D_n \frac{\partial^2(\Delta n)}{\partial x^2} \quad \text{_____ (8.107)}$$

This is continuity equation for excess electrons. Similarly, we can write continuity equation for excess holes as:

$$\frac{\partial(\Delta p)}{\partial t} = -\frac{\Delta p}{\tau_p} - \frac{\partial(\Delta p)}{\partial x} \mu_p E + D_p \frac{\partial^2(\Delta p)}{\partial x^2} \quad \text{_____ (8.108)}$$

Equations (8.107) and (8.108) can be represented in short by using the drift and diffusion current densities of excess electrons and holes. For electrons,

$$J_n = \Delta n e \mu_n E + D_n e \frac{\partial(\Delta n)}{\partial x} \quad \text{_____ (8.109)}$$

Differentiating Equation (8.109) with respect to 'x', we get:

$$\frac{\partial J_n}{\partial x} = \frac{\partial(\Delta n)}{\partial x} e \mu_n E + D_n e \frac{\partial^2(\Delta n)}{\partial x^2}$$

$$(\text{or}) \quad \frac{1}{e} \frac{\partial J_n}{\partial x} = \frac{\partial(\Delta n)}{\partial x} \mu_n E + D_n \frac{\partial^2(\Delta n)}{\partial x^2} \quad \text{_____ (8.110)}$$

Equation (8.110) replaces the last two terms in Equation (8.107). So, Equation (8.107) becomes:

$$\frac{\partial(\Delta n)}{\partial t} = -\frac{\Delta n}{\tau_n} + \frac{1}{e} \frac{\partial J_n}{\partial x} \quad \text{_____ (8.111)}$$

Similarly for holes,

$$\frac{\partial(\Delta p)}{\partial t} = -\frac{\Delta p}{\tau_p} - \frac{1}{e} \frac{\partial J_p}{\partial x} \quad \text{_____ (8.112)}$$

Equations (8.111) and (8.112) represent another form of representing continuity equations of excess electrons and holes, respectively.

## 8.10 Hall effect

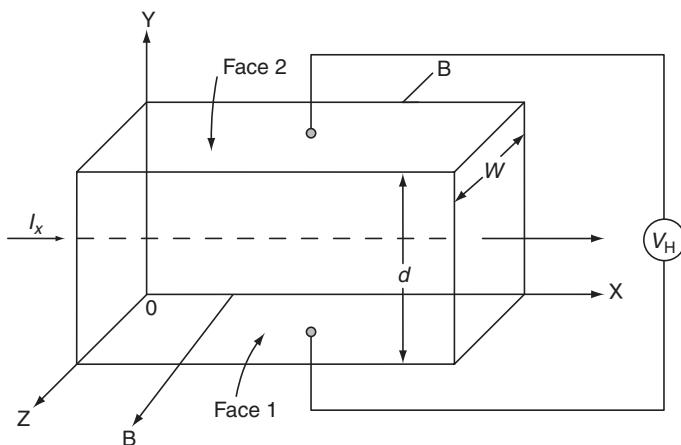
When magnetic field is applied perpendicular to a current-carrying conductor, then a voltage is developed in the material perpendicular to both magnetic field and current in the conductor. This effect is known as Hall effect and the voltage developed is known as Hall voltage ( $V_H$ ). Hall effect is useful to identify the nature of charge carriers in a material and hence to decide whether the material is n-type semiconductor or p-type semiconductor, also to calculate carrier concentration and mobility of carriers.

Hall effect can be explained by considering a rectangular block of an extrinsic semiconductor in which current is flowing along the positive X-direction and magnetic field  $B$  is applied along Z-direction as shown in Fig. 8.12.

Suppose if the semiconductor is n-type, then mostly the carriers are electrons and the electric current is due to the drifting of electrons along negative X-direction or if the semiconductor is p-type, then mostly the carriers are holes and the electric current is due to drifting of the holes along positive X-direction. As these carriers are moving in magnetic field in the semiconductor, they experience Lorentz force ( $F_L$ ) equal to  $Bev_d$ , where  $v_d$  is the drift velocity of the carriers.

The direction of this force can be obtained by applying Fleming's left-hand rule in electromagnetism. [If we stretch the thumb, fore finger and middle finger in three perpendicular directions so that the fore finger is parallel to the magnetic field and the middle finger is parallel to the current direction, then thumb represents the direction of force on the current-carrying carriers]. The Lorentz force is exerted on the carriers in the negative Y-direction. Due to Lorentz force, more and more carriers will be deposited at the bottom face [face 1] of the conductor. The deposition of carriers at the bottom face is continued till the repulsive force due to accumulated charge, balances the Lorentz force. After some time of the applied voltage, both the forces

**Figure 8.12** Hall effect



become equal in magnitude and act in opposite direction, then the potential difference between the top and bottom faces is equal to Hall voltage and that can be measured.

$$\text{At equilibrium, the Lorentz force on a carrier } F_L = Bev_d \quad \dots \quad (8.113)$$

$$\text{and the Hall force } F_H = eE_H \quad \dots \quad (8.114)$$

where  $E_H$  is the Hall electric field due to accumulated charge.

$$\text{At equilibrium, } F_H = F_L$$

$$eE_H = Bev_d$$

$$\therefore E_H = Bv_d \quad \dots \quad (8.115)$$

If 'd' is the distance between the upper and lower surfaces of the slab, then the Hall field

$$E_H = \frac{V_H}{d} \quad \dots \quad (8.116)$$

In n-type material,  $J_x = -nev_d$

$$\text{(or)} \quad v_d = -\frac{J_x}{ne} \quad \dots \quad (8.117)$$

where  $n$  is free electron concentration, substituting Equation (8.117) in (8.115) gives:

$$E_H = \frac{-BJ_x}{ne} \quad \dots \quad (8.118)$$

For a given semiconductor, the Hall field  $E_H$  is proportional to the current density  $J_x$  and the intensity of magnetic field 'B' in the material.

$$\text{i.e. } E_H \propto J_x B$$

$$\text{(or)} \quad E_H = R_H J_x B \quad \dots \quad (8.119) \quad \text{where } R_H = \text{Hall coefficient}$$

Equations (8.118) and (8.119) are same so, we have:

$$R_H J_x B = \frac{-BJ_x}{ne} \quad \text{(or)} \quad R_H = \frac{-1}{ne} = \frac{-1}{\rho} \quad \dots \quad (8.120)$$

where  $\rho$  is charge density. Similarly for p-type material,

$$R_H = \frac{1}{ne} = \frac{1}{\rho} \quad \dots \quad (8.121)$$

Using Equations (8.120) and (8.121), carrier concentration can be determined.

Thus, the Hall coefficient is negative for n-type material. In n-type material, as more negative charge is deposited at the bottom surface, so the top face acquires positive polarity and the Hall field is along negative Y-direction. The polarity at the top and bottom faces can be measured by applying probes. Similarly, in case of p-type material, more positive charge is deposited at the bottom surface. So, the top face acquires negative polarity and the Hall field is along positive Y-direction. Thus, the sign of Hall coefficient decides the nature of (n-type or p-type) material. The Hall coefficient can be determined experimentally in the following way:

Multiplying Equation (8.119) with 'd', we have:

$$E_H d = V_H = R_H J_x B d \quad \dots \quad (8.122)$$

From Fig. 8.12, we know the current density ( $J_x$ )

$$J_x = \frac{I_x}{Wd}$$

Then, Equation (8.122) becomes:

$$V_H = R_H \frac{I_x}{Wd} Bd = R_H \frac{I_x B}{W} \quad (\text{or}) \quad R_H = \frac{V_H W}{I_x B} \quad (8.123)$$

Substituting the measured values of  $V_H$ ,  $I_x$ ,  $B$  and  $W$  in Equation (8.123),  $R_H$  is obtained. The polarity of  $V_H$  will be opposite for  $n$ - and  $p$ -type semiconductors.

The mobility of charge carriers can be found by using the Hall effect, for example, the conductivity of electrons is:

$$\sigma_n = ne\mu_n$$

$$(\text{or}) \quad \mu_n = \frac{\sigma_n}{ne} = \sigma_n R_H \quad (8.124)$$

Using Equations (8.123) and (8.124), we get:

$$\mu_n = \frac{\sigma_n V_H W}{I_x B}$$

## 8.11 Direct and indirect band gap semiconductors

Based on the structure of energy bands, semiconductors are classified into: (i) Direct band gap semiconductors and (ii) Indirect band gap semiconductors.

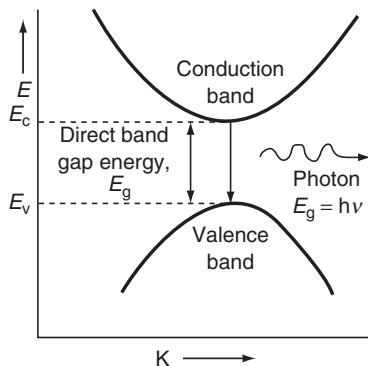
This has been explained in the following way:

The electrons and holes present in a Semiconductor possess energies corresponding to allowed bands but none of them possesses energies correspond to energy gap. The energy of electrons and holes comprises both potential energy and kinetic energy. As they possess kinetic energy, they possess momentum. As shown in Figs. (8.13) and (8.14), graphs have been plotted between energy ( $E$ ) versus momentum ( $\hbar K$ ) or propagation vector ( $K$ ) for direct band gap and indirect band gap semiconductors. In both the figures, the lower curves represent the variation of  $E$  with  $K$  for holes in the valence band and the upper curves represent the variation of  $E$  with  $K$  for electrons in the conduction band.

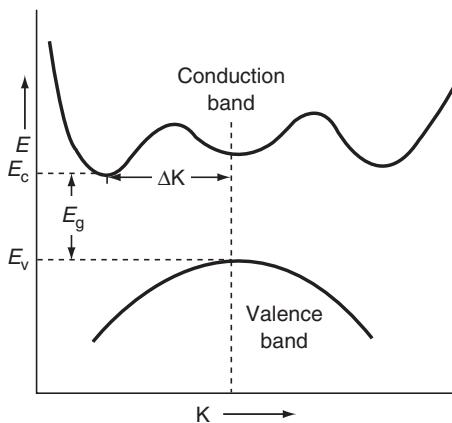
It can be seen that the energy difference between the bottom of conduction band and the top of the valence band varies with  $K$ . The energy gap of the semiconductor is equal to the energy difference between minimum energy of conduction band and maximum energy of valence band. If the maximum energy of valence band is exactly below the minimum energy of conduction band and both the above energies are at the same  $K$  value, then the material is direct band gap semiconductor (Fig. 8.13). The electron transition between these bands causes emission or absorption of a photon. The conservation of energy and momentum is obeyed during this transition. In direct band gap transition, the momentum of electron remains almost the same because the momentum of the emitted photon  $\left(\frac{h\nu}{c}\right)$  is very small.

As shown in Fig. (8.14), the  $K$  value corresponds to the maximum energy of valence band and the minimum energy of conduction band are different also between these  $K$  values, there exists large probability of transition. The semiconductors which possess this type of band structure are called indirect band gap

**Figure 8.13 E-K diagram for direct band gap semiconductor**



**Figure 8.14 E-K diagram for indirect band gap semiconductor**



semiconductors. When transition takes place between the minimum of conduction band and maximum of valence band, then the difference in energy is generated in the form of phonons. Phonons are the quanta of crystal lattice vibrations. The generated phonon has wave vector,  $\Delta K$  equal to the difference in the above-said  $K$  values.

If  $E_{ph}$  is the energy of a phonon and  $h\nu$  is the energy of a emitted photon, then the energy gap  $E_g$  of the indirect band gap semiconductor is:

$$E_g = h\nu + E_{ph}$$

Examples for indirect band gap semiconductors are Germanium and Silicon. Similarly, an example for direct band gap semiconductors is GaAs. This material has been used in the manufacture of LEDs and semiconductor lasers.

## 8.12 Formation of p-n junction

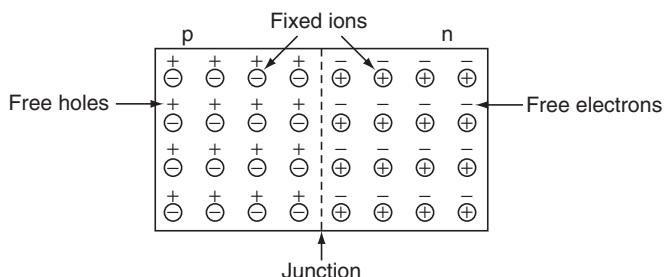
It is not possible to make a single piece of p-n junction by placing a p-type semiconductor material in contact with n-type semiconductor material, because even if the surfaces of contact are very smooth, the area of contact is less at atomic scale. Also, discontinuities in the crystal structure at the junction will be large. The p-n junction can be formed by different methods. They are (i) Grown junction method, (ii) Alloying method and (iii) Diffusion method. These are described below.

**(i) Grown junction method:** In this method, an impure semiconductor crystal is grown from n-type (or p-type) melt to some extent and the melt is counter doped by enough p-type (or n-type) impurity and the crystal is allowed to grow further. To begin with, the molten material contains donor impurity. After growing the crystal to some extent acceptor impurity is added, so that the acceptor impurity concentration dominates donor impurity concentration, and the crystal grown further will be a p-type semiconductor. A p-n junction is formed between these n-type and p-type materials.

**(ii) Alloying method:** In this method a pillet or foil of indium (trivalent impurity) is melted on a n-type germanium semiconductor material at a high temperature of about  $500^{\circ}\text{C}$ , so that indium and some amount of the germanium is melted. A puddle of molten Ge-In mixture will be formed. This molten indium will slowly dissolve in the semiconductor crystal to some extent like liquid solution and on slow cooling, recrystallization takes place forming n-region and p-region. Here the base material is n-type (or p-type) and the regrown material is p-type (or n-type) so that a p-n junction is formed between the two regions.

**(iii) Diffusion method:** Inside a chamber a p-type (or n-type) semiconductor material is heated to gaseous phase. The chamber also contains n-type (or p-type) base material. The gaseous atoms at elevated temperature diffuse into the base material, so that a diffused p-n junction is formed. Fig. 8.15 shows the p-n junction immediately after its formation.

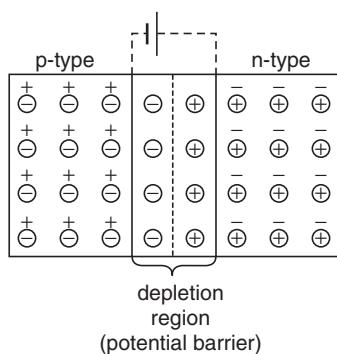
**Figure 8.15 Newly made p-n junction**



The charges in the circles represent impurity ions and uncircled charges represent free carriers. The plus (+) signs represent holes and minus (-) signs represent free electrons. The atomic plane that joins the p-side and n-side regions is called p-n junction. In the p-region, the electrons present in the upper energy levels of valence band goes to the acceptor energy level. Hence, a large number of negative ions and holes are formed. In the n-region the electrons present in the donor energy level goes to the conduction band so

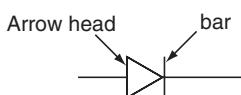
that large number of positive ions and free electrons are formed. Immediately after the formation of the junction, a large number of holes near the junction in the p-region and a large number of free electrons near the junction in the n-region are seen. Due to thermal energy these carriers may diffuse through the junction. Thus the holes diffuse from p-side to n-side and electrons diffuse from n-side to p-side. The diffusion carriers find large number of opposite charges, hence electron-hole recombinations takes place, due to recombination a pair of opposite charges are lost soon after the formation of p-n junction. The number of free charge carriers are continuously reduced due to recombinations and the junction becomes devoid of free charge carriers. Hence the p-n junction is known as the depletion region. Far away from the junction free charge carriers are present. This leaves negative (acceptor) ions near the junction in the p-region and positive (donor) ions near the junction in the n-region. These ions will form a barrier for further diffusion of free charge carriers. This is called potential barrier or junction barrier. At 300 K it is about 0.3 V for Ge and 0.7 V for Si. Fig. 8.16(a) shows the p-n junction with potential barrier.

**Figure 8.16 (a) p-n junction shown with potential**



A p-n junction is known as the semiconductor diode. It is represented by the symbol shown in Fig. 8.16(b). The arrow indicates the direction of easier conventional current flow.

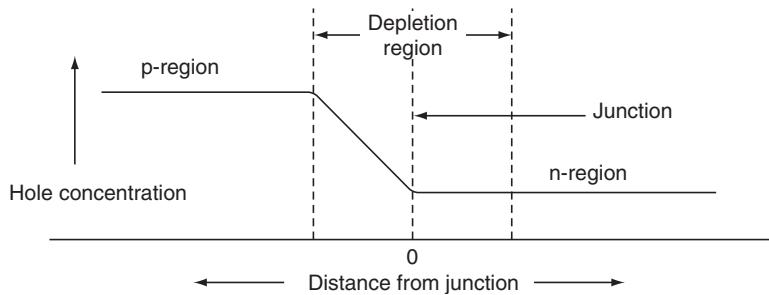
**Figure 8.16 (b) p-n diode symbol**



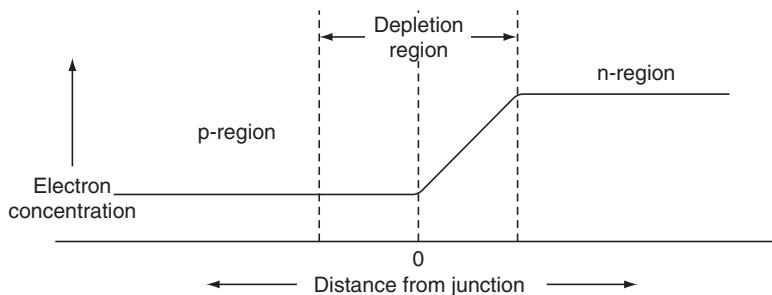
The potential barrier stops the flow of charge carriers from one side to the other side because, the positive charges on the n-side (adjacent to the junction) repels the holes crossing from the p-side to the n-side and vice versa.

The electron and hole concentrations are non-uniform in the junction region of the material, hence the potential varies with distance as shown in Fig. 8.17.

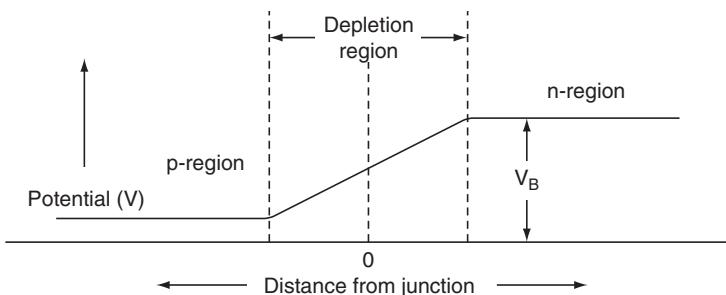
**Figure 8.17 (a) Variation of hole concentration with distance from junction**



**Figure 8.17 (b) Variation of electron concentration with distance from junction**



**Figure 8.17 (c) Variation of potential with distance from junction**

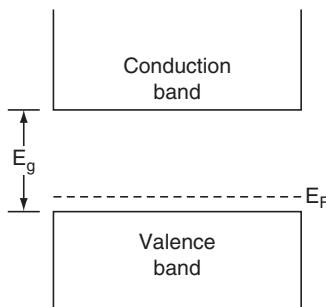


The hole concentration remains constant throughout the p-region. Similarly electron concentration remains constant throughout the n-region. In the depletion region, there is a variation in electron and hole concentrations as shown in the above figures. The n-side of the depletion region contains positive ions, so it is at a higher potential than the p-side of the depletion region which contains negative ions.

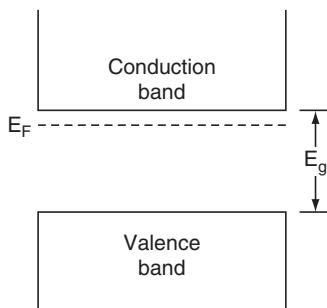
## 8.13 Energy band diagram of p-n diode

The band diagram of isolated p-type and n-type materials are shown in Figs. 8.18(a) and (b)

**Figure 8.18 (a) Band diagram of p-type material**



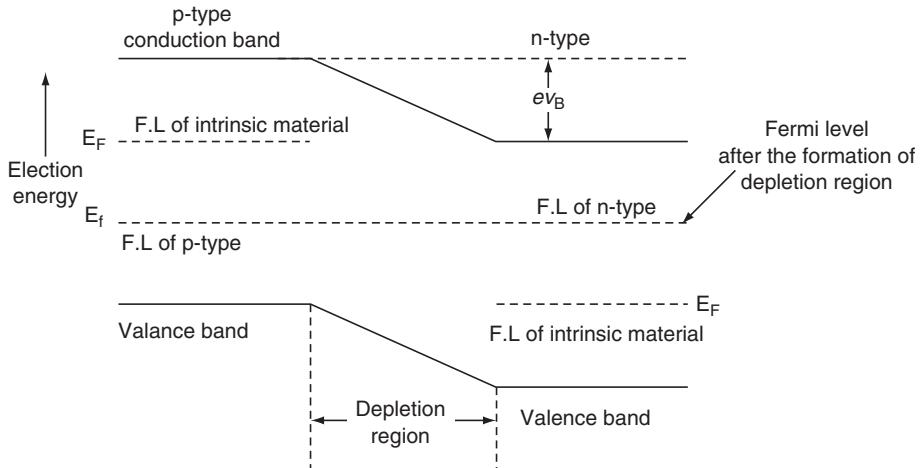
**Figure 8.18 (b) Band diagram of n-type material**



The Fermi level lies close to the conduction band in n-type material and it is close to valence band in p-type material. When a p-n diode is made with p-type and n-type materials, then flow of free charge carriers takes place at the junction. As the charge carriers flow from one side of the junction to the other side, the potential and hence the position of the Fermi level changes. In equilibrium state the Fermi level in both sides of the junction is at the same level. The energy band diagram for a p-n diode is shown in Fig. 8.19. The width of the depletion region is of the order of  $10^{-8}$ m. The potential developed across the barrier is represented by  $V_B$ .

The Fermi level in p-type material is close to the top of valence band and in n-type material it is close to the bottom of conduction band. When contact is made between p- and n-type materials then electrons in the conduction band of n-type material travel across the junction (leaving positive ions) and combine with holes in the valence band of p-type material (negative ions are formed). The flow of electrons from n- to p-side takes place until the Fermi level in both regions adjust to the same level. Unneutralised immobile charge will remain at the junction, this is called the space charge region. The space charge produces an internal potential,  $V_B$ . The conduction band of p-type move upwards by  $eV_B$  over the conduction band of n-type.

**Figure 8.19 Energy band diagram of p-n diode**



## 8.14 Diode equation

The general characteristics of a p-n diode can be represented by an equation called Shockley's equation for the forward and reverse bias regions:

$$I = I_s \left[ e \frac{V_D}{\eta V_T} - 1 \right]$$

where

$I$  = Diode current

$I_s$  = Reverse saturation current

$V_D$  = Forward biased voltage across the diode

$\eta$  = Identity factor, this depends on the construction and operating conditions  
= 1 to 2, usually taken as 1

$V_T$  = Thermal voltage =  $\frac{k_B T}{q}$

$k_B$  = Boltzmann's constant =  $1.38 \times 10^{-23}$  J/K

$T$  = Absolute temperature in Kelvin

$q$  = magnitude of electronic charge =  $1.6 \times 10^{-19}$  C

## 8.15 p-n junction biasing

The free carriers can be made to cross the junction by increasing their kinetic energy by some external means. The kinetic energy (K.E) of carriers can be increased by applying electric potential externally across the junction. As the electric potential across the junction increases, the K.E of free electrons also increases. When the K.E of carriers attain the energy of the potential barrier ( $eV_B$ ) between p-region and n-region, the carriers start crossing the junction.

Suppose the positive terminal of a battery is connected to the p-type and the negative terminal to the n-type of a p-n junction, a large current flows through the junction, and the p-n junction is said to be forward biased. If terminals of battery are interchanged, then very small current flows through the junction and it is said to be reverse biased. The forward biasing and reverse biasing of a p-n diode is described below.

**(i) Forward bias:** To forward bias a p-n junction, the positive terminal of the battery is connected to the p-side of the diode and the negative terminal of the battery is connected to the n-side of the diode as shown in Fig. 8.20 (a). The symbolic representation of p-n diode in the forward bias circuit is shown in Fig. 8.20 (b).

Figure 8.20 (a) Forward biasing of the p-n junction

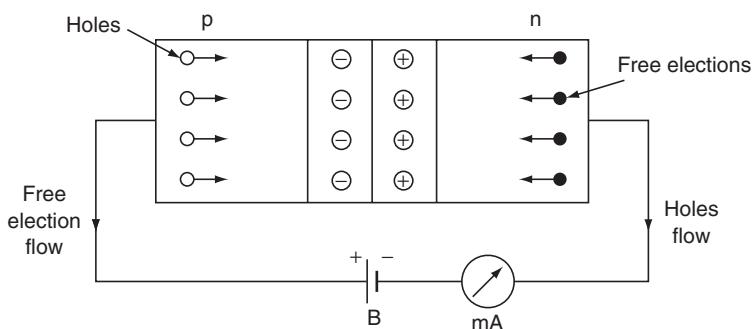
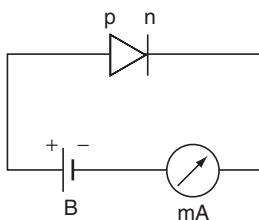


Figure 8.20 (b) Symbolic representation of p-n diode in forward bias



The negative terminal of battery connected to n-type material can drive the free electrons towards the junction and the positive terminal of battery connected to p-type material of the diode can drive the holes towards the junction, so that the width of potential barrier becomes thin and the carriers easily cross the junction. As large number of carriers cross the junction, large amount of electric current pass through the junction. This circuit is called a forward bias circuit and the current is called forward bias current. The p-n junction offers low electrical resistance to forward bias current.

**(ii) Reverse biasing:** As shown in Fig. 8.21(a), the positive terminal of battery is connected to n-region and the negative terminal of battery is connected to p-region of the diode, in a reverse biased p-n junction. The negative terminal of the battery attracts the holes in the p-region and the positive terminal of the battery attracts the electrons in the n-region. Hence, the width of the potential barrier and hence the barrier potential increases. This prevents the flow of charge carriers across the junction. Thus the diode offers high resistance to the current. However very little leakage current pass through the junction due to minority carrier flow. Fig. 8.21(b) shows the symbolic representation of a p-n junction in reverse bias.

Figure 8.21 (a) Reverse biasing of the p-n junction

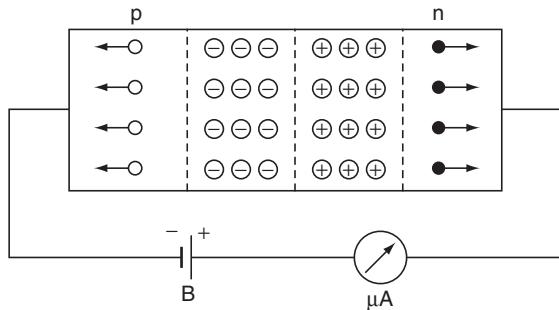
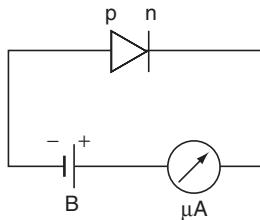


Figure 8.21 (b) Symbolic representation of a p-n diode in reverse bias

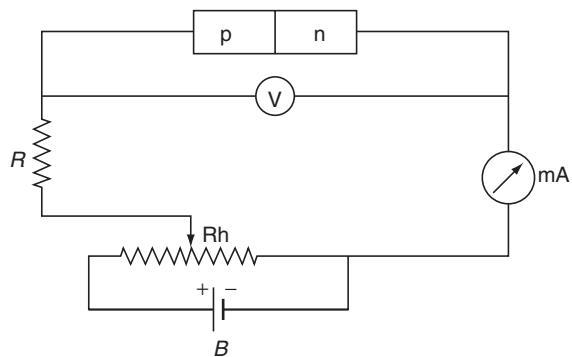


## 8.16 V-I characteristics of p-n diode

A diode shows variation in electric current passing through it when the biasing voltage is varied. V-I characteristics of the diode have been studied separately for both forward bias and reverse bias.

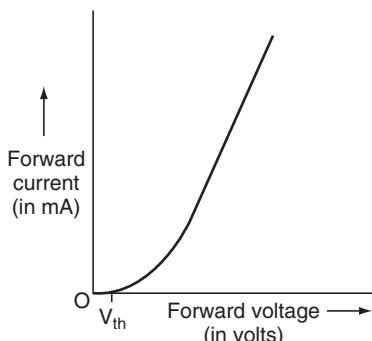
**(i) Forward bias:** The circuit diagram for a p-n diode in forward bias is shown in Fig. 8.22.

Figure 8.22 Circuit for forward biased p-n diode



By varying the rheostat contact, the voltage applied to the diode can be slowly increased. The voltage applied across the diode can be recorded with a voltmeter connected in parallel to the diode. To control the flow of current through the diode, a resistor  $R$  is connected in series to it. A milliammeter reads the current through the diode. The voltage applied across the diode is gradually increased in steps and current in the circuit is noted. As shown in Fig. 8.23. A graph is plotted between the applied voltage versus current through the diode for forward bias. It is seen that the current rises exponentially with the applied voltage. At room temperature a potential of 0.3 V is required to start the current flow in the circuit for Ge and it is 0.7 V for Si. This voltage is known as threshold voltage ( $V_{th}$ ) or cut-in-voltage. This is practically the same as barrier voltage,  $V_B$ . For  $V < V_B$ , the current flow is negligible. As the applied voltage is increased beyond the threshold value the forward current increases sharply.

**Figure 8.23** The V-I characteristics for forward biased p-n diode



**(ii) Reverse bias:** The circuit diagram for a p-n diode in reverse bias is shown in Fig. 8.24. In reverse bias, the battery connections are opposite to those for forward biasing. As the voltage is increased, a small current starts flowing in the reverse direction due to opposite battery connections. This current is measured using microammeter. The potential barrier width increases with reverse voltage and hence the diode offers a very high electrical resistance. Practically, the current through the diode is negligible. The small current is due to flow of minority carriers and is known as reverse saturation current. As the applied voltage is slowly increased, at a particular value of voltage the potential barrier breaks down and a very large amount of current pass through the diode. This voltage is known as breakdown voltage,  $V_{Br}$ . A graph plotted between current and voltage is shown in Fig. 8.25. The forward and reverse bias characters can also be represented in a single graph as shown in Fig. 8.26.

**Figure 8.24** Circuit for reverse biased p-n diode

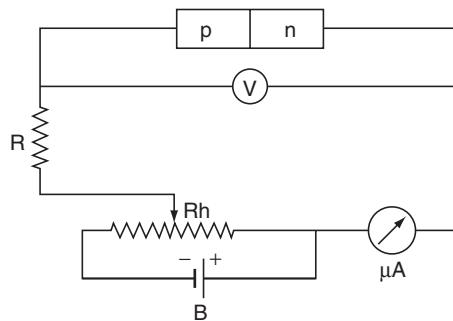


Figure 8.25 V-I characteristics for reverse biased p-n diode

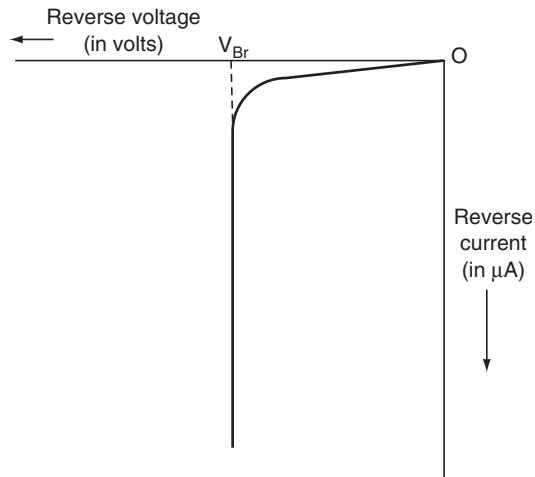
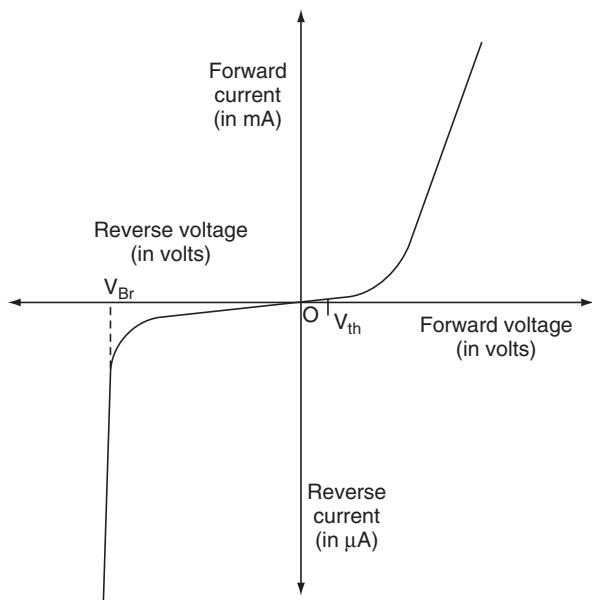


Figure 8.26 V-I characteristics of p-n diode



## 8.17 p-n diode rectifier

A p-n diode is used in a circuit to convert a.c supply into d.c supply. The process of converting a.c supply into d.c supply is called rectification. A rectifier is a device that permits current to flow through it in one direction only. We have mainly two different types of rectifiers (i) Half-wave rectifier and (ii) Full-wave rectifier.

**(i) Half-wave rectifier:** The half-wave rectifying circuit is shown in Fig. 8.27(a). The circuit consists of a single crystal p-n diode and load resistor,  $R_L$ . These are connected in series with the secondary winding of a transformer (or a.c source). The rectifier conducts current only during the positive half cycles of input a.c supply. Let the input a.c supply have sinusoidal wave form as shown in Fig. 8.27(b). During each positive half cycle of a.c supply voltage, the diode is in forward bias and conducts current through the circuit in the direction shown in Fig. 8.27(a).

Figure 8.27 (a) Half wave rectifier

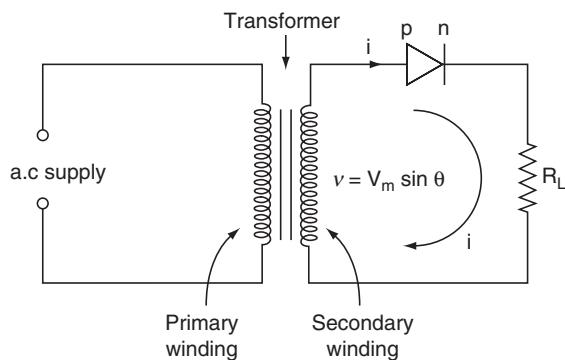


Figure 8.27 (b) Input Voltage of half wave rectifier

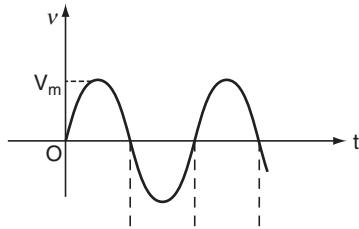
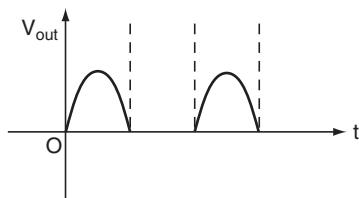


Figure 8.27 (c) Output voltage of half wave rectifier



The diode conducts only the positive half-cycles of input current, for which it offers practically no resistance. Below the cut-in-voltage there is no current in the circuit. So, here onwards we consider an ideal diode. During each negative half cycle of input voltage the diode is in reverse bias and it offers infinite electrical

resistance. Thus, no current passes through the diode and hence through the load resistance,  $R_L$ . The output voltage across the load,  $V_{out}$  shown in Fig. 8.27(c). It consists of a series of positive half-cycle voltage pulses of input. The current due to  $V_{out}$  always flows through the load,  $R_L$  in the same direction. Hence pulses of d.c output is obtained across  $R_L$ . These pulses of output are smoothed with the help of a filter circuit.

Here we see some more points relating half-wave rectifier.

**(a) Output average current ( $I_{av}$ ):** This is represented by  $I_{av}$ .

For one cycle

$$\begin{aligned} I_{av} = I_{dc} &= \frac{1}{2\pi} \int_0^\pi i \, d\theta = \frac{1}{2\pi} \int_0^\pi \frac{V_m \sin \theta}{r_f + R_L} \\ &= \frac{V_m}{2\pi(r_f + R_L)} \int_0^\pi \sin \theta \, d\theta = \frac{V_m}{2\pi(r_f + R_L)} [-\cos \theta]_0^\pi \\ &= \frac{V_m}{2\pi(r_f + R_L)} \times 2 = \frac{V_m}{\pi(r_f + R_L)} = \frac{I_m}{\pi} \end{aligned} \quad (1)$$

where  $I_{dc}$  = d.c current in the circuit

$r_f$  = forward bias diode resistance

$V_m$  = maximum peak voltage

$i$  = instantaneous a.c current.

**(b) Output d.c power,  $P_{dc}$ :**

This is represented by

$$P_{dc} = I_{dc}^2 \times R_L = \left( \frac{I_m}{\pi} \right)^2 \times R_L \quad (2)$$

**(c) Rectifying efficiency ( $\eta$ ):** This is the ratio of output d.c power to the applied input a.c power.

$$\text{Rectifying efficiency } (\eta) = \frac{\text{output d.c power}}{\text{input a.c power}}$$

Equation (2) represents output d.c power. The input a.c power is given by  $P_{ac} = I_{rms}^2 (r_f + R_L)$  (3)

Using equation (2) and equation (3), we have

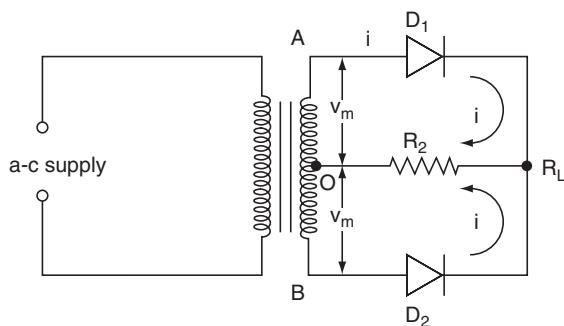
$$\eta = \frac{\left( \frac{I_m}{\pi} \right)^2 \times R_L}{\left( \frac{I_m}{2} \right)^2 (r_f + R_L)} = \frac{0.406 R_L}{r_f + R_L} = \frac{0.406}{1 + \frac{r_f}{R_L}} \approx 0.406 \quad (\text{Since } r_f \ll R_L)$$

$\therefore$  Maximum rectifying efficiency of half-wave rectifier is 0.406 or 40.6%

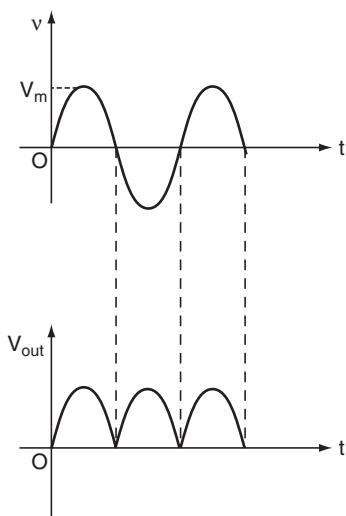
**(ii) Full-wave rectifier:** In full wave rectifier, current flows through load resistor,  $R_L$  in the same direction for both half cycles of a.c input. Usually there are two configurations for full wave rectification (a) Central tapped full wave rectifier and (b) Bridge rectifier.

**(a) Centre-tapped transformer full-wave rectifier:** The circuit diagram of centre tapped full wave rectifier is shown in Fig. 8.28. It consists of two diodes  $D_1$  and  $D_2$  connected to the secondary of centre tapped transformer [tapped at 'O'] so that each diode uses one half cycle of input a.c supply. The sinusoidal input voltage is shown in Fig. 8.28(b) and the output voltage across the load resistor,  $R_L$  is shown in Fig. 8.28(c). The working of this rectifier is explained below.

**Figure 8.28 (a) Circuit diagram of centre tapped transformer full wave rectifier**



**Figure 8.28 (b) Sinusoidal voltage (c) Full wave rectified voltage across load**

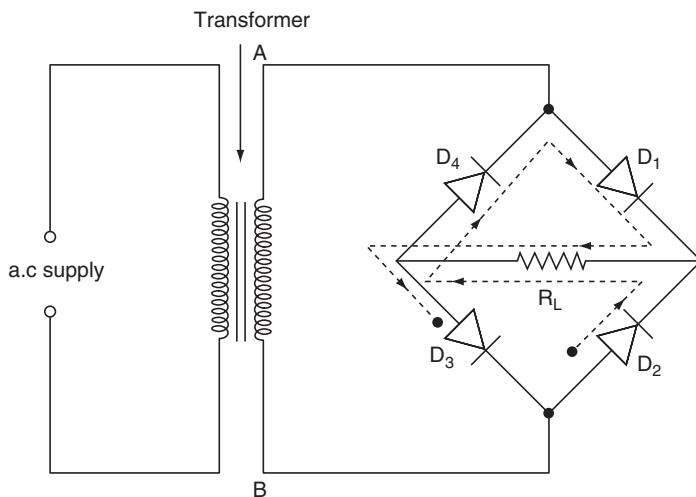


During the positive half-cycles of input voltage, the end A of the secondary winding is positive and the end B of secondary winding is negative. This makes the diode  $D_1$  forward biased and the diode  $D_2$  reverse biased. So the diode  $D_1$  conducts current through load resistor,  $R_L$  and the upper half of secondary winding, whereas  $D_2$  does not conduct current during positive half cycles. During the negative half cycle of input voltage, the end B of the secondary winding is positive and the end A of secondary winding is negative. This makes the diode  $D_2$  forward biased and the diode  $D_1$  reverse biased. So, the diode  $D_2$  conducts current through load resistor,  $R_L$  and in the lower half of the secondary winding, whereas  $D_1$  does not conduct current during negative half cycles.

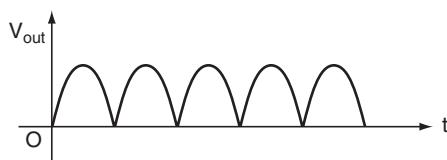
It is seen that for both half cycles of input a.c voltage, the current that shown in Fig. 8.28(c) will flow in the same direction through the load resistor  $R_L$ . So we say that d.c is obtained across the load resistor.

**(b) Full-wave bridge rectifier:** The circuit diagram of a full wave bridge rectifier is shown in Fig. 8.29(a). This bridge rectifier uses four diodes. The use of two more extra diodes in bridge rectifier is less costly than the use of centre tapped transformer as discussed earlier. So bridge rectifier is more popular.

**Figure 8.29 (a) Bridge rectifier**



**Figure 8.29 (b) The output voltage across the load,  $R_L$  in bridge rectifier**



As shown in Fig. 8.29(a), the transformer secondary winding is connected to the diagonally opposite ends of the bridge rectifier. Between the other two diagonally opposite ends of the bridge, a load resistance,  $R_L$  is connected. During the positive half cycles of secondary voltage, the end A of secondary winding is positive and the end B is negative. This positive voltage makes the diodes  $D_1$  and  $D_3$  to be forward biased whereas diodes  $D_2$  and  $D_4$  are reverse biased. The diodes  $D_1$  and  $D_3$  are in series with the load resistance,  $R_L$ . So current flows from A to B through load resistance,  $R_L$ . The conventional current is shown by dotted arrows. During the negative half-cycles of secondary voltage the end B of secondary winding is positive and the end A is negative. This voltage makes the diodes  $D_1$  and  $D_3$  reverse biased. The diodes  $D_2$  and  $D_4$  are in series with the load resistance,  $R_L$  and current flows from B to A through load resistance,  $R_L$ . For both the positive and negative half cycles of a.c supply, the current flows in the same direction through the load resistance  $R_L$ . The output voltage ( $V_{out}$ ) across the load resistance,  $R_L$  is shown in Fig. 8.29(b). Here we will see some more points relating to full wave rectifier.

- (i) **Peak Inverse Voltage (PIV):** In bridge rectifier, the peak inverse voltage of each diode is equal to the maximum secondary voltage ( $V_m$ ) of the transformer. Whereas in the case of centre-tapped transformer,

$V_m$  is the maximum voltage across half secondary winding. Hence the peak inverse voltage is twice the maximum voltage across the half secondary winding of centre-tapped transformer i.e. PIV =  $2V_m$ .

- (ii) **D.C output power:** The d.c output power,  $P_{dc}$  is

$$P_{dc} = I_{dc}^2 \times R_L = \left( \frac{2I_m}{\pi} \right)^2 \times R_L \quad \dots \quad (1)$$

- (iii) **A.C input power:** The a.c input power is given by

$$P_{ac} = I_{rms}^2 (r_f + R_L)$$

For full-wave rectifier, we have

$$I_{rms} = \frac{I_m}{\sqrt{2}}$$

$$\therefore P_{ac} = \left( \frac{I_m}{\sqrt{2}} \right)^2 (r_f + R_L) \quad \dots \quad (2)$$

- (iv) **Full-wave rectification efficiency ( $\eta$ ):**

From equations 1 and equation 2 we can write

$$\begin{aligned} \eta &= \frac{P_{dc}}{P_{ac}} = \frac{(2I_m/\pi)^2 R_L}{\left( \frac{I_m}{\sqrt{2}} \right)^2 (r_f + R_L)} \\ &= \frac{8}{\pi^2} \times \frac{R_L}{(r_f + R_L)} = \frac{0.812 R_L}{r_f + R_L} = \frac{0.812}{1 + \frac{r_f}{R_L}} \approx 0.812 \quad \text{or} \quad 81.2\% \end{aligned}$$

This is double the efficiency due to half-wave rectifier

- (v) **Ripple factor:** It is the ratio of r.m.s value of a.c component to the d.c component in the rectifier output

$$\therefore \text{Ripple factor} = \frac{\text{r.m.s value of a.c component}}{\text{Value of d.c component}} - \frac{I_{ac}}{I_{dc}}$$

For half-wave rectifier the ripple factor is 1.21 or 121% and for full wave rectifier it is 0.48 or 48%

- (vi) **Frequency:** The frequency of a.c component in full-wave rectification is twice the frequency of a.c supply.

## 8.18 Light emitting diode [LED]

On forward biasing a p-n diode, energy is given off in the form of heat in some diodes, while photons are emitted in addition to heat in some other diodes. A p-n diode specially prepared to produce visible and IR light on forward biasing is called light emitting diode. On forward biasing a LED, the majority carriers present

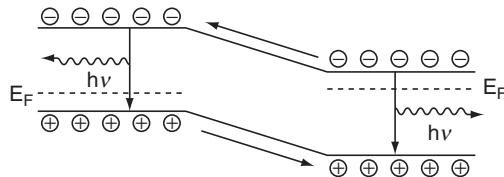
in the respective regions of diode cross the p-n junction. The free electrons at the n-side move towards the p-side and holes at the p-side move towards the n-side of the diode. The free electrons that enter the p-side from the n-side are called minority carriers in the p-region and vice versa.

This increases the local minority carrier population than the normal value. This is known as minority carrier injection. The excess minority carriers diffuse away from the junction and produce recombinations with majority carriers. For example, the excess minority electrons in the conduction band of the p-region recombine with the majority holes in the valence band of the p-region and emit photons. Here the electrons make downward transition from conduction band to valence band for recombination with holes and the difference of energy will be emitted in the form of photons of energy  $E_g$ . Similar action takes place in the n-region also. Under reverse bias no photons are emitted. The above process has been shown with the energy band diagram shown in Fig. 8.30. The wave length of emitted photon in given by

$$\lambda = \frac{hc}{E_g} \quad (1)$$

where  $h$  = Planck's constant =  $6.626 \times 10^{-34}$  Js.

**Figure 8.30** Band diagram showing injection electroluminescence in forward biased LED



The basic structure of LED is shown in Fig. 8.31 (a), and its standard symbol in Fig. 8.31(b)

**Figure 8.31** (a) Basic structure of LED

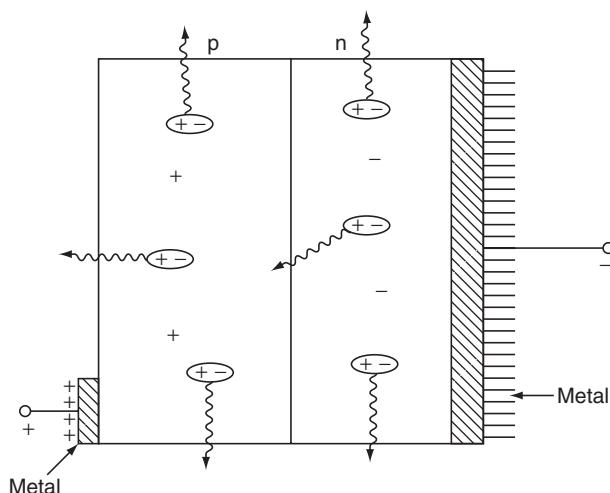
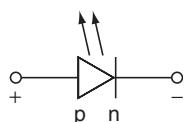


Figure 8. 31 (b) Symbol of LED



The contact area of electrode on p-type material is smaller to permit the emergence of a large number of photons when the device is forward biased. The Si and Ge semiconductor diodes will not emit photons on forward biasing but heat is dissipated at the junction. The following table give the various LED materials and the colour of emitted waves.

Table: Different LED materials in visible region

Material	Colour
GaP	Green
SiC	Blue
GaN	Blue
AlInGaP	Yellow
GaAsP [Direct band gap]	Red
GaAsP [Indirect band gap]	yellow

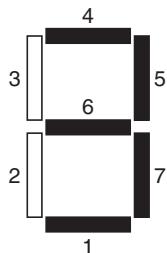
The emitted photons move in random directions. Some of them will be absorbed in the material. To get large photon emissions per second, a large number of electron-hole recombinations should take place per second. To have a large recombination rate, the doping concentration in n- and p-regions should be high. There is large concentration of electrons in the conduction band of n-region and large concentration of holes in the valence band of p-region. It is essential that light should be emitted from one side of the junction and most of the light emitted should come out of the device. For this, the device is made of an asymmetrically doped junction. The impurity concentration in the n-region should be higher than in the p-region. Then injection of carriers proceed in one direction.

Electrons are injected in large numbers into the p-region. Thus, the large number of photons released in the p-region reaches the surface and becomes visible without loss. As photons pass through the p-region some of them get absorbed. This can be reduced by making the p-region very thin. Also, the photons that fall on the interface between the p-type material and air causes total internal reflection if the angle of incidence at the interface is greater than critical angle ( $\theta_c$ ). Suppose  $n_1$  and  $n_2$  are the refractive indices of air and semiconductor respectively then  $\theta_c = \sin^{-1} \left( \frac{n_1}{n_2} \right)$ . If the refractive index of the LED material is about 3.3 to 3.8. Then the

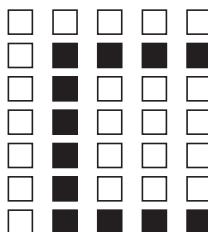
critical angle will come to  $15^\circ$  to  $18^\circ$ . So the rays that strike the surface at angles less than this come out and the rest get internally reflected. This problem can be overcome by enclosing the LED in an epoxy resin, whose refractive index lies between air and the LED material. From equation (1), the semiconductor should have an energy gap between 1.7 eV and 3.0 eV, to get emission in the visible region. So LEDs are fabricated from GaP and GaAsP. LEDs operate at low voltages and currents, typically at 1.5 V and 10 mA. The reverse breakdown voltage is very low, usually 3 V.

LEDs are used as indicators, as light sources in fibre optic communication, etc. A number of LEDs are grouped to form a seven-segment display as shown in Fig. 8.32(a). The decimal numbers 0 to 9 can be displayed using the seven segments. The LEDs can also be arranged in the form of a  $5 \times 7$  matrix as shown in Fig. 8.32(b) to get a decimal number or an alphabetical character. Such a display is known as an alpha numeric display. The number 3 is shown in Fig. 8.32 (a) and the alphabet 'C' is shown in Fig. 8.32 (b).

**Figure 8.32 (a) Seven-segment display**



**Figure 8.32 (b) LED array displaying alphabet 'C'**



## 8.19 Liquid crystal display (LCD)

Liquid crystals are the intermediate phases between liquid and crystal. LCDs do not generate light energy, but simply alter or control the existing light to make selected areas appear bright or dark. Liquid crystals have orientational order but lack positional order. The material that is used in liquid crystal display is 4-methoxy - 4' n-butyl benzylidene aniline (MBBA) molecules. It can act as a liquid crystal between the temperatures of  $21^{\circ}\text{C}$  to  $48^{\circ}\text{C}$ . It has an elongated rod-like structure. There are three phases in liquid crystals. They are smetic, nematic and cholesteric. In smetic phase the molecules are cigar shaped and are arranged in layers. The molecules can move forward and backward but not up and down. In nematic phase all the molecular axes are parallel to each other, but it is not a layered structure. This can be considered as a one-dimensional liquid. In the cholesteric phase the molecules are plate-shaped and this is a stack of thin layers. As one goes down the stack, the direction of orientation rotates in the form of a screw. This phase of crystals possess double refraction. The other liquid crystal is pentyl cyano biphenyl. This has nematic form in the temperature range of  $18^{\circ}\text{C}$  to  $35^{\circ}\text{C}$ .

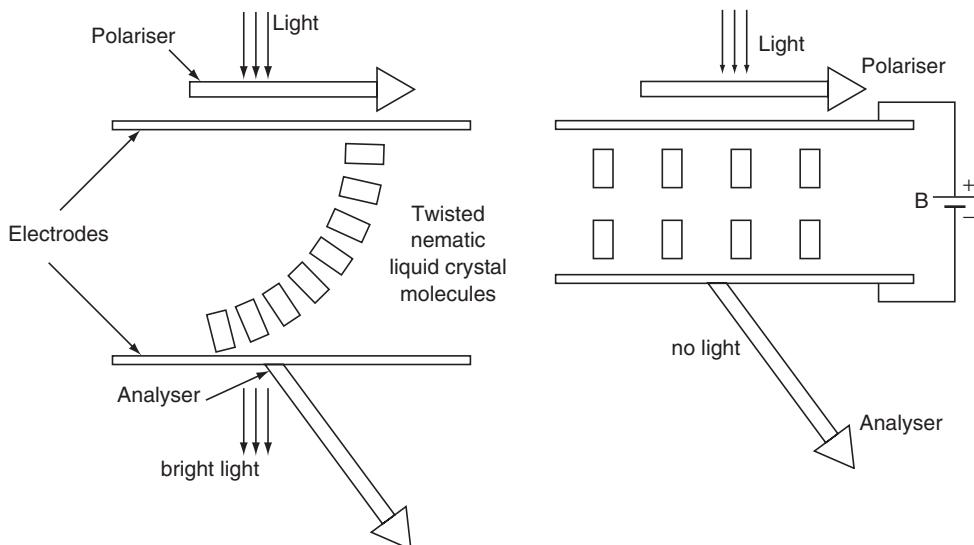
### Properties of liquid crystals:

1. Liquid crystals are very sensitive to temperature, electric field, mechanical stress, etc. Change in any of the above parameters causes change in the optical properties of liquid crystals.
2. As temperature changes the cholesteric phase can change the colour of radiation. This fact is used to measure the temperature of children, and also in thermography to detect breast cancer.
3. Nematic phase is widely used for displays. The display is based on the change of polarisation during the application of electric field.

There are two types of liquid crystal displays (i) Dynamic scattering display and (ii) Twisted nematic field effect display. The dynamic scattering display is not presently used because of its short life time and larger power consumption during operation. In case of twisted nematic field effect display, a thin layer of liquid crystal material of 10–20  $\mu\text{m}$  thick is kept in between two glass plates coated with transparent tin oxide on the inner side surfaces, which acts as electrodes as shown in Fig. 8.33(a). In the absence of applied electric field, the top glass plate is rotated through 90°, this causes the liquid crystal molecules also to be twisted through 90°. Above the top glass plate, a polariser and below the bottom glass plate, an analyser are kept in crossed positions. When light is allowed to pass through the liquid crystal cell and through the crossed polariser and analyser, the cell appears bright due to additional phase difference introduced by twisting. When an electric field is applied, the liquid crystal molecules orient themselves parallel to the field direction as shown in Fig. 8.33(b). Hence the cell appears dark due to the crossed polariser and analyser.

**Figure 8.33**

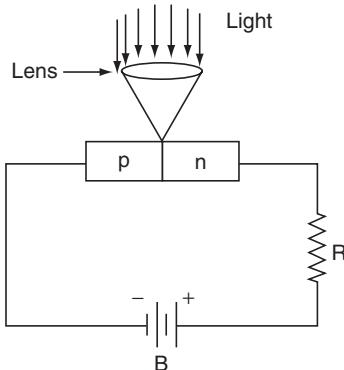
(a) Twisted nematic field effect display in the absence of applied electric field (b) Twisted nematic field effect display under applied electric field



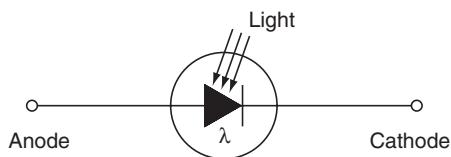
## 8.20 Photodiodes

A photo diode is a reverse biased semiconductor p-n diode whose reverse current increases with the increase in intensity of light incident at the junction. When light is incident on the p-n junction of a photo diode, the atoms at the junction absorb the energy of photons and create more free electrons and holes. These additional carriers increase the reverse current. As the intensity of incident light on the junction increases the reverse current also increases. The basic biasing arrangement and construction of a photodiode is shown in Fig. 8.34(a). Its standard symbol is shown in Fig. 8.34(b). The lens is used to concentrate the light to the junction region.

**Figure 8.34 (a) The basic biasing arrangement and construction of a photodiode**

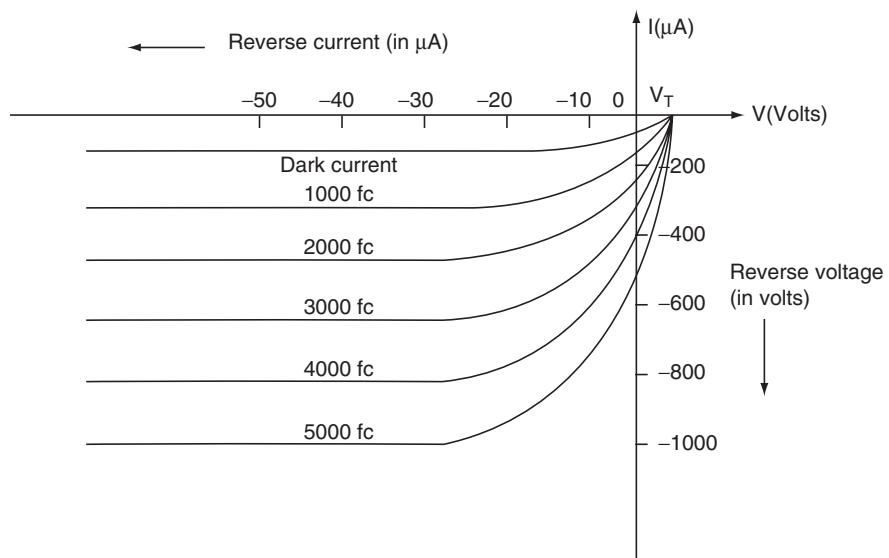


**Figure 8.34 (b) Symbol of photodiode**



The diode has a few microamperes of reverse saturation current due to thermally generated minority carriers in the n- and p-type materials. When light is incident on the junction, the minority carriers increase and hence the level of reverse current increases. The graph shown in Fig. 8.35 has been plotted between the reverse saturation current and the applied voltage for different intensity levels of light incident on the junction. The reverse current that exists when no light is incident on the junction is known as dark current. The equal spacings between curves show that for the same increment in the luminous flux, the increase in the reverse saturation current is the same. This indicates that the photodiode has good linearity.

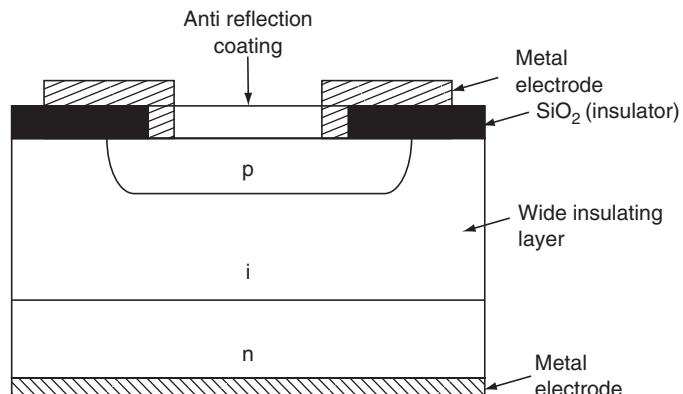
**Figure 8.35** Photodiode characteristics



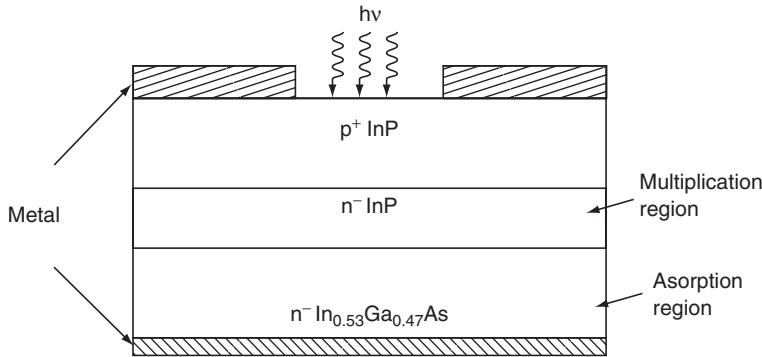
We have two different photodiodes (i) p-i-n photodiode and (ii) Avalanche photodiode.

**(i) p-i-n photodiode:** The structure of this diode is shown in Fig. 8.36. It consists of a p-n junction separated by a wide insulating layer (i). On biasing a large electric field exists across this layer. This field sweeps the excess holes and excess electrons across the insulating layer 'i' by drift. These excess carriers contribute to the photo current. For biasing the diode, two metal electrodes are present, one at the bottom and the other at the top of the layers. This is used in switching and logic circuits, and to detect laser pulses.

**Figure 8.36** Structure of p-i-n diode



**(ii) Avalanche photodiode:** Under high reverse bias voltage, breakdown of the p-n junction takes place resulting in a current gain of nearly 1000. This is known as avalanche breakdown.

**Fig. 8.37 Avalanche photodiode**


The product of current gain and band width is 100 GHz. Hence they are biased at microwave frequencies. Fig. 8.37 shows the structure of an avalanche photodiode. Holes are swept from InGaAs region to the InP junction, where avalanche multiplication takes place. Separation of absorption and multiplication regions reduces the junction leakage current.

**Applications:** These diodes find large number of applications. We will see a few of them.

**(i) Alarm circuit using photodiode:** Photodiodes are used in alarm systems fixed to doors of houses. The light from light source is allowed to fall on a photodiode fitted to the doorway. As long as there is no break of light on the photodiode, constant reverse current passes. If a person passes through the door, then there is a break in the light beam falling on the photodiode, so the photo current drops to its dark current level. This causes an alarm to sound.

**(ii) Counting of objects:** In industries, the objects that pass on a conveyer belt are counted using a photodiode. Here a light beam from a source passes across the conveyer to a photodiode. If an object passes on the conveyer then the light beam is broken resulting in dark current in the circuit, and causes the count to increase by one.

## Formulae

$$1. \quad n = \int_{E_C}^{\infty} g_e(E) f_e(E) dE$$

$$2. \quad f_e(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$

$$3. \quad g_e(E) = \frac{\pi}{2} \left[ \frac{8m_e^*}{h^2} \right]^{1/2} \left[ E - E_c \right]^{1/2}$$

$$4. \quad n = 2 \left[ \frac{2m_e^* \pi k_B T}{h^2} \right]^{1/2} \exp\left[\frac{-\left(E_C - E_F\right)}{k_B T}\right]$$

$$5. \quad n = N_C \exp\left[\frac{-\left(E_C - E_F\right)}{k_B T}\right] \quad \text{where } N_C = 2 \left[ \frac{2m_e^* \pi k_B T}{h^2} \right]$$

$$6. \quad P = \int_{-\infty}^{E_V} g_h(E) f_h(E) dE$$

$$7. f_h(E) = 1 - f_e(E) = \frac{1}{1 + \exp\left[\frac{E_F - E}{k_B T}\right]}$$

$$9. P = 2 \left[ \frac{2m_h^* \pi k_B T}{h^2} \right]^{3/2} \exp\left[\frac{-(E_F - E_V)}{k_B T}\right]$$

$$11. E_F = \frac{E_C + E_V}{2} + \frac{3}{4} k_B T \ln\left(\frac{m_h^*}{m_e^*}\right)$$

$$\text{If } m_h^* \approx m_e^*, E_F = \frac{E_C + E_V}{2}$$

$$13. n_i = 2 \left[ \frac{2\pi k_B T}{h^2} \right]^{3/2} \left( \frac{m_e^* m_h^*}{m_e^* m_h^*} \right)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right)$$

$$\text{if } m_e^* = m_h^* = m$$

$$n_i = 2 \left[ \frac{2\pi m k_B T}{h^2} \right]^{3/2} \exp\left(\frac{-E_g}{2k_B T}\right) \\ = C T^{3/2} \exp\left(\frac{-E_g}{2k_B T}\right)$$

$$\text{where } C = 2 \left[ \frac{2\pi m k_B}{h^2} \right] = 4.83 \times 10^{21}$$

$$19. \rho_i = \frac{1}{\sigma_i} = A \exp\left[\frac{E_g}{2k_B T}\right]$$

$$21. n + N_A^- = p + N_D^+$$

$$23. N_D^+ = N_D \left[ \frac{1}{1 + \exp\left[\frac{E_F - E_D}{k_B T}\right]} \right]$$

$$25. E_F = \frac{E_C + E_D}{2} + \frac{1}{2} k_B T \ln\left(\frac{N_D}{N_C}\right) \text{ for n-type}$$

$$26. N_A^- \approx p; p_p \approx N_A$$

$$8. g_h(E) = \frac{\pi}{2} \left( \frac{8m_h^*}{h^2} \right)^{3/2} (E_V - E)^{1/2}$$

$$10. P = N_v \exp\left[\frac{-(E_F - E_V)}{k_B T}\right]$$

$$\text{where } N_v = 2 \left[ \frac{2m_h^* \pi k_B T}{h^2} \right]^{3/2}$$

$$12. np = n_i^2 \quad \text{and}$$

$$n_i = (N_v N_c)^{1/2} \exp\left[\frac{-E_g}{2k_B T}\right]$$

$$14. I = I_e + I_h, I_e = neA v_{de}, J_e = ne v_{de} = \sigma_e E$$

$$15. v_{de} = \mu_e E, \sigma_e = ne\mu_e, \sigma_h = pe\mu_h$$

$$16. \sigma = \sigma_e + \sigma_h = e[n\mu_e + p\mu_h]$$

$$17. \sigma_i = n_i e [\mu_e + \mu_h]$$

$$18. \sigma_i = n_i e \gamma T^{-3/2}$$

$$20. \frac{\Delta T}{T} = \frac{2k_B T}{E_g} \ln 2$$

$$22. N_A^- = \frac{N_A}{1 + \exp\left[\frac{(E_A - E_F)}{k_B T}\right]}$$

$$24. n_n \approx N_D^+ \approx N_D; P_n \approx \frac{n_i^2}{N_D}$$

$$25. (a) E_F = \frac{E_V + E_A}{2} - \frac{k_B T}{2} \ln\left(\frac{N_A}{N_v}\right) \text{ for p-type}$$

$$27. \Delta p = (\Delta p)_0 \exp\left[-t\left(\frac{1}{\tau_B} + \frac{1}{\tau_s}\right)\right]$$

28.  $\Delta p = (\Delta p)_0 e^{-t/\tau}$

29.  $J_n = \sigma_n E = nev_{de}$

30.  $v_{de} = \mu_n E$

31.  $\sigma = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p = \frac{1}{\rho}$

32.  $\sigma_i = n_i e(\mu_n + \mu_p) = \frac{1}{\rho_i}$

33.  $J_{drift} = J_{n,drift} + J_{p,drift} = ne\mu_n E + pe\mu_p E$

34.  $J_{diff} = J_{n,diff} = J_{p,diff}$

35.  $J_n = J_{n,drift} + J_{p,diff}$

$$= D_n e \frac{\partial(\Delta n)}{\partial x} - D_p e \frac{\partial(\Delta p)}{\partial x}$$

$$= ne\mu_n E + D_n e \frac{\partial(\Delta n)}{\partial x}$$

36.  $J_p = J_{p,drift} + J_{p,diff}$

37.  $J_{total} = J_n + J_p$

$$= pe\mu_p E - D_p e \frac{\partial(\Delta p)}{\partial x}$$

$$= ne\mu_n E + D_n e \frac{\partial(\Delta n)}{\partial x} + pe\mu_p E - D_p e \frac{\partial(\Delta p)}{\partial x}$$

38.  $\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{k_B T}{e}$  at 300 K,

$$39. \frac{\partial(\Delta n)}{\partial t} = \frac{-\Delta n}{\tau_n} + \frac{\partial(\Delta n)}{\partial x} \mu_n E + D_n \frac{\partial^2(\Delta n)}{\partial x^2}$$

$$\frac{k_B T}{e} = 26 \text{ mV}$$

$$(\text{or}) \quad \frac{\partial(\Delta n)}{\partial t} = \frac{-\Delta n}{\tau_n} + \frac{1}{e} \frac{\partial J_n}{\partial x}$$

40.  $\frac{\partial(\Delta p)}{\partial t} = \frac{-\Delta p}{\tau_p} - \frac{\partial(\Delta p)}{\partial x} \mu_p E + D_p \frac{\partial^2(\Delta p)}{\partial x^2}$

41.  $E_H = \frac{-BJ_x}{ne} = R_H J_x B$

$$(\text{or}) \quad \frac{\partial(\Delta p)}{\partial t} = \frac{-\Delta p}{\tau_p} - \frac{1}{e} \frac{\partial J_p}{\partial x}$$

$$R_H = \frac{-1}{ne} = \frac{-1}{\rho} \text{ for n-type}$$

42.  $R_H = \frac{1}{ne} = \frac{1}{\rho}$  for p-type

43.  $R_H = \frac{V_H W}{I_x B}$

44.  $\mu_n = \frac{\sigma_n}{ne} = \sigma_n R_H = \frac{\sigma_n V_H W}{I_x B}$

45.  $I = I_s \left[ e \frac{V_D}{\eta V_T} - 1 \right]$  (Shockley's equation)

46.  $I_{av} = \frac{I_m}{\pi}$  (for half-wave rectifier)

## Solved Problems

1. Find the resistivity of an intrinsic semiconductor with intrinsic concentration of  $2.5 \times 10^{19}$  per  $\text{m}^3$ . The mobilities of electrons and holes are  $0.40 \text{ m}^2/\text{V}\cdot\text{s}$  and  $0.20 \text{ m}^2/\text{V}\cdot\text{s}$ .

**Sol:** Given data are:

$$\text{Intrinsic concentration } (n_i) = 2.5 \times 10^{19}/\text{m}^3$$

$$\text{Mobility of electrons } (\mu_n) = 0.40 \text{ m}^2/\text{V}\cdot\text{s}$$

The mobility of holes ( $\mu_p$ ) = 0.20 m<sup>2</sup>/V-s

The conductivity of an intrinsic semiconductor ( $\sigma_i$ ) =  $n_i e [\mu_n + \mu_p]$

$$\text{The resistivity } (\rho_i) = \frac{1}{\sigma_i} = \frac{1}{n_i e [\mu_n + \mu_p]}$$

$$= \frac{1}{2.5 \times 10^{19} \times 1.6 \times 10^{-19} [0.40 + 0.20]}$$

$$= \frac{1}{2.5 \times 1.6 \times 0.6} = 0.4166 \Omega\text{-m.}$$

2. Calculate the number of donor atoms per m<sup>3</sup> of n-type material having resistivity of 0.25 Ω-m, the mobility of electrons is 0.3 m<sup>2</sup>/V-s.

**Sol:** We know:

$$\frac{1}{\sigma} = \rho = \frac{1}{n e \mu_n}$$

[Since  $n$  = number of free electron per m<sup>3</sup> ≈ number of donor atoms in n-type]

$$\text{So } n = \frac{1}{\rho e \mu_n} = \frac{1}{0.25 \times 1.6 \times 10^{-19} \times 0.3} = 8.333 \times 10^{19} \text{ per m}^3$$

3. At 300 K, find the diffusion coefficient of electrons in silicon. Given the mobility of electrons ( $\mu_n$ ) is 0.21 m<sup>2</sup>/V-s.

**Sol:** From Einstein's equation, we know:

$$\frac{D_n}{\mu_n} = \frac{K_B T}{e}$$

$$D_n = \mu_n \frac{K_B T}{e} = \frac{0.21 \times 1.38 \times 10^{-23} \times 300}{1.6 \times 10^{-19}} = 54.34 \times 10^{-4} \text{ m}^2/\text{s}$$

4. The Hall coefficient ( $R_H$ ) of a semiconductor is  $3.22 \times 10^{-4}$  m<sup>3</sup> C<sup>-1</sup>. Its resistivity is  $8.50 \times 10^{-3}$  Ω-m. Calculate the mobility and carrier concentration of the carriers.

**Sol:** Since  $R_H$  is positive, so the given semiconductor is p-type.

$$\text{So } R_H = \frac{1}{p e} \text{ where } p = \text{hole concentration}$$

$$(\text{or}) \quad p = \frac{1}{R_H e} = \frac{1}{3.22 \times 10^{-4} \times 1.6 \times 10^{-19}} = 19.4 \times 10^{21} \text{ m}^{-3}$$

Mobility of holes  $\mu_p$  is:

$$\mu_p = \frac{\sigma_p}{p e} = \sigma_p R_H = \frac{R_H}{\rho} ; \text{ where } \rho = \text{resistivity} = 8.50 \times 10^{-3} \Omega\text{-m}$$

$$\mu_p = \frac{3.22 \times 10^{-4}}{8.50 \times 10^{-3}} = 0.0378 \text{ m}^2/\text{V-s}$$

5. Mobilities of electrons and holes in a sample of intrinsic germanium at 300 K are  $0.36 \text{ m}^2/\text{V-s}$  and  $0.17 \text{ m}^2/\text{V-s}$ , respectively. If the resistivity of the specimen is  $2.12 \Omega\text{-m}$ , compute the intrinsic concentration.

**Sol:** Mobility of electrons ( $\mu_e$ ) =  $0.36 \text{ m}^2/\text{V-s}$

Mobility of holes ( $\mu_h$ ) =  $0.17 \text{ m}^2/\text{V-s}$

Resistivity  $\rho_i = 2.12 \Omega\text{-m}$

Energy gap ( $E_g$ ) = ?

$$\sigma_i = \frac{1}{\rho_i} = n_i e (\mu_e + \mu_h)$$

$$\frac{1}{2.12} = n_i \times 1.6 \times 10^{-19} [0.36 + 0.17]$$

$$n_i = \frac{10^{19}}{2.12 \times 1.6 \times 0.53} = 556.25 \times 10^{16}/\text{m}^3$$

6. The following data are given for intrinsic germanium at 300 K  $n_i = 2.4 \times 10^{19}/\text{m}^3$ ;  $\mu_e = 0.39 \text{ m}^2/\text{V-s}$ ;  $\mu_h = 0.19 \text{ m}^2/\text{V-s}$ . Calculate the resistivity of the sample.

(Set-1–Sept. 2007), (Set-2–Sept. 2006), (Set-1–May 2003)

$$\text{Sol: } \rho_i = \frac{1}{n_i e (\mu_e + \mu_h)}$$

$$n_i = 2.4 \times 10^{19}/\text{m}^3; \mu_e = 0.39 \text{ m}^2/\text{V-s}; \mu_h = 0.19 \text{ m}^2/\text{V-s}$$

$$\rho_i = \frac{1}{2.4 \times 10^{19} \times 1.6 \times 10^{-19} \times (0.39 + 0.19)} = \frac{1}{2.4 \times 1.6 \times 0.58} = 0.449 \text{ } \Omega\text{-m}$$

7. The electron and hole mobilities in a silicon sample are  $0.135$  and  $0.048 \text{ m}^2/\text{V-s}$ , respectively. Determine the conductivity of intrinsic Si at 300 K if the intrinsic carrier concentration is  $1.5 \times 10^{16} \text{ atoms/m}^3$ . The sample is doped with  $10^{23}$  phosphorous atoms/ $\text{m}^3$ . Determine the hole concentration and conductivity.

(Set-3–May 2004), (Set-4–May 2003)

**Sol:** Mobility of electrons ( $\mu_e$ ) =  $0.135 \text{ m}^2/\text{V-s}$

Mobility of holes ( $\mu_h$ ) =  $0.048 \text{ m}^2/\text{V-s}$

Intrinsic carrier concentration ( $n_i$ ) =  $1.5 \times 10^{16}/\text{m}^3$

$$\text{Conductivity } (\sigma) = n_i e (\mu_e + \mu_h) = 1.5 \times 10^{16} \times 1.6 \times 10^{-19} [0.135 + 0.048]$$

$$= 1.5 \times 1.6 \times 0.183 \times 10^{-3} = 0.439 \times 10^{-3}/\Omega\text{-m.}$$

Doping concentration,  $N_D = 10^{23}$  phosphorous atoms/ $\text{m}^3$

hole concentration,  $p = ?$

conductivity ( $\sigma_n$ ) = ?

$$p = \frac{n_i^2}{N_D} = \frac{(1.5 \times 10^{16})^2}{10^{23}} = 2.25 \times 10^9 \text{ m}^{-3}$$

$$\sigma_n = N_D e \mu_e = 10^{23} \times 1.6 \times 10^{-19} \times 0.135 = 2.16 \times 10^3 \text{ } \Omega\text{-m}.$$

8. The  $R_H$  of a specimen is  $3.66 \times 10^{-4} \text{ m}^3/\text{c}$ . Its resistivity is  $8.93 \times 10^{-3} \text{ } \Omega\text{-m}$ . Find  $\mu$  and  $n$ .

(Set-1-May 2004), (Set-2-May 2003)

**Sol:** Since  $R_H$  is positive, the given specimen is p-type material,  $R_H = \frac{1}{pe}$

$$\left. \begin{array}{l} \text{Carrier concentration} \\ [\text{hole concentration}] \end{array} \right\} (p) = \frac{1}{R_H e} = \frac{1}{3.66 \times 10^{-4} \times 1.6 \times 10^{-19}} = 1.7 \times 10^{22} \text{ m}^{-3}$$

$$\text{Mobility } (\mu) = \sigma_H R_H = \frac{R_H}{\rho_H} = \frac{3.66 \times 10^{-4}}{8.93 \times 10^{-3}} = 4.099 \times 10^{-2} \text{ m}^2/\text{V-s}$$

9. Find the conductivity of intrinsic silicon at 300 K. It is given that  $n_i$  at 300 K in silicon is  $1.5 \times 10^{16}/\text{m}^3$  and the mobilities of electrons and holes in silicon are  $0.13 \text{ m}^2/\text{V-s}$  and  $0.05 \text{ m}^2/\text{V-s}$ , respectively

(Set-2-May 2003)

**Sol:** Intrinsic concentration ( $n_i$ ) =  $1.5 \times 10^{16}/\text{m}^3$

$$\text{Mobility of electrons } (\mu_e) = 0.13 \text{ m}^2/\text{V-m}$$

$$\text{Mobility of holes } (\mu_h) = 0.05 \text{ m}^2/\text{V-m}$$

$$\text{Conductivity } (\sigma) = n_i e (\mu_e + \mu_h) = 1.5 \times 10^{16} \times 1.6 \times 10^{-19} (0.13 + 0.05)/\text{m} \cdot \text{A}$$

$$= 4.32 \times 10^{-4}/\text{m} \cdot \text{A}$$

10. A pure silicon material has an intrinsic concentration of  $1.5 \times 10^{16}/\text{m}^3$  at 300 K. If it is doped with donor impurity atoms at the rate of 1 in  $10^9$  atoms of silicon, then calculate its conductivity. Assume that all the impurity atoms are ionized. Given that the atomic weight of silicon is 28.09, density =  $2.33 \times 10^3 \text{ kg/m}^3$  electron and hole mobilities are  $0.14 \text{ m}^2/\text{V-s}$  and  $0.05 \text{ m}^2/\text{V-s}$ , respectively.

**Sol:** Given data are:

$$\text{Intrinsic concentration } (n_i) = 1.5 \times 10^{16}/\text{m}^3$$

$$\text{Atomic weight of silicon } (A) = 28.09$$

$$\text{Density of silicon } (D) = 2.33 \times 10^3 \text{ kg/m}^3$$

$$\text{Electron mobility } (\mu_e) = 0.14 \text{ m}^2/\text{V-s}$$

$$\text{Hole mobility } (\mu_h) = 0.05 \text{ m}^2/\text{V-s}$$

$$\text{No. of silicon atoms per unit volume } (N) = \frac{N_A \times D}{A}$$

$$= \frac{6.025 \times 10^{26} \times 2.33 \times 10^3}{28.09} = 5 \times 10^{28}/\text{m}^3$$

Since the doping concentration is 1 in  $10^8$  silicon atoms

$$\therefore \text{Electron concentration } (n) = \frac{N}{10^8} = \frac{5 \times 10^{28}}{10^8} = 5 \times 10^{20}/\text{m}^3$$

$$\begin{aligned} \text{From law of mass action, hole concentration } p &= \frac{n_i^2}{n} = \frac{1.5 \times 10^{162}}{5 \times 10^{20}} \\ &= 4.5 \times 10^{11}/\text{m}^3 \end{aligned}$$

$$\begin{aligned} \therefore \text{Conductivity } (\sigma) &= e[n\mu_e + p\mu_h] = 1.6 \times 10^{-19}[5 \times 10^{20} \times 0.14 + 4.5 \times 10^{11} \times 0.05] \\ &= 1.6 \times 10^{-19}[70,000 \times 10^{15} + 0.0000225 \times 10^{15}] = 1.6 \times 10^{-19} \times 70,000.0000225 \times 10^{15} \\ &= 11.2/\Omega\text{-m} \end{aligned}$$

11. Pure germanium at 300 K has a density of charge carriers  $2.5 \times 10^{19}/\text{m}^3$ . A specimen of pure germanium is doped with donor impurity atoms at the rate of one impurity atom for every  $10^6$  atoms of germanium. Assuming that all the impurity atoms are ionized, find the resistivity of the doped germanium if the electron and hole mobilities are  $0.36 \text{ m}^2/\text{V-s}$  and  $0.18 \text{ m}^2/\text{V-s}$ , respectively and the number of germanium atoms/unit volume is  $4.2 \times 10^{28}$  atoms/ $\text{m}^3$ .

**Sol:** Given data are:

$$\text{Density of charge carriers } (n_i) = 2.5 \times 10^{19}/\text{m}^3$$

$$\text{Mobility of electrons } (\mu_e) = 0.36 \text{ m}^2/\text{V-s}$$

$$\text{Mobility of holes } (\mu_h) = 0.18 \text{ m}^2/\text{V-s}$$

Since doping concentration is 1 in  $10^6$

$$\begin{aligned} \text{Hence, impurity atoms per } \text{m}^3 &= \frac{\text{No. of germanium atoms in } \text{m}^3}{10^6} \\ &= \frac{4.2 \times 10^{28}}{10^6} = 4.2 \times 10^{22}/\text{m}^3 \end{aligned}$$

As all the impurity atoms are ionized,

$$\text{So, the number of free electrons per } \text{m}^3 = n = 4.2 \times 10^{22}/\text{m}^3$$

The hole concentration  $p$  is obtained from law of mass action as:

$$np = n_i^2$$

$$p = \frac{n_i^2}{n} = \frac{(2.5 \times 10^{19})^2}{4.2 \times 10^{22}} = 1.488 \times 10^{16}/\text{m}^3$$

$$\text{Resistivity } (\rho_i) = \frac{1}{\sigma_i} = \frac{1}{ne\mu_e + pe\mu_h} = \frac{1}{e[n\mu_e + p\mu_h]}$$

$$\begin{aligned}
 &= \frac{1}{1.6 \times 10^{-19} [4.2 \times 10^{22} \times 0.36 + 1.488 \times 10^{16} \times 0.18]} \\
 &= \frac{1}{1.6 \times 10^{-19} [1512 \times 10^{19} + 0.0002678 \times 10^{19}]} \\
 &= \frac{1}{1.6 \times 1512.0002678} = 4.13 \times 10^{-4} \Omega\text{-m}
 \end{aligned}$$

12. An intrinsic Ge at room temperature with a carrier concentration of  $2.4 \times 10^9 \text{ m}^{-3}$  is doped with one Sb atom in  $10^6$  Ge atoms. What would be the concentration of holes if the Ge atom concentration is  $4 \times 10^{28} \text{ m}^{-3}$ ?

**Sol:** Carrier concentration in Ge at room temperature,  $(n + p) = 2.4 \times 10^9 \text{ m}^{-3}$

Doping concentration of Sb atoms = 1 in  $10^6$  Ge atoms

Concentration of Ge atoms,  $N = 4 \times 10^{28} \text{ m}^{-3}$

Since Sb atoms are pentavalent atoms, their ionization contributes free electrons and positive ions in the material, but holes will not be affected.

$$\begin{aligned}
 \text{So, hole concentration, } p &= \frac{1}{2} \times \text{carrier concentration} \\
 &= \frac{1}{2} \times 2.4 \times 10^9 \text{ m}^{-3} = 1.2 \times 10^9 \text{ m}^{-3}.
 \end{aligned}$$

13. Calculate the density of donor atoms to produce an n-type material with  $0.2 \Omega\text{-m}$  resistivity and  $0.35 \text{ m}^2 \text{V}^{-1}$  electron mobility.

**Sol:** Resistivity of the material,  $\rho = 0.2 \Omega\text{-m}$

Mobility of electrons,  $\mu_n = 0.35 \text{ m}^2 \text{V}^{-1}$

Density of donor atoms,  $n = ?$

Electrical conductivity,  $\sigma_e = ne\mu_e$

$$\text{or } n = \frac{\sigma_e}{e \mu_e} = \frac{1}{\rho e \mu_e} = \frac{1}{0.2 \times 1.602 \times 10^{-19} \times 0.35} = 8.92 \times 10^{19} \text{ electron/m}^3$$

14. If resistivity of an intrinsic semiconductor is  $5 \Omega\text{-m}$  at  $300 \text{ K}$  and  $2.5 \Omega\text{-m}$  at  $320 \text{ K}$ , what would be its energy gap?

**Sol:** Resistivity at  $300 \text{ K}$ ,  $\rho_1 = 5 \Omega\text{-m}$

Resistivity at  $320 \text{ K}$ ,  $\rho_2 = 2.5 \Omega\text{-m}$

Energy gap of intrinsic semiconductor,  $E_g = ?$

For intrinsic semiconductor,

We know  $\sigma = A \exp\left(\frac{-E_g}{2K_B T}\right)$  where  $A$  is constant

$$\rho = \frac{1}{\sigma} = \frac{1}{A \exp\left(\frac{-E_g}{2K_B T}\right)}$$

$$\rho_1 \propto \exp\left(\frac{E_g}{2K_B T_1}\right) \quad \text{and} \quad \rho_2 \propto \exp\left(\frac{E_g}{2K_B T_2}\right)$$

$$\frac{\rho_1}{\rho_2} = \frac{\exp\left(\frac{E_g}{2K_B T_1}\right)}{\exp\left(\frac{E_g}{2K_B T_2}\right)} = \exp\left[\frac{E_g}{2K_B} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

$$l_n \left( \frac{\rho_1}{\rho_2} \right) = \frac{E_g}{2K_B} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$

$$E_g = \frac{2K_B \ln\left(\frac{\rho_1}{\rho_2}\right)}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} = \frac{2 \times 1.38 \times 10^{-23} \ln\left(\frac{5}{2.5}\right)}{\left(\frac{1}{300} - \frac{1}{320}\right)} = \frac{1.913 \times 10^{-23}}{2.0833 \times 10^{-4}} = 0.918 \times 10^{-19} \text{ J}$$

$$= \frac{0.918 \times 10^{-19}}{1.602 \times 10^{-19}} \text{ eV} = 0.573 \text{ eV}$$

15. Find the diffusion coefficient of electrons in Silicon at 300 K if  $\mu_e$  is  $0.19 \text{ m}^2/\text{V-s}$ .

(Set-2–Sept. 2007), (Set-3–May 2007), (Set-4–June 2003), (Set-2–May 2004)

**Sol:** Probability of electrons,  $\mu_e = 0.19 \text{ m}^2/\text{V-s}$

Temperature of specimen,  $T = 300 \text{ K}$

Diffusion coefficient of electrons,  $D_n = ?$

$$D_n = \frac{\mu_e K_B T}{e}, \text{ where } K_B = \text{Boltzmann constant}$$

$$= 1.38 \times 10^{-23} \text{ J/K}$$

and  $e = \text{charge on electrons} = 1.6 \times 10^{-19} \text{ C}$

$$D_n = \frac{0.19 \times 1.38 \times 10^{-23} \times 300}{1.6 \times 10^{-19}} = 4.92 \times 10^{-3} \text{ m}^2/\text{sec}$$

16. The resistivity of an intrinsic semiconductor is  $4.5 \Omega\text{-m}$  at  $20^\circ \text{C}$  and  $2.0 \Omega\text{-m}$  at  $32^\circ \text{C}$ . What is the energy band gap?

(Set-4–May 2004)

**Sol:**  $\rho_1 = 4.5 \Omega\text{-m}$

$$\rho_2 = 2.0 \Omega\text{-m}$$

$$T_1 = 20^\circ \text{C} = 293 \text{ K}$$

$$T_2 = 32^\circ\text{C} = 305 \text{ K}$$

Energy band gap,  $E_g = ?$

We know:

$$\text{Resistivity, } \rho = A \exp\left[\frac{E_g}{2k_B T}\right]$$

where  $A = \text{constant}$

$k_B = \text{Boltzmann constant}$

$$= 1.38 \times 10^{-23} \text{ J/K}$$

$$\frac{\rho_1}{\rho_2} = \frac{A \exp\left[\frac{E_g}{2k_B T_1}\right]}{A \exp\left[\frac{E_g}{2k_B T_2}\right]} = \exp\left[\frac{E_g}{2k_B} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

Taking logarithm on both sides, we get:

$$\begin{aligned} \ln\left(\frac{\rho_1}{\rho_2}\right) &= \frac{E_g}{2k_B} \left(\frac{1}{T_1} - \frac{1}{T_2}\right) \\ E_g &= \frac{2k_B}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} \ln\left(\frac{\rho_1}{\rho_2}\right) \\ &= \frac{2 \times 1.38 \times 10^{-23}}{\frac{1}{293} - \frac{1}{305}} \times \ln\left(\frac{4.5}{2.0}\right) \text{ J} \\ &= 1.6669 \times 10^{-19} \text{ J} = 1.04 \text{ eV} \end{aligned}$$

17. A load resistance of  $500 \Omega$  is connected in series with a silicon diode, and to this an a.c voltage of peak value 20 V is applied. The forward resistance of diode is  $10 \Omega$ . Find (i) the peak current and (ii) the peak output voltage.

**Sol:** Load resistance,  $R_L = 500 \Omega$

Peak input voltage,  $V_m = 20 \text{ V}$

Forward resistance of diode,  $r_f = 10 \Omega$

Barrier voltage,  $V_B = 0.7 \text{ V}$

$$V_m = V_B + I_f (r_f + R_L)$$

$$\therefore I_m \frac{V_m - V_B}{r_f + R_L} = \frac{20 - 0.7}{10 + 500} = \frac{19.3}{510} = 37.8 \text{ mA}$$

$$\begin{aligned} \text{Peak output voltage} &= I_m \times R_L = 37.8 \text{ mA} \times 500 \Omega \\ &= 18.9 \text{ V.} \end{aligned}$$

18. A load resistance of  $1000 \Omega$  is connected to a full-wave rectifier having ideal diodes. If the alternate voltage supplied to the diodes is  $200 - 0 - 200 \text{ Volts (rms)}$ , then calculate (i) the average d.c voltage, (ii) average d.c current and (iii) ripple voltage.

**Sol:** The load resistance,  $R_L = 1000 \Omega$

rms voltage,  $V_{\text{rms}} = 200 \text{ V}$

$$\text{The peak current, } I_m = \frac{V_m}{R_L} = \frac{V_{\text{rms}} \times \sqrt{2}}{R_L}$$

$$= \frac{200 \times \sqrt{2}}{1000} = 0.2828 \text{ A}$$

$$\text{The average d.c current, } I_{dc} = \frac{2I_m}{\pi} = \frac{2 \times 0.2828}{\pi} = 0.18 \text{ A}$$

The d.c voltage across the load,  $V_{dc} = I_{dc} \times R_L = 0.18 \times 1000 = 180$  V

$$\text{Ripple factor, } \gamma = \sqrt{\frac{V_{\text{rms}}^2}{V_{\text{dc}}^2} - 1} = \sqrt{\frac{(200)^2}{(180)^2} - 1} = 0.4843$$

$$\text{Ripple voltage, } \gamma \times V_{dc} = 0.4843 \times 180 = 87.17 \text{ V}$$

## Multiple Choice Questions

- The electrical conductivity of a semiconductor at absolute zero of temperature is: ( )  
(a) finite (b) very large  
(c) zero (d) none
  - At room temperature, the conduction band electrons are \_\_\_\_\_ that of valence band holes in an intrinsic semiconductor. ( )  
(a) less than (b) greater than  
(c) equal to (d) none
  - If  $m_h^* > m_e^*$ , then the position of Fermi energy level is: ( )  
(a) at the centre of energy gap (b) just above the centre of energy gap  
(c) just below conduction band (d) just above valence band
  - The carrier concentration in an intrinsic semiconductor \_\_\_\_\_ with increase of temperature. ( )  
(a) increases (b) decreases  
(c) remains the same (d) none
  - Electrical current in an intrinsic semiconductor is due to: ( )  
(a) conduction band electrons (b) valence band holes  
(c) both (a) and (b) (d) None
  - At 300K, the intrinsic concentration in a semiconductor having energy gap nearly equal to 1 eV is: ( )  
(a)  $10^{10}/\text{m}^3$  (b)  $10^{15}/\text{m}^3$  (c)  $10^{20}/\text{m}^3$  (d)  $10^{17}/\text{m}^3$
  - The mobility ( $\mu$ ) of a carrier is proportional to: ( )  
(a)  $T^{-3/2}$  (b)  $T^{3/2}$   
(c)  $T^{-2/3}$  (d)  $T^{2/3}$

8. The conductivity of silicon increases by \_\_\_\_\_ times by adding 10 parts of boron per million parts of silicon. ( )
- (a) 10 (b) 100 (c) 1000 (d) 10,000
9. In n-type material, the majority carriers are: ( )
- (a) valence band electrons (b) conduction band electrons  
 (c) valence band holes (d) electrons and holes
10. The phosphorous atoms in silica crystal create donor energy level, \_\_\_\_\_ eV below the conduction band of silica. ( )
- (a) 0.01 (b) 0.1 (c) 0.045 (d) 0.45
11. With increase of temperature, the Fermi energy level moves \_\_\_\_\_ in n-type semiconductors. ( )
- (a) upwards (b) downwards  
 (c) uncharged (d) None
12. At room temperature, in n-type material, ( )
- (a) large number of holes exist (b) large number of positive ions exist  
 (c) large number of negative ions exist (d) None
13. At 0 K, in n-type material, the Fermi energy level lies: ( )
- (a) at the centre of energy gap  
 (b) at the centre of donor energy level and bottom of conduction band  
 (c) at the centre of acceptor energy level and top energy level of valence band  
 (d) None of the above
14. Minority carrier life time is defined as the time taken by the minority carriers to decay to \_\_\_\_\_ % of initial carriers. ( )
- (a) 67 (b) 33 (c) 37 (d) 25
15. The ratio of diffusion coefficient to mobility of carriers is proportional to: ( )
- (a)  $T$  (b)  $T^2$  (c)  $1/T$  (d)  $1/T^2$
16. According to Einstein, the ratio of diffusion coefficient to mobility is equal to: ( )
- (a)  $\frac{2k_B T}{e}$  (b)  $\frac{e}{2k_B T}$   
 (c)  $\frac{k_B T}{e}$  (d)  $\frac{e}{k_B T}$
17. If the Hall coefficient is negative, then the semiconductor is: ( )
- (a) n-type (b) p-type (c) intrinsic (d) None
18. If  $n$  and  $\mu_e$  are the free electron concentration and mobility of electrons, then the conductivity,  $\sigma_e$  is [ $e$  = charge on an electron] ( )
- (a)  $\frac{ne}{\mu_e}$  (b)  $ne \mu_e$   
 (c)  $\frac{\mu_e}{ne}$  (d)  $\frac{1}{ne\mu_e}$

19. An intrinsic semiconductor atom possesses \_\_\_\_\_ valence electrons. ( )  
 (a) 1 (b) 2 (c) 3 (d) 4
20. At 0 K, valence band of a semiconductor has full of electrons and conduction band of a semiconductor has: ( )  
 (a) full of electrons (b) no electrons  
 (c) partially filled with electrons (d) None of the above
21. The maximum energy possessed by an electron at absolute zero of temperature is called: ( )  
 (a) Fermi energy (b) de Broglie energy  
 (c) energy gap energy (d) None of the above
22. The drift velocity produced in a carrier per unit applied electric field is called its: ( )  
 (a) mobility (b) current density  
 (c) Hall effect (d) None of the above
23. The slope of a straight line drawn between  $\ln \rho_i$  versus  $1/T$  for an intrinsic semiconductor is equal to \_\_\_\_\_. [ $\rho_i$  = resistivity and  $T$  = temperature in Kelvin]. ( )  
 (a)  $E_g/k_B$  (b)  $E_g/2k_B$  (c)  $2E_g/k_B$  (d)  $E_g/3k_B$
24. The mobility of electrons is \_\_\_\_\_ that of holes. ( )  
 (a) less than (b) equal to  
 (c) larger than (d) None of the above
25. At room temperature, the conductivity of Si and Ge becomes double for \_\_\_\_\_ and \_\_\_\_\_ rise of temperature. ( )  
 (a) 5°C and 10°C (b) 10°C and 5°C (c) 10°C and 15°C (d) 20°C and 15°C
26. At room temperature, a semiconductor possesses \_\_\_\_\_ coefficient of resistivity. ( )  
 (a) positive (b) negative (c) zero (d) None
27. By doping \_\_\_\_\_ group atoms in silica crystal, a n-type semiconductor is obtained. ( )  
 (a) first (b) second (c) third (d) fifth
28. Boron atoms in silica crystal creates \_\_\_\_\_ energy level in the energy gap of silica. ( )  
 (a) acceptor (b) donor (c) both a & b (d) None
29. With increase of temperature, the Fermi energy level moves \_\_\_\_\_ in p-type semiconductor. ( )  
 (a) downwards (b) upwards (c) left (d) right
30. The product  $np$  varies by changing: ( )  
 (a) temperature (b) pressure  
 (c) humidity (d) doping concentration
31. At room temperatures, in n-type material, the free electron concentration is almost equal to the number of \_\_\_\_\_ atoms present per unit volume of the material. ( )  
 (a) acceptor (b) donor (c) both a & b (d) None
32. An electron-hole recombination results in: ( )  
 (a) release of energy (b) absorption of energy

- (c) both a & b (d) None

33. The diffusion current is proportional to \_\_\_\_\_ of charge carriers. ( )  
(a) concentration gradient (b) drift velocity  
(c) mobility (d) None

34. The electrical conductivity of semiconductors lies in between \_\_\_\_\_ and dielectrics. ( )  
(a) plastics (b) metals (c) ceramics (d) None

35. The electron vacancies in valence band of a semiconductor will exist as: ( )  
(a) positive ions (b) holes (c) negative ions (d) None

36. In semiconductors both free electrons and \_\_\_\_\_ participate in electrical conduction. ( )  
(a) holes (b) positive ions (c) negative ions (d) None

37. Above room temperature, a semiconductor possesses \_\_\_\_\_ coefficient of temperature resistance. ( )  
(a) negative (b) positive  
(c) both a & b (d) None

38. At 300K, the electron and hole diffusion coefficients of silica material is  $3.6 \times 10^{-3} \text{ m}^2/\text{s}$  and \_\_\_\_\_  $\text{m}^2/\text{s}$ . ( )  
(a)  $1.3 \times 10^{-3}$  (b)  $2.3 \times 10^{-3}$  (c)  $3.2 \times 10^{-3}$  (d)  $0.5 \times 10^{-3}$

39. At 300 K the electron and hole diffusion coefficients of germanium is  $10 \times 10^{-3} \text{ m}^2/\text{s}$  and \_\_\_\_\_  $\text{m}^2/\text{s}$ . ( )  
(a)  $2 \times 10^{-3}$  (b)  $5 \times 10^{-3}$  (c)  $10 \times 10^{-3}$  (d)  $3.6 \times 10^{-3}$

40. A p-n junction can be formed by the \_\_\_\_\_ method. ( )  
(a) grown junction (b) alloying (c) diffusion (d) All the above

41. Immediately after the formation of a p-n junction ( )  
(a) electrons in the valence band of the p-region goes to the acceptor level  
(b) electrons in the donor energy level of the n-region goes to the conduction band  
(c) a large number of holes near the junction in the p-region and a large number of free electrons near the junction in the n-region are seen  
(d) All the above

42. At 300 K, the potential barrier at the junction is ( )  
(a) 0.3 V for Ge (b) 0.7 V for Si (c) both a and b (d) none of the above

43. The n-side of the depletion region contains positive ions, so it is at \_\_\_\_\_ potential than the p-side of the depletion region. ( )  
(a) higher (b) lower (c) both a and b (d) none of the above

44. The Fermi energy level is ( )  
(a) close to the conduction band in n-type.  
(b) close to the valence band in p-type.  
(c) at the centre of energy gap in n- and p-type.  
(d) Both a and b.

45. The Fermi level in both sides of the p-n junction in equilibrium is at the \_\_\_\_\_ level ( )





72. Liquid crystals are sensitive to ( )  
 (a) temperature      (b) electric field      (c) mechanical stress      (d) All the above
73. The reverse current in a photo diode \_\_\_\_\_ with the increase in intensity of light incident at the junction ( )  
 (a) increases      (b) decreases      (c) no change      (d) None of the above
74. The reverse current that exists when no light is incident at the junction of a photo diode is known as ( )  
 (a) dead current  
 (b) dark current  
 (c) break down current  
 (d) None of the above.
75. The current gain in avalanche photo diode after avalanche break down is ( )  
 (a) 10      (b) 100      (c) 1000      (d) 50
76. Photo diodes are used in ( )  
 (a) alarm circuits      (b) counting of objects in industries  
 (c) both a and b      (d) None of the above.

## Answers

1. c	2. c	3. b	4. a	5. c	6. d	7. a	8. c	9. b	10. c	11. b
12. b	13. b	14. c	15. a	16. c	17. a	18. b	19. d	20. b	21. a	22. a
23. b	24. c	25. c	26. b	27. d	28. a	29. b	30. a	31. b	32. a	33. a
34. b	35. b	36. a	37. a	38. a	39. b	40. d	41. d	42. c	43. a	44. d
45. a	46. b	47. b	48. a	49. a	50. c	51. b	52. a	53. a	54. c	55. b
56. b	57. a	58. b	59. c	60. d	61. c	62. c	63. d	64. a	65. d	66. c
67. b	68. a	69. d	70. d	71. d	72. d	73. a	74. b	75. c	76. c	

## Review Questions

- Derive the continuity equation for conduction electrons. (Set-4–June 2005), (Set-2–May 2004)
- Derive an expression for the density of holes in the valence band of an intrinsic semiconductor. (Set-1–Sept. 2008), (Set-1–Sept. 2007), (Set-2–Sept. 2006), (Set-1–May 2003)
- Explain Hall effect. Show that for a n-type semiconductor the Hall coefficient  $R_H = -\frac{1}{ne}$ . (Set-1–May 2004), (Set-2–May 2003)
- Explain the effect of temperature and dopent on the Fermi level in a semiconductor. (Set-2–May 2003)
- Describe the drift and diffusion currents in a semiconductor. Derive their expressions and deduce Einstein's relation. (Set-1–May 2006), (Set-4–Nov. 2004), (Set-4–Nov. 2003)
- Explain the effect of temperature on resistivity of a semiconductor. (Set-3–Sept. 2007), (Set-1–May 2007), (Set-2–June 2005)
- Derive an expression for the number of electrons per unit volume in the conduction band of an intrinsic semiconductor.

(Set-3, Set-4–Sept. 2008), (Set-3–Sept. 2007), (Set-1–May 2007), (Set-3, Set-4–Sept. 2006),  
(Set-2–June 2005), (Set-1–Nov. 2003)

8. State the expression for the density of electrons and holes in an intrinsic semiconductor. Derive the expression for Fermi level.  
(Set-1–Nov. 2004), (Set-2–Nov. 2003)
9. Derive the relation between the intrinsic carrier concentration and absolute temperature.  
(Set-1–Nov. 2004), (Set-2–Nov. 2003)
10. When donor impurities are added to a semiconductor, the concentration of holes decreases. Explain with reasons.  
(Set-1–June 2005), (Set-3–Nov. 2004), (Set-3–Nov. 2003)
11. Show that the Fermi level is nearer to the conduction band in a n-type semiconductor.  
(Set-1–June 2005), (Set-3–Nov. 2004), Set-3–Nov. 2003)
12. Discuss the variation of conductivity with temperature of an n-type semiconductor.  
(Set-1–June 2005), (Set-3–Nov. 2004), (Set-3–Nov. 2003)
13. What physical law is manifested in the continuity equation?  
(Set-4–June 2005), (Set-2–May 2004)
14. Explain the effect of temperature on resistivity of a semiconductor.  
(Set-3, Set-4–Sept. 2006), (Set-1–Nov. 2003)
15. Distinguish between metals, semiconductors and insulators.  
(Set-3–Sept. 2007), (Set-1–May 2007), (Set-3, Set-4–Sept. 2006), (Set-1–Nov. 2003)
16. Explain the difference between metals and semiconductors from the consideration of temperature coefficient of resistivity.  
(Set-3–May 2004), (Set-4–May 2003)
17. Explain the applications of Hall effect.  
(Set-4–May 2004)
18. Write a note on diffusion length.  
(Set-4–May 2004)
19. Explain n-type and p-type semiconductors. Indicate on an energy level diagram, the conduction and valence bands, donor and acceptor levels from intrinsic and extrinsic semiconductors.  
(Set-4–Sept. 2007), (Set-4–May 2006), (Set-2–Nov. 2004)
20. Explain the detailed mechanism of current conduction in n- and p-type semiconductors.  
(Set-4–Sept. 2007), (Set-4–May 2006), (Set-2–Nov. 2004)
21. Distinguish between intrinsic and extrinsic impurity semiconductors with suitable examples.  
(Set-4–Sept. 2008), (Set-1–Sept. 2007), (Set-2–Sept. 2006), (Set-1–May 2003)
22. Derive an expression for the carrier concentration in n-type extrinsic semiconductors.  
(Set-3–May 2008)
23. Write a note on intrinsic semiconductors.  
(Set-3–May 2008), (Set-3–Sept. 2008)
24. Derive the continuity equation for electrons.  
(Set-3–May 2007), (Set-2–Sept. 2007)
25. What physical law is manifested in the continuity equation?  
(Set-2–Sept. 2007), (Set-3–May 2007)
26. Distinguish between intrinsic and extrinsic semiconductors with suitable examples.  
(Set-1–Sept. 2008)
27. Write notes on direct band gap and indirect band gap semiconductors.  
(Set-2–Sept. 2008)
28. Show that for a p-type semiconductors the Hall coefficient,  $R_H = \frac{1}{ne}$   
(Set-2–Sept. 2008)
29. What is an intrinsic semiconductor? Derive equations for electron and hole concentration in an intrinsic semiconductor at room temperature  $TK$ .

30. Derive an equation for Fermi energy level of an intrinsic semiconductor at temperature  $TK$ , by equating electron and hole densities. Comment on the position of Fermi energy level.
31. Distinguish between intrinsic and extrinsic semiconductors. Obtain an expression for carrier concentration in an extrinsic semiconductor.
32. Explain extrinsic semiconductors with the help of energy band diagrams and specify the position of Fermi energy level in n-type and p-type semiconductors.
33. Derive an equation for the conductivity of an intrinsic semiconductor in terms of carrier concentration and the mobilities of carriers. Explain the method of obtaining energy gap of a semiconductor.
34. Obtain equations for drift and diffusion current densities of electrons and holes.
35. Write short notes on Einstein's relations.
36. What is Hall effect? Explain. What are the uses of Hall effect?
37. Point out the importance of continuity equations. Deduce the continuity equation for the electrons in a p-type material.
38. Obtain the equation for the conductivity of an intrinsic semiconductor in terms of carrier concentration and carrier mobility.
39. What do you understand by drift and diffusion currents in the case of a semiconductor? Deduce Einstein's relation relating to these currents.
40. Explain with necessary theory the concept of minority carrier life time in an extrinsic semiconductor.
41. Derive the expression for the densities of electrons and holes in the conduction and valence bands, respectively. The Fermi level in an intrinsic semiconductor lies approximately half-way between the top of the valence band and the bottom of conduction band.
42. What is an intrinsic semiconductor? Write the expression for electron concentration and hole concentration and deduce from them that the Fermi energy level is at the middle of the conduction band and valence band of the intrinsic semiconductor.
43. Using the expressions of electron concentration and hole concentration for an intrinsic semiconductor, show that the product of these two concentrations is independent of the Fermi level of any type of semiconductor.
44. Derive an expression for the carrier concentration in a p-type semiconductor using Fermi-Dirac statistics.
45. Prove that the recombination rate in an extrinsic semiconductor is indirectly proportional to its minority carrier life time.
46. Derive the continuity equation in the non-equilibrium condition of semiconductors and write the practical implications of minority carrier lifetime in appliances.
47. Derive an expression for the density of holes in the valency band in an intrinsic semiconductor.
48. Derive an equation of continuity in semiconductors involving drift and diffusion mechanisms of carriers.
49. Explain the concept of drift and diffusion current. How are they different?
50. Derive an expression for electron and hole concentrations for an intrinsic semiconductor.
51. Explain charge neutrality in an intrinsic semiconductor.
52. Define Fermi level. Assuming the expressions for electron and hole concentration, show that Fermi level lies half-way between the valence band and the conduction band.
53. Deduce the continuity equation for electrons in p-type material.

54. Derive the expression for conductivity of an intrinsic semiconductor.
55. What are mobility and drift current? Obtain Einstein's relation for doped semiconductors.
56. Explain Hall effect.
57. Derive an expression for density of electrons in the conduction band for an n-type semiconductor.
58. What is an extrinsic semiconductor? Discuss the variation of the Fermi level with temperature for an n-type semiconductor.
59. Explain the different methods to form a semiconductor p-n junction.
60. Draw and explain the energy band diagram of a p-n junction.
61. Mention and explain Shockley's diode equation.
62. What is diode biasing? Explain the forward and reverse biasing of a p-n diode.
63. Explain half-wave rectification using p-n diode.
64. What is full-wave rectification? Explain full-wave rectification with centre tap transformer and bridge circuits.
65. Write notes on (i) LEDs, (ii) LCDs and (iii) photodiodes.



## CHAPTER

# 9

# Superconductivity

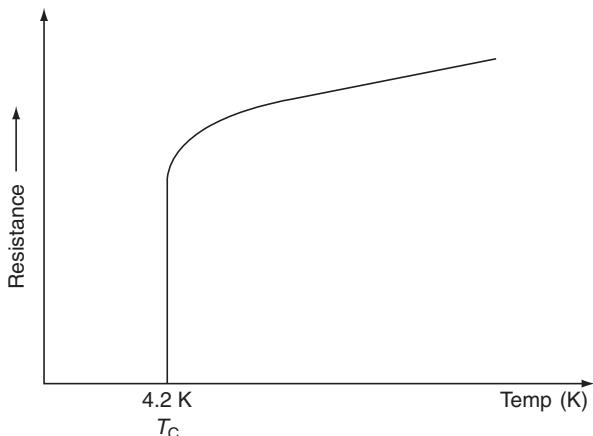
## 9.1 Introduction

From free electron theory of metals, we know that by decreasing the temperature of a perfect metal, the thermal vibrations and electron scattering of ions (or atoms) decrease and hence the electrical resistance of the substance decreases. One would expect that the electrical resistance of a substance may become zero as its temperature reaches 0 K. Based on this point, experiments were conducted on many substances by scientists. In 1911, Kammerling Onnes found that the electrical resistance of pure mercury vanishes suddenly at 4.2 K as shown in Fig. 9.1. This temperature is called its superconducting transition temperature and denoted as  $T_c$ . The superconducting transition temperature of a few important materials is shown below.

Material	Transition Temperature ( $T_c$ ) (in K)
Hg	4.15
CuS	1.6
Nb	9.3
$\text{Nb}_3\text{Au}$	11.5
$\text{Nb}_3\text{Sn}$	18.0
$\text{Nb}_3\text{Ge}$	23.2
$\text{YBa}_2\text{Cu}_3\text{O}_7$	90
$\text{Tl}_2\text{Ga}_2\text{Ba}_2\text{Cu}_4\text{O}_{10}$	125

Above the superconducting transition temperature, the material possesses normal resistance and is said to be in the normal state. Below this temperature, the resistance of the material becomes zero and its

**Figure 9.1 Variation of resistance with decrease of temperature for mercury**

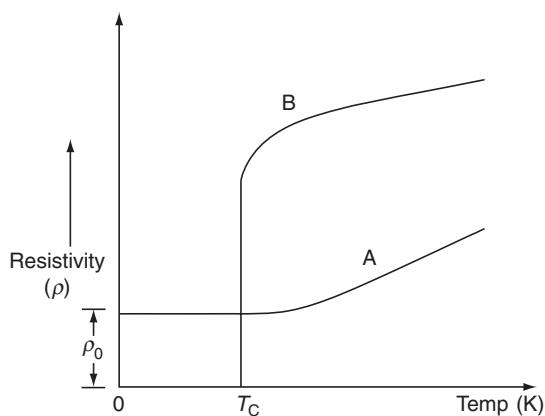


conductivity reaches infinity. This state of the material is called superconducting state. Now, the superconducting transition temperature can be defined as the temperature at which the material changes from normal state to superconducting state as it is cooled. The total disappearance of electrical resistance of these few substances is called **superconductivity** and the materials which exhibit this property are called **superconductors**.

The electrical resistivity of a material is caused by electron scattering. This is due to: (a) temperature, (b) impurities and (c) crystal defects. Figure 9.2 shows the variation of electrical resistivity of an impure defective material and pure perfect material with temperature. Curve 'A' shows the presence of electrical resistance even at 0 K; this is due to defects and impurities in the material and curve 'B' shows the superconductivity of pure perfect crystalline material.

**Figure 9.2**

**Shows the variation of electrical resistivity with decrease of temperature. Curve A for a defective impure crystal and curve B for a perfect pure crystal**

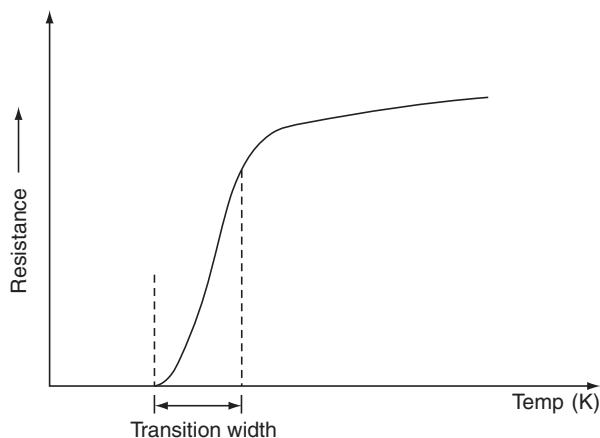


## 9.2 General features of superconductors

Superconductors show many features. We could study these features one by one as shown below:

- Persistent current:** The electrical current in a superconductor, in superconducting state remains for a very long time. This can be proved by placing a superconducting loop of material in magnetic field and lowering its temperature to below its superconducting transition temperature ( $T_c$ ) and the magnetic field is removed. This causes dc current in the superconductor loop and the current remains for a very long period without attenuation. File and Mills determined the time taken by the super current to reduce to  $1/e$  of its initial value is more than 1,00,000 years. This indicates that the dc current in a superconducting material is persistent.
- Normally, superconductivity has been observed in metals having valence electrons between 2 and 8 and not 1.
- Some good conductors of electricity at room temperature will not show superconductivity at low temperatures. For example, gold, silver, copper, sodium, crystalline iron, ferromagnetic and anti-ferromagnetic materials.
- The materials which possess high resistance at room temperatures will show superconductivity at low temperatures. For example, amorphous thin films of beryllium, bismuth and iron. Under pressure, antimony, bismuth and tellurium show superconductivity.
- By reducing the temperature of a material, it changes from normal to superconducting state. This transition is sharp in case of pure perfect metals and is broad for metals containing impurities as shown in Fig. 9.3.

**Figure 9.3** Shows the transition width of impure metals



- Isotopic effect:** Transition temperature ( $T_c$ ) of a superconducting substance varies with isotopic mass ( $M$ ). For example, the transition temperature of three isotopes of mercury is shown below.

Isotopic Mass ( $M$ ) of Hg	Transition Temperature [ $T_c$ in K]
199	4.161
200	4.153
204	4.126

It has been observed that  $T_C \propto M^{-\beta}$  (or)  $T_C M^\beta = \text{constant}$ . For large number of materials,  $\beta \approx +0.5$ .

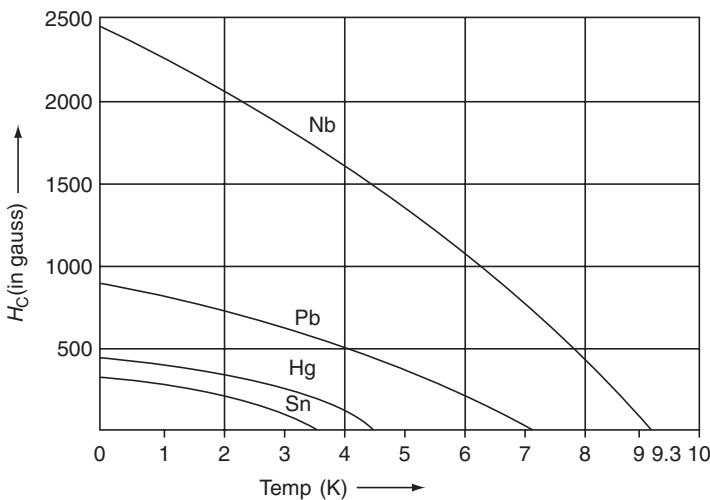
$$\text{so } T_C M^{1/2} = \text{constant.}$$

However, deviations from this value have been observed for some materials.

**7. Effect of magnetic field:** By applying magnetic field of sufficient strength, the superconductivity of a material can be destroyed. The minimum magnetic field strength required to destroy superconductivity of a substance, below  $T_C$  is called critical magnetic field ( $H_C$ ) at that temperature.  $H_C$  varies with temperature. This variation has been shown for a number of superconducting elements in Fig. 9.4.

Figure 9.4

Shows the variation of critical magnetic field with temperature for a few elements



From the graph, we see that the critical magnetic field for different elements will be different at different temperatures. Also it shows for a material, the critical magnetic field increases with decrease of temperature below  $T_C$ . At  $T_C$ , no magnetic field is required to change the material from superconducting to normal state. Maximum magnetic field is required to destroy superconductivity at 0 K. The critical magnetic field at 0 K is  $H_0$ . The critical magnetic field ( $H_C$ ) at any temperature ' $T$ ' below  $T_C$  can be represented as:

$$H_C = H_0 \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right]$$

**8. Critical currents:** Suppose a material carries electric current in superconducting state, this current produces magnetic field. If this magnetic field exceeds critical magnetic field ( $H_C$ ) at that temperature  $T (< T_C)$ , then normal resistance will be included in the material and it will be in the normal state. Hence, it is not possible to pass large currents through a superconductor. The maximum current that can be passed through a superconductor in superconducting state is called critical current, represented by  $I_C$ .

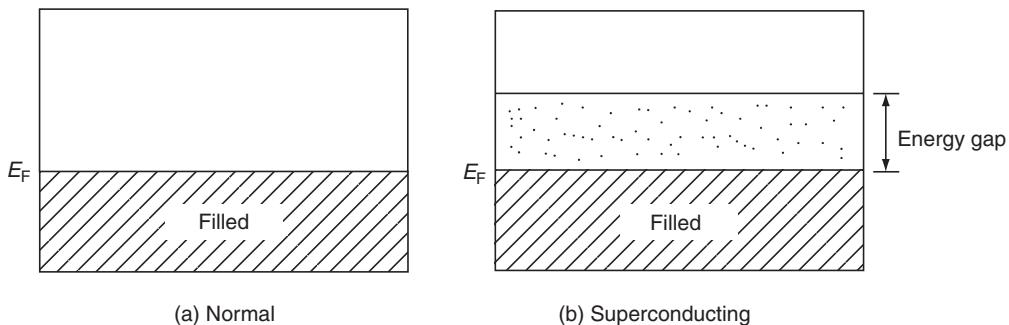
**9. AC Resistivity:** The current in a superconductor in normal state is carried by normal electrons only. When the material changes from normal state to superconducting state, then few normal electrons are converted

into super electrons which carry dc current in superconducting state without any electrical resistance. If a constant dc current is flowing in a superconductor, there is no resistance in the material; hence, no electric field in the material. If we apply dc voltage source to a superconductor [below  $T_c$ ], then current will not increase suddenly but at the rate at which the electrons accelerate in the electric field. This indicates the presence of electric field in the material. If we apply ac voltage source to the superconductor, then the superelectrons accelerate in the forward and backward direction; they lag behind the field because of inertia. Also under ac fields, current is carried not only by superelectrons but also by normal electrons; this adds resistance to superconductor [below  $T_c$ ]. Under high frequency ac voltages, a superconductor behaves as a normal material because under ac voltages, electric field exists in the material that excites superelectrons to go into higher states where they behave as normal electrons.

**10. Entropy:** Entropy is the measure of disorder in a material. By reducing the temperature of a material, it goes into superconducting state. Also thermal vibrations and entropy of the material get reduced. In all superconducting materials, entropy decreases as they change from normal to superconducting state. The electrons in superconducting state are more ordered than in normal state.

**11. Heat Capacity and energy gap:** At all temperatures in normal state, the heat capacity of a superconductor is almost the same. A sudden change in heat capacity at the transition temperature was observed. Again in superconducting state, heat capacity changes exponentially with temperature. This suggests the existence of an energy gap at the Fermi gas of the material. This energy gap is represented in Fig. 9.5.

**Figure 9.5** Represents the existence of energy gap in superconductors

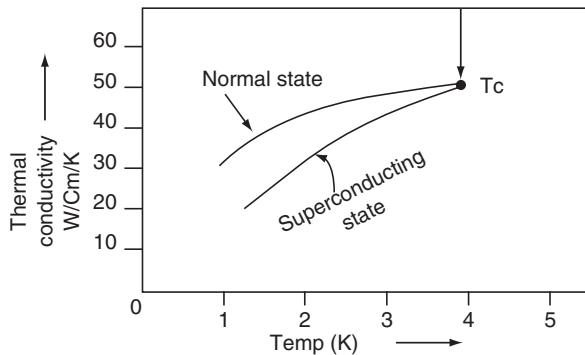


This energy gap separates the superconducting electrons and normal electrons. The superconducting electrons lie below the energy gap and the normal electrons are above it. The width of this energy gap is not constant as we see in case of an insulator. In insulators, the energy gap is attached to the lattice and the width of energy gap will not vary with temperature. In case of superconductors, the width of energy gap at Fermi gas increases by decreasing temperature below  $T_c$ . This energy gap attains maximum at 0 K and reduces to zero at  $T_c$ . Giaever confirmed the existence of energy gap in superconductors by electron tunnelling observation across the superconducting junctions.

**12. Thermal conductivity:** It has been observed that the thermal conductivity of a material in superconducting state is less than in normal state. By applying sufficient magnetic field, a material changes from superconducting state to normal state below  $T_c$ . In normal state, all free electrons participate in thermal conductivity; hence, the thermal conductivity is large. Whereas in superconducting state, the materials have superelectrons

**Figure 9.6**

**Shows the variation of thermal conductivity of tin in normal and superconducting states**



and normal electrons, the superelectrons will not participate in thermal conductivity; so, thermal conductivity is less. A sudden drop in thermal conductivity has been observed when a material changes from normal to superconducting state at a temperature below  $T_C$ . The thermal conductivities of tin as a function of temperature in normal and superconducting state are shown in Fig. 9.6.

**13. Mechanical effects:** Experimentally, it was found that the superconducting transition temperature and critical magnetic field change slightly by applying mechanical stress on it. Small changes in volume, coefficient of thermal expansion and bulk modulus of elasticity were seen when a material changes from normal state to superconducting state.

**14. Acoustic attenuation:** When sound wave propagates through a metal, then the ions will be slightly displaced from their original positions. These displacements produce microscopic electric fields. These fields increase the energy of electrons present near the Fermi surface. So, the wave is attenuated. This attenuation has been expressed in terms of attenuation coefficient,  $\alpha$  of the acoustic waves. The ratio of  $\alpha$  in superconducting state to normal state of a material has been expressed as:

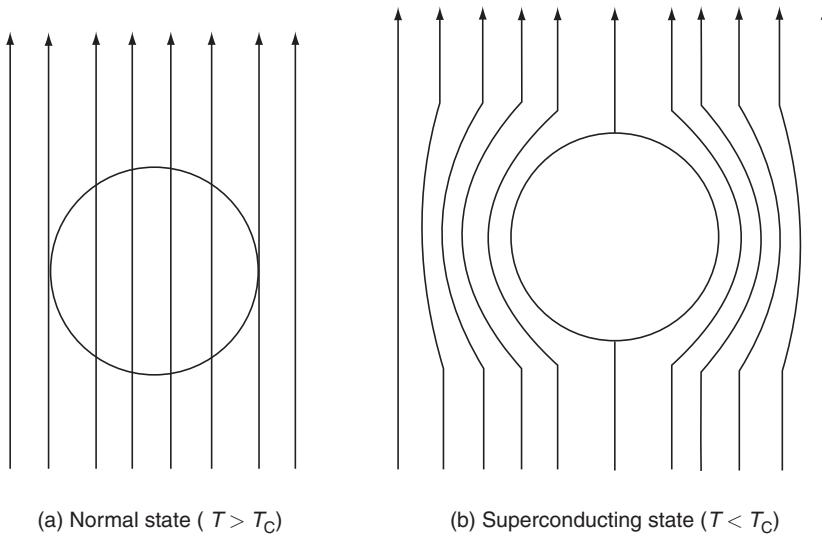
$$\frac{\alpha_s}{\alpha_n} = \frac{2}{1 + \exp\left(\frac{\Delta E}{K_B T}\right)}$$

$$\text{At low temperatures, } \frac{\alpha_s}{\alpha_n} = 2 \exp\left(-\frac{\Delta E}{K_B T}\right).$$

**15. Flux exclusion or Meissner effect:** In 1933, Meissner and Ochsenfeld found the exclusion of magnetic flux lines by a superconductor below  $T_C$ . They reduced the temperature of a long superconductor in magnetic field. They observed that the superconductor pushes the magnetic lines of force out of the body at some low temperature,  $T_C$  as shown in Fig. 9.7. When the material is in normal state, the magnetic force of lines pass through it. The magnetic induction ( $B$ ) inside the material is given as

$$B = \mu_0(H + M) = \mu_0 H(1 + \chi).$$

**Figure 9.7** Figure shows the superconductor in applied magnetic field ( $H$ )



where  $\mu_0$  is the magnetic permeability of free space.  $H$  is the intensity of applied magnetic field,  $M$  is the magnetization of the material and  $\chi$  is the magnetic susceptibility given as  $\chi = M/H$ .

When the temperature reaches below  $T_C$ , the material enters into superconducting state and it expels the magnetic force lines. So,  $B = 0$  inside the material. From the above equation, we write  $0 = \mu_0 (H + M)$

$$\Rightarrow H = -M \quad \text{or} \quad \chi = -1.0.$$

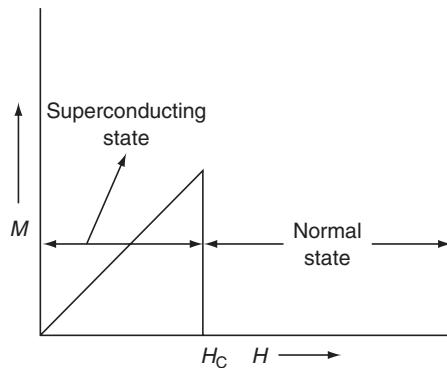
In superconducting state, inside the material magnetization takes place which is equal in magnitude and opposite in direction to the applied field. The superconductor is a perfect diamagnetic material (since  $\chi = -1.0$ ). The exclusion of magnetic lines from a superconductor when it is cooled in magnetic field to below its transition temperature is called Meissner effect.

### 9.3 Type-I and Type-II superconductors

Depending on the way of transition from superconducting state to normal state by the application of magnetic field, superconductors are divided into Type-I and Type-II superconductors. In case of Type-I superconductors, as we increase the intensity of applied magnetic field, inside the material opposing magnetization takes place up to some applied magnetic field, up to this applied magnetic field, the material is completely diamagnetic and it is in superconducting state. As the applied field reaches the critical value,  $H_C$ , all of a sudden the magnetic force lines pass through the material and the material changes sharply from superconducting state to normal state as shown in Fig. 9.8. This effect (Type-I superconductivity) was first noted by Silsbee in 1916. So, this effect is also called Silsbee effect. The critical magnetic field,  $H_C$  for Type-I superconductors is of the order of 0.1 Tesla or less so, high magnetic fields cannot be produced using Type-I superconductors. These are called soft superconductors. Almost all elements show Type-I superconductivity.

Figure 9.8

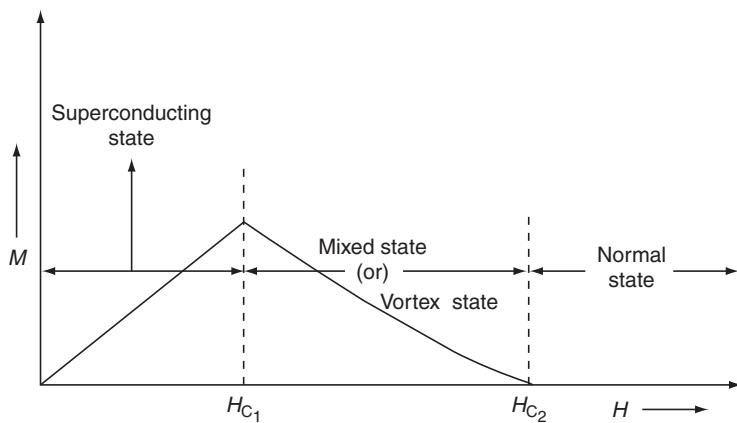
Shows the relation between magnetization and applied magnetic field for Type-I superconductors



In case of Type-II superconductors, as we increase the intensity of applied magnetic field, in the material opposing magnetization takes place up to some applied magnetic field  $H_{C_1}$ , called lower critical magnetic field. Up to this magnetic field, the material completely expels the magnetic force lines. The material is completely diamagnetic and it is in superconducting state. If the applied magnetic field exceeds  $H_{C_1}$ , slowly the magnetic force lines pass through the material and the transition from superconducting to normal state takes place gradually. The penetration of magnetic force lines through the material increases gradually from  $H_{C_1}$  to  $H_{C_2}$ . At  $H_{C_2}$ , the magnetic force lines completely pass through the material and the material changes completely from superconducting state to normal state. Above  $H_{C_2}$ , the material is in normal state. The variation of magnetization with applied magnetic field in Type-II superconductors is shown in Fig. 9.9.

Figure 9.9

Figure shows the variation of magnetization with applied magnetic field for Type-II superconductors



Type-II superconductivity was discovered by Schubnikov et al. in 1930s. The critical magnetic field  $H_{C_2}$  for Type-II superconductors is of the order of 10 Tesla.  $H_{C_2}$  is called upper critical field. Type-II superconductors with a large amount of magnetic hysteresis are called hard superconductors. Type-II superconductors are alloys or transition metals with high values of electrical resistivity.

## 9.4 Penetration depth

In 1935, F. London and H. London obtained an expression for penetration of applied magnetic field into superconducting material from the surface by adding: (i) Meissner effect i.e., the magnetic induction ( $B$ ) inside a superconducting material is equal to zero ( $B = 0$ ) and (ii) zero resistivity i.e., the intensity of electric field ( $E$ ) in a superconductor in superconducting state is equal to zero ( $E = 0$ ) to Maxwell's electromagnetic equations. According to them, the applied magnetic field does not drop to zero at the surface of the superconductor [in superconducting state] but decreases exponentially as given by the equation:

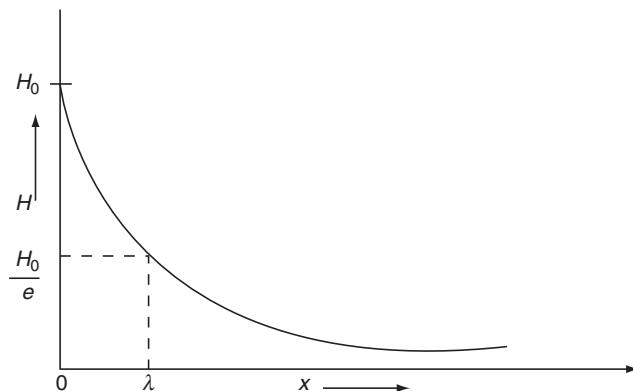
$$H = H_0 \exp\left(\frac{-x}{\lambda}\right)$$

where  $H$  is the intensity of magnetic field at a depth  $x$  from the surface,  $H_0$  is the intensity of magnetic field at the surface and  $\lambda$  is called London penetration depth. London penetration depth is defined as the distance from the surface of the superconductor to a point inside the material at which the intensity of magnetic field is  $\left(\frac{1}{e}\right)$  of the magnetic field at the surface [i.e.,  $H_0/e$ ]. The variation of intensity of magnetic field with distance from the surface into the material for tin is shown in Fig. 9.10.

The magnetic field is likely to penetrate to a depth of 10 to 100 nm from the surface of a superconductor. If the superconducting film or filament is thinner than this value, then its properties are significantly different from that of the bulk material. For example, the critical magnetic field increases with a decrease in thinness. The value of  $\lambda$  for some materials is given below.

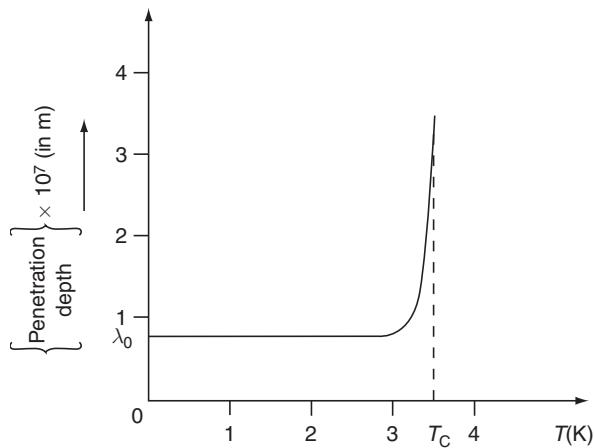
**Figure 9.10**

Figure shows the variation of the intensity of magnetic field with distance into the material for tin



Material	$\lambda$ (in nm)
Mercury	70
Aluminium	50
Tin	50
Lead	39
Indium	64

Figure 9.11 Variation of penetration depth in tin



The penetration depth is not constant but varies with temperature as shown in Fig. 9.11 for tin.

From the figure, we know that the penetration depth is independent of temperature, but the penetration depth increases rapidly and approaches infinity as the temperature approaches the transition temperature of the material. The London penetration depth at temperature  $T (< T_c)$  can be obtained using the equation

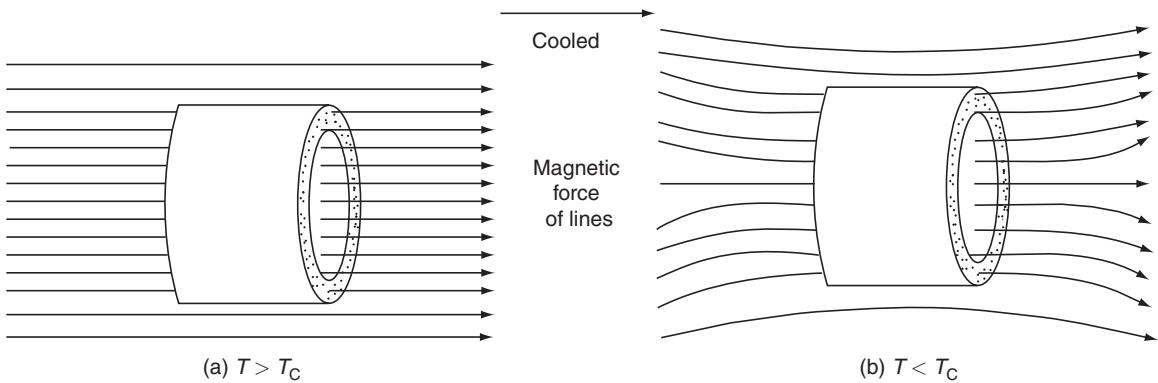
$$\lambda = \frac{\lambda_0}{\left[1 - \left(\frac{T}{T_c}\right)^4\right]^{1/2}}$$

where  $\lambda_0$  is the London penetration depth at 0 K.

## 9.5 Flux quantization

We know that electric charge is quantized in terms of integral multiples of charge on an electron [ $1.6 \times 10^{-19}$  C]. Similarly, the magnetic flux lines passing through a superconducting loop due to persistent current is quantized

**Figure 9.12** Sample cooled in the presence of magnetic field



in terms of integral multiples of  $\frac{h}{2e}$  ( $= 2 \times 10^{-15}$  Webers). Flux quantization can be proved with the help of a superconducting material in the form of a hollow cylinder or ring.

Magnetic field is applied on the superconducting ring in normal state as shown in Fig. 9.12. As its temperature is reduced to below critical temperature, the material expels the magnetic lines of force and enters into superconducting state. Persistent current is set up in the material this current will remain in the material even if the applied magnetic field is removed. This persistent current sets up magnetic force lines in the ring. This magnetic flux adjusts itself such that the total flux through the cylinder is quantized in integral multiples of  $\left(\frac{h}{2e}\right)$  (i.e.,  $n \frac{h}{2e}$ ). If the persistent current in the superconductor decreases, then the magnetic flux also decreases and adjust to integral multiples of  $\left(\frac{h}{2e}\right)$ . Here,  $2e$  is the charge on a pair of electrons. Experimentally, it was found that the value of  $h/2e$  is equal to  $2.07 \times 10^{-15}$  webers. It confirms the existence of an electron pair in the superconductor in superconducting state. This is very well agreed with the Cooper pair concept. The Cooper pair concept plays a major role in BCS theory.

## 9.6 Quantum tunnelling

As shown in Fig. 9.13(a), if a thick insulating layer is sandwiched between two metals, then electric current will not pass through this insulating layer. If the insulating layer is very thin ( $\approx 10$  to  $20$  Å), then there is a large probability for electrons to pass from one metal to another through this insulating layer by quantum mechanical process called tunnelling. If both the metals are normal conductors, then the  $V - I$  characteristics is a straight line as shown in Fig. 9.13(b).

In 1961, Giaever took a system in which an insulating layer of  $10$  nm thick has been sandwiched between a normal metal and a superconductor as shown in Fig. 9.14(a). Gradually, an increasing potential has been applied between the metal and superconductor by connecting them to electrodes. Up to certain voltage,  $V_C$ , there is no current in the circuit, afterwards the current increases as shown in Fig. 9.14(b).

Figure 9.13

(a) Shows an insulator sandwiched between two metals;  
 (b) V-I characteristics for the system shown in Fig. 9.13(a)

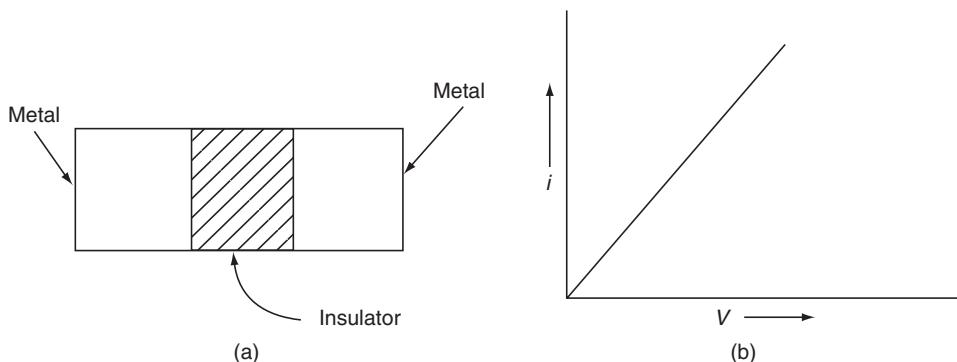
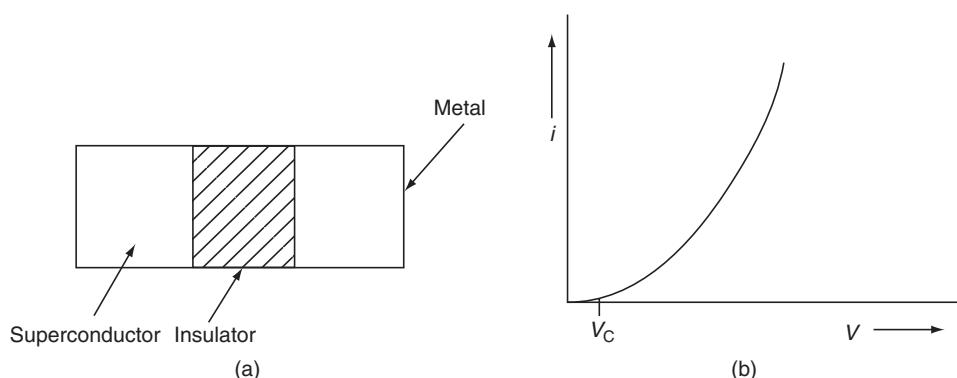


Figure 9.14

(a) Figure shows the sandwich of an insulator between a normal metal and a superconductor; (b) V-I characteristics for the system shown in Fig. 9.14(a)



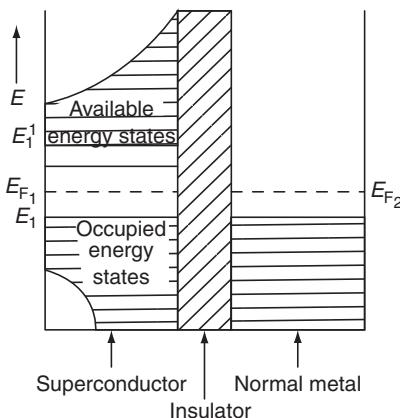
The flow of current through this insulating layer has been explained on the basis of quantum mechanical tunnelling of electrons. Quantum theory says that an electron on one side of the insulator [barrier] has a certain probability of tunnelling through it, if there is an allowed available equal energy electron state on the other side of the barrier. The quantum tunnelling for the above system can be explained with the aid of electron states in the energy space. Figure 9.15 shows the energy level diagram for the sandwich consisting of superconductor, insulator and metal at 0 K. The Fermi energy levels of these materials adjust to a same height after sandwiching.

The electron tunnelling in the above sandwich can be explained in the following way: When voltage is not applied across the sandwich, then electrons are filled upto the Fermi energy level  $E_{F_2}$  in the normal metal. At this energy, there is a forbidden energy band in superconductor. So, electron states in the superconductor are not available for the electrons present at  $E_{F_2}$  in normal metal.

So, electron tunnelling will not take place. Suppose voltage ( $V$ ) is applied across the sandwich, then the electrons present at the Fermi energy level or near to it in the normal metal gain energy and will go to higher

Figure 9.15

Figure shows the energy level diagram for the sandwich consisting of superconductor–insulator and normal metal



energy level. By the continuous increase of voltage across the sandwich, the electrons present at the Fermi energy level or near to it will go to excited states. The voltage across the barrier is raised such that the electrons in a metal should raise to a height of  $E_1^1$  or higher than that. Then, the electrons in the normal metal can see vacant energy levels in superconductor and tunnel through the insulating layer and reaches the superconducting material. Thus, quantum tunnelling takes place. Obviously, there is no current until the voltage becomes equal to  $V_C$  so that  $eV_C$  is equal to energy gap  $E_1^1 - E_{F_2}$ . Thus, the flow of electrons through a thin insulating layer has been explained based on the quantum mechanical tunnelling process.

## 9.7 Josephson's effect

In 1962, Josephson passed electrical current consisting of correlated pairs of electrons across an insulating gap ( $\sim 10 \text{ \AA}$ ) between two superconductors. This effect is known as Josephson effect.

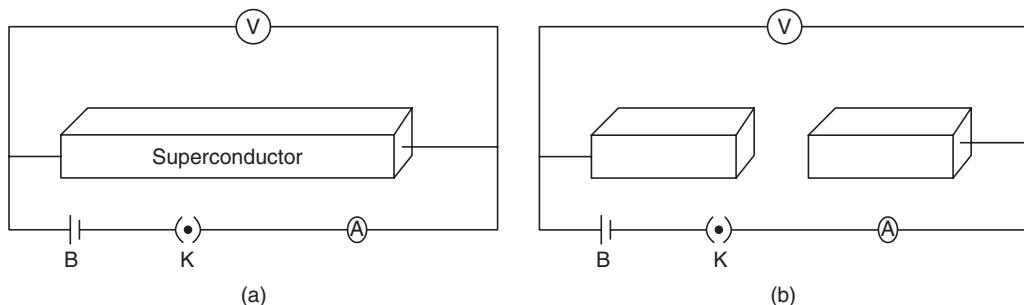
Josephson effect can be explained in the following way. As shown in Fig. 9.16(a), a rectangular superconducting bar is connected in series with a battery ( $B$ ), plug key ( $K$ ) and an ammeter ( $A$ ). A voltmeter ( $V$ ) is connected across the superconductor. Since the superconductor has zero resistance, so the voltmeter shows zero reading. Whereas the ammeter shows the current through the superconductor. Next, the superconductor is cut into two pieces as shown in Fig. 9.16(b). If the gap between the two pieces is about 1 cm, then current will not flow through the superconductor pieces, so ammeter shows zero reading and the voltmeter shows the open circuit voltage of the battery. If the gap between the superconducting pieces is reduced to 1 nm, then the voltmeter reading drops to zero and the ammeter shows dc current through the superconducting pieces and across the gap between the superconducting pieces [Josephson Junction]. That is without any applied voltage across the gap, dc current passes through the insulating gap. This effect is known as dc Josephson effect.

The gap between the superconducting pieces is slightly increased and the applied voltage is increased, the current passes through the gap also increased so that a small dc voltage exists across the gap. Now, a high-frequency electromagnetic radiation is observed from the gap. That is the gap emits a high-frequency electromagnetic rays. This indicate a high-frequency ac current through the gap. This effect is known as ac Josephson effect.

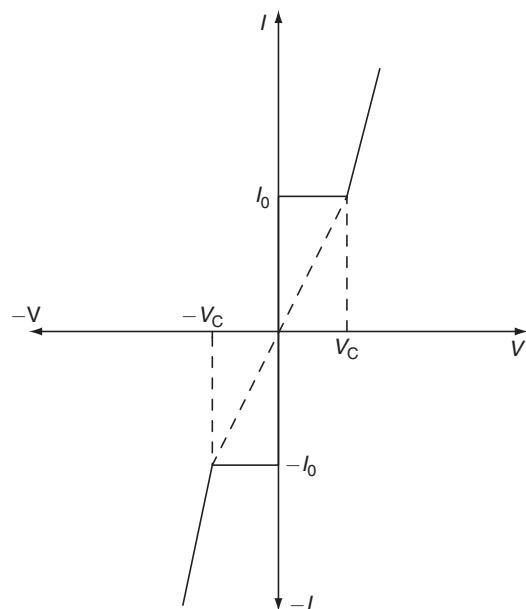
The  $V$ - $I$  characteristics of a Josephson junction is shown in Fig. 9.17. With zero applied voltage across the Josephson's junction, a dc current passes across the junction. As shown in figure, the dc current is in

**Figure 9.16**

Shows Josephson's effect: (a) Current through superconductor bar and (b) The bar is cut into two pieces with a narrow gap between them



**Figure 9.17** V-I characteristics of a Josephson's junction



between  $I_0$  to  $-I_0$ , where  $I_0$  is the maximum dc current under no applied voltage across the junction. This current is due to the quantum mechanical tunnelling of Cooper pairs of electrons across the junction. These electrons tunnel from one superconductor to another across the junction (barrier) and returns to the first conductor through the external circuit. If current exceeds  $I_0$ , then a potential difference develops across the junction. This indicates resistance in the junction. The change from zero to finite resistance is not related to the elimination of superconductivity.

The current across the junction can be represented as  $I = I_0 \sin \phi$ , where  $\phi$  is the phase difference between the waves associated with Cooper pairs of electrons on two sides of the gap. As shown in Fig. 9.17, whenever current exceeds  $I_0$ , a potential difference ( $V$ ) exists across the junction. This shows that the Cooper

pairs on both sides of the junction differ by an energy equal to  $2eV$ , where  $2e$  is the charge on a Cooper pair of electrons. Since in superconductors, current is carried by Cooper pairs of electrons, if a Cooper pair passes across the gap, then it emits a photon of energy ( $\hbar\nu$ ) equal to  $2eV$ . Then, the frequency of emitted radiation is

$$\nu = \frac{2eV}{\hbar}. \text{ This is the oscillating frequency of sinusoidal current across the gap.}$$

The phase difference  $\phi = 2\pi t/T = 2\pi t\nu$

$$= 2\pi t \left( \frac{2eV}{\hbar} \right) = \left( \frac{4\pi eV}{\hbar} \right) t$$

Suppose the potential difference across the gap is 1 mV, then the frequency is of the order of 480 GHz, this lies in the microwave region. This enables to construct microwaves resonators.

## 9.8 BCS theory

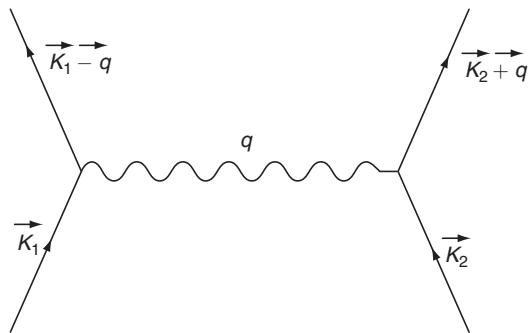
The existence of energy gap and long-range electronic order in superconducting state pointed that electrons in superconductor are somehow bound together. The positively charged ions screen the Coulomb repulsive forces between electrons. In 1950, Frohlich and Bardeen concluded that a moving electron inside a crystal distorts the crystal lattice and this distortion is quantized in terms of virtual phonons. That means the reaction between an electron and lattice phonons represent the vibrations of crystal lattice in a solid. The electron-phonon interaction can cause resistance or superconductivity. The interaction of electrons and virtual phonons causes superconductivity. We know generally that superconductors are always poor conductors at room temperature and the best conductor do not become superconductors. For example, gold, silver and copper at low temperatures.

In 1957, Bardeen, Cooper and Schriffer put forward a theory [called BCS theory] [Jhon Bardeen received noble prize twice in physics; in 1947, he invented transistor and later he developed the key concepts of photocopy machine] which explains very well for all the properties shown by superconductors, such as zero resistance, Meissner effect, etc. This theory involves electron interactions through phonons. The basis for BCS theory is: (i) isotopic effect and (ii) specific heat of superconductors. Isotopic effect,  $T_c M^{1/2} = \text{constant}$ , infers that the transition to superconducting state must involve the dynamics of motions, lattice vibrations and phonons. Also as  $T_c \rightarrow 0$ , then  $M$  approaches infinity. This suggests non-zero transition temperature and finite mass of ions.

### Description

Suppose an electron approaches a positive ion core in the crystal, then the electron makes an attractive interaction with a positive ion. This attractive interaction sets in motion the positive ion and this ion motion distorts the lattice. This distortion of lattice is quantized in terms of phonons. At that instant, if another electron approaches the distorted lattice, then the interaction between this second electron and distorted lattice takes place; this interaction lowers the energy of second electron. Now, the two electrons interact through the lattice distortion or the phonon field and results in the lowering of energy of the electrons. The lowering of energy indicates that an attractive force exists between the electrons. This attractive interaction is larger if the two electrons have opposite spin and momenta. This interaction is called electron-lattice-electron interaction or electron-electron interaction through

**Figure 9.18** Electron-electron interaction through phonons



phonons as a mediator. Cooper stated that the presence of an attractive interaction even weak in between two electrons in a superconductor makes them to form a bound pair. Cooper showed that the lowering of energy leads to the formation of a bound state. Such bound pairs of electrons formed by the interaction between the electrons with opposite spin and momenta are known as Cooper pairs. This interaction can be represented in terms of the wave vector of electrons as shown in Fig. 9.18. Let an electron having wave vector  $K_1$  emits a virtual phonon  $q$  and this phonon is absorbed by another electron having wave vector  $K_2$ , then  $K_1$  is scattered as  $K_1 - q$  and  $K_2$  as  $K_2 + q$ . Conservation of energy is not satisfied in this reaction. This process is called virtual because virtual phonons are involved in this process.

In this interaction, phonon exchange takes place between electrons. If the phonon energy exceeds electronic energy, then the interaction is attractive and the attractive force between these two electrons exceeds the usual repulsive force. These two electrons which interact attractively in the phonon field are called Cooper pairs. The Cooper pair of electrons are said to be in the bound state or in the condensed state so that their energy is less than in the free state. The difference of energy of these electrons between these two states is equal to the binding energy of Cooper pair. Below critical temperature, the electron-lattice-electron interaction is stronger than electron-electron coulomb interaction, so electrons tend to pair up. The pairing is complete at 0 K and is completely broken at critical temperature. According to quantum theory, a wave function could be associated with a Cooper pair by treating it as a single entity. The Cooper pairs do not get scattered in the material and the conductivity becomes infinite which is named as superconductivity. The best conductors such as gold, silver and copper do not exhibit superconductivity because the electrons in these metals move freely in the lattice that, the electron-lattice interaction is virtually absent and the Cooper pairs will not form. Hence, these metals will not show superconductivity.

BCS theory explains the energy gap in superconductors in the following way: The energy gap at the Fermi surface is the energy difference between the free state of the electron and its paired state. The energy gap is a function of temperature. The energy gap is maximum at 0 K because pairing is complete at this temperature. At transition temperature, the energy gap reduces to zero because pairing is dissolved. The existence of energy gap in superconductors can be proved by the absorption of electromagnetic waves in microwave region. At temperature close to 0 K, a superconductor does not absorb energy of incident radiation until the energy of the incident radiation exceeds the width of the gap ( $2\Delta$ ) after absorption of energy, the electrons become free or normal.

## Coherent length

The paired electrons (Cooper pair) are not scattered because they smoothly ride over the lattice points or to the lattice imperfections. The Cooper pairs are not slowed down. Hence, the substance does not possess any electrical resistivity. Superconductivity is due to the mutual interaction and correlation of electrons over a considerable distance called coherent length ( $\epsilon_0$ ). It is found to be of the order of  $10^{-6}$  m. The coherent length is defined as the maximum distance up to which the state of paired electrons are correlated to produce superconductivity. The ratio of London penetration depth ( $\lambda$ ) to the coherence length ( $\epsilon_0$ ) is represented as

$$(K) = \lambda/\epsilon_0 \text{ is a number. For Type-I superconductors, } K < \frac{1}{\sqrt{2}} \text{ and for Type-II superconductors, } K > \frac{1}{\sqrt{2}}.$$

The intrinsic coherence ( $\epsilon_0$ ) is related to the energy gap as  $\epsilon_0 \approx \frac{\hbar v_F}{2\Delta}$  where  $2\Delta$  is the energy gap.

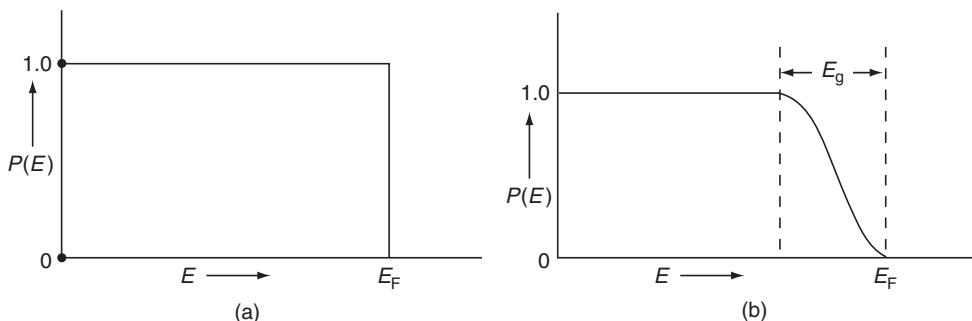
## BCS ground state

Fermi gas in the ground state is bounded by Fermi surface, excited state of an electron can be formed by taking an electron from the Fermi surface to just above it. According to BCS theory in superconducting state, there is an attractive interaction between the electrons [Cooper pairs]. In this case, we cannot form an excited state unless we supply an energy which exceeds the energy of attraction between electrons. These electron states are known as BCS ground states. This implies that the energy of Cooper pairs of electrons or BCS ground state is separated by a finite energy gap  $E_g (= 2\Delta)$  from the lowest excited energy state (Fermi energy). Further, the Cooper pairs are situated within about  $K_B \theta_D$  of the Fermi energy where  $\theta_D$  is the Debye temperature. The energy gap is situated about the Fermi surface of the Fermi state. The probability of occupation of the ground state in terms of one particle states is shown in Fig. 9.19(a).

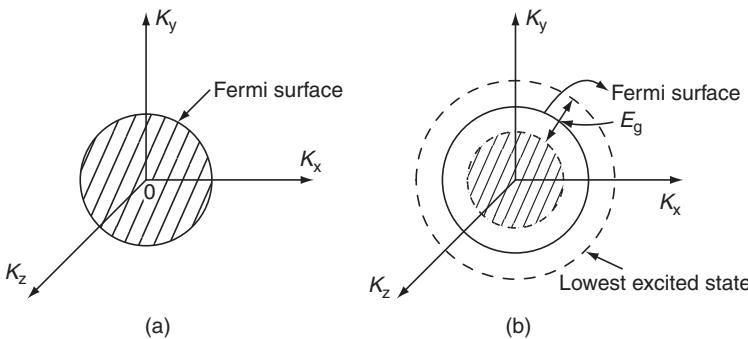
BCS ground state of superconductor is shown in Fig. 9.20. Figure 9.20(a) shows the ground state of Fermi gas and Fig. 9.20(b) shows the BCS ground state of electrons with an attractive interaction between them, states near  $E_F$  are filled in accordance with the probability shown in Fig. 9.19(b). The lowest excited state is separated from the ground state in this case by an energy gap  $E_g$ .

The total energy (T.E) of the BCS state is lower than that of the Fermi state. The total energy of the BCS state consists of K.E and attractive P.E, whereas that of Fermi state comprises K.E only. Thus, the attractive P.E reduces the T.E of the BCS state. This is in agreement with experimental observations on the superconducting and normal states.

**Figure 9.19 (a) Ground state of Fermi gas; (b) BCS ground state**



**Figure 9.20 (a) Ground state of Fermi gas; (b) BCS ground state of an electron gas**



## 9.9 Applications of superconductivity

Superconductors find many applications. Some of them are mentioned below:

### 9.9.1 Magnetic applications

#### a. Superconducting magnets

Similar to electromagnets, superconducting magnets can also be formed by using coils of wire made up of superconducting material. To obtain magnetic fields from electromagnets, current should be maintained in the coil, whereas in superconducting coils, current once introduced into the coil will remain for a very long time and during this period magnetic field can be obtained, provided the temperature of the coil is maintained below its transition temperature [usually at liquid helium temperature]. The benefit of using superconducting magnets instead of electromagnets is the cost of power required to maintain superconductors at low temperature will be 1000 times less than the cost of power required in case of electromagnets to produce the same magnetic field. The size of superconducting magnets is less than that of electromagnets. Superconducting magnets are made of Type-II superconducting material because strong magnetic fields is of the order of 20 Tesla can be produced. Of the many superconducting materials, niobium-titanium (Nb Ti), a Type-II superconducting material, is mostly used because it can be easily drawn into thin wires.

The superconducting coils are used in electric machines, transformers and magnetic resonance imaging (MRI) instruments. MRI instruments are used in hospitals to obtain human body cross-sectional images. This process is much safer than using X-rays. Superconductor coils are used in magnetically levitated vehicles and in high-resolution nuclear magnetic resonance (NMR) instruments. Using NMR instruments, molecular structure of chemical compounds can be known. Superconducting coils are used in NMR imaging equipment, this equipment is used in hospitals for scanning the whole human body and diagnose medical problems.

#### b. Magnetic bearings

Meissner effect is used in these bearings. Mutual repulsion between two superconducting materials due to opposite magnetic fields is used in the construction of magnetic bearings. There is no friction in these bearings.

## 9.9.2 Electrical applications

### a. Loss-less power transmission

DC current through an ordinary metallic wire causes heating effect called Joule's heating that is proportional to  $i^2 R$ . This means an amount of electrical energy equal to  $i^2 R$  is wasted for every second. This dc power loss can be eliminated by passing current through a superconductor wire. For ac, the superconductors shows resistance.

### b. Superconductor fuse and breaker

We know some insulating materials that show superconductivity at low temperatures, thin films of such materials can be used instead of fuse because when more than critical current pass through them, then they change into normal state. In normal state, they are insulators. They would not conduct current, so it will act as a fuse. In breaker, a long thin film of superconductor is used. In normal state, this film possesses high resistance. In this, lead is used.

### c. Cryotron switch

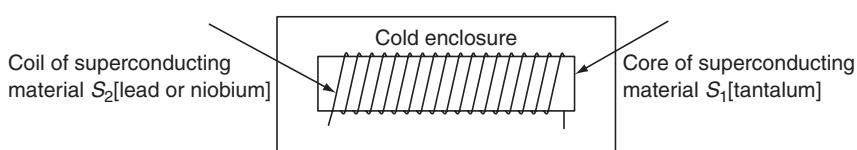
In this device, the resistance of a superconducting material can be made to zero or normal value by applying magnetic field of strength just below and above its critical magnetic field.

The device consists of a thick straight wire (or core), made up of some superconducting material  $S_1$ , on the surface of this another long thin wire made up of some other superconducting material  $S_2$ , has been wounded. This is called coil. The superconducting materials  $S_1$  and  $S_2$  are selected in such a way that the transition temperature of  $S_1$  should be less than that of  $S_2$ , hence the critical magnetic field of  $S_1$  is less than the critical magnetic field of  $S_2$ , at some temperature ' $T$ ' below their transition temperatures. This set-up is immersed in a cold enclosure as shown in Fig. 9.21. The temperature in the enclosure should be less than the transition temperature of  $S_1$  and  $S_2$ , so that the core and coil is in superconducting state.

The current flowing through the coil is adjusted such that the magnetic field produced is very close to the critical magnetic field of core at that temperature. Now, by slightly increasing the current through the coil, the core can be changed from superconducting to normal state; again by slightly reducing the current through the coil, the core can be brought back to superconducting state. Because by increasing the current through the coil, the magnetic field produced will exceed the critical magnetic field of core again by decreasing the current through the coil, the magnetic field produced can be brought below the critical magnetic field of core. Even the core changes to normal state, the coil will be in the superconducting state because of its high transition temperature. Thus, the resistance of core is made ON or OFF by external control, so that this arrangement functions as a switch. Cryotron may be used as an element in flip-flop.

To produce low temperature in the enclosure, the liquid helium [ $T_C = 4.2$  K] is used, then the core material could be tantalum [ $T_C = 4.38$  K] and coil material will be lead [ $T_C = 7.2$  K] or niobium [ $T_C = 9.3$  K].

**Figure 9.21** Cryotron switch



### 9.9.3 Computer applications

A closed superconducting ring [or a circular ring of superconductor] is used in memory cell. When persistent current in superconducting state passes through it, then it is said to be in '1' state. In normal state, current will not pass through it, then it is said to be in '0' state. Thus, the superconducting memory cell is a binary system.

### 9.9.4 Josephson junction devices

A very small gap between superconductors forms a junction called Josephson Junction. The devices which use such junctions are called Josephson Junction device. The dc Josephson effect is used in the construction of sensitive magnetometers. These devices can measure magnetic fields accurately up to  $10^{-11}$  gauss. AC Josephson effect is used to generate and detect electromagnetic radiations from radio frequencies to infrared frequencies.

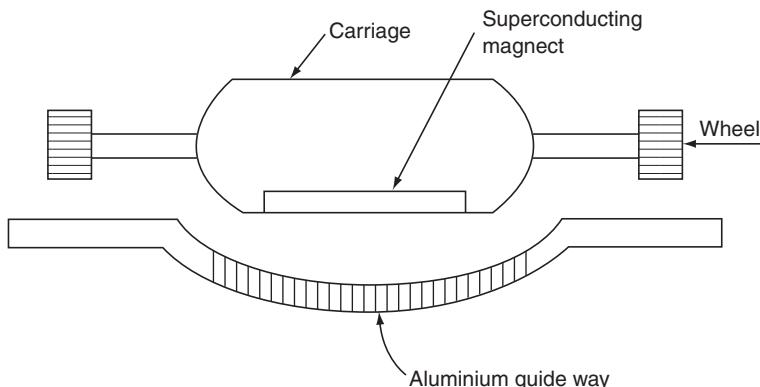
### 9.9.5 Maglev vehicles

Maglev vehicles means magnetically levitated vehicles. These vehicles are made to stay afloat above the guide way. So, it is not in contact with guide way. High speeds can be achieved with less energy. It is based on Meissner effect.

The Maglev vehicle is shown in Fig. 9.22. It consists of superconducting magnet at its base. There is a segmented aluminium guide way above which the maglev can be made to afloat by magnetic repulsion. The magnetic repulsion is in between the superconducting magnet at the bottom of Maglev and the magnetic field obtained by passing current through electric coils arranged in the aluminium guide way.

During the motion of the vehicle, only the part of the guided way over which the vehicle is located is actuated instantaneously. For this purpose, the guide way is formed into a large number of segments provided with coils. The currents in the segmented guide way not only levitate the vehicle but also help to move. Usually, the vehicle is levitated above the guide way by 10 to 15 cm. The vehicle is provided with retractable wheels. Once the vehicle is levitated in air, the wheels are pulled into the body, while stopping the wheels are drawn out and the vehicle slowly settles on the guide way after running a certain distance. Maglev train has been constructed in Japan, it runs at a speed of 500 km/h.

**Figure 9.22 Maglev vehicle**



### 9.9.6 Medical applications

#### a. Superconducting sensitive magnetometer

Superconducting quantum interference devices (SQUIDs) are used in the construction of superconducting sensitive magnetometers. Basically, SQUIDs are superconducting rings that are used in magnetic flux storage devices. The quantization of magnetic flux in SQUID is the basis for construction of sensitive magnetometer. With the aid of good electronic feedback circuit, SQUIDs can measure magnetic field strengths that are less than 1/1000 of a quantum of magnetic flux. SQUIDs are used in medical diagnostics of heart and brain. They can measure the magnetic fields generated by heart brain signals. They are of the order of  $10^{-14}$  Tesla. The SQUIDs are used to measure the voltages associated with brain, chest and cardiac activity. Earth magnetic field can be measured accurately using SQUIDs and a magnetic map can be constructed. This map helps us to detect mineral and oil deposits inside the earth.

#### b. Superconductors in medicine

(i) Human blood contains iron in certain percentage. Iron supplies oxygen to various parts of the body. If the iron content is less, then oxygen supply will be reduced and if iron content is more then it causes heart attack. The disease caused due to the variation of iron content in blood is called haemochromatosis. It is difficult to diagnose this disease, often overlooked. Doctors can detect this disease easily and quickly using superconducting susceptometer. In this instrument, superconducting magnet and SQUIDs are used.

(ii) A disease that produces disorder in nervous system of brain is called epilepsy. This disorder causes fits and brain malfunctions. The epileptic attacked part of the brain is short circuited. If the disease is severe in certain part of the brain, there the nerve pathways get jammed and the person receives meaningless signals from that damaged region. The only permanent cure for epilepsy is to operate and remove the damaged portion of the brain. The short-circuited epileptic centre produces distinctive magnetic signals. Doctors can locate the damaged portion of the brain by placing an array of a dozen SQUID magnetometers around the patient head and magnetic signals received by the magnetometers are fed to a computer. Computer analysis gives a three-dimensional picture of the activity within the brain. Doctors can locate the damaged portion of the brain in the image. This technique is known as magnetoencephalography.

### Formulae

$$1. \quad TM^{1/2} = \text{constant}$$

$$2. \quad H_c = H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right]$$

$$3. \quad \frac{\alpha_s}{\alpha_n} = 2 \exp \left[ \frac{-\Delta E}{K_B T} \right]$$

$$4. \quad B = \mu_0 (H + M) = \mu_0 H (1 + \chi)$$

$$5. \quad \lambda = \frac{\lambda_0}{\left[ 1 - \left( \frac{T}{T_c} \right)^4 \right]^{1/2}}$$

$$6. \quad \nu = \frac{2eV}{h}$$

**Solved Problems**

1. The critical field for niobium is  $1 \times 10^5$  amp/m at 8 K and  $2 \times 10^5$  amp/m at absolute zero. Find the transition temperature of the element.

(Set-2–May 2008)

**Sol:** Critical magnetic field at 8 K,  $H_c = 1 \times 10^5$  amp/m

$$T = 8 \text{ K}$$

$$\text{Critical magnetic field at } 0 \text{ K}, H_0 = 2 \times 10^5 \text{ amp/m}$$

$$\text{Transition temperature, } T_c = ?$$

$$H_c = H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right]$$

$$\frac{H_c}{H_0} = 1 - \left( \frac{T}{T_c} \right)^2 \quad \text{or} \quad \left( \frac{T}{T_c} \right)^2 = 1 - \frac{H_c}{H_0}$$

$$\therefore T_c^2 = \frac{T^2}{1 - \frac{H_c}{H_0}} = \frac{8^2}{1 - \frac{1 \times 10^5}{2 \times 10^5}} = \frac{8^2}{1 - \frac{1}{2}} = 2 \times 8^2$$

$$T_c = \sqrt{2} \times 8 = 11.3 \text{ K}$$

2. A Josephson junction having a voltage of  $8.50 \mu\text{V}$  across its terminals, then calculate the frequency of the alternating current.  
[Planck's constant =  $6.626 \times 10^{-34} \text{ J}\cdot\text{sec}$ ]

(Set-1–May 2008)

**Sol:** Voltage across the junction,  $V = 8.50 \mu\text{V}$

$$= 8.5 \times 10^{-6} \text{ V}$$

Frequency of alternating current,  $\nu = ?$

$$\nu = \frac{2eV}{h} = \frac{2 \times 1.6 \times 10^{-19} \times 8.5 \times 10^{-6}}{6.626 \times 10^{-34}}$$

$$= 4.1 \times 10^9 \text{ Hz}$$

3. A super conducting material has a critical temperature of 3.7 K, and a magnetic field of 0.0306 tesla at 0 K. Find the critical field at 2 K.

(Set-2–May 2007)

**Sol:**  $T_c = 3.7 \text{ K}$

$$T = 2 \text{ K}$$

$$H_0 = 0.0306 \text{ T}$$

$$H_c = ?$$

$$H_c = H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right]$$

$$= 0.0306 \left[ 1 - \left( \frac{2}{3.7} \right)^2 \right] = 0.0306 \times 0.7078$$

$$= 0.02166 \text{ Tesla}$$

4. A long superconducting wire produces a magnetic field of  $200 \times 10^3$  A/m on its surface due to current through it at temperature  $T (< T_c)$ . Its critical magnetic field at 0 K is  $250 \times 10^3$  A/m. The critical temperature of the material of wire is 12 K. Find the value of  $T$ .

**Sol:**  $H_c = H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right] \Rightarrow \frac{H_c}{H_0} = 1 - \left( \frac{T}{T_c} \right)^2$

$$\left( \frac{T}{T_c} \right)^2 = 1 - \frac{H_c}{H_0} \Rightarrow T^2 = T_c^2 \left( 1 - \frac{H_c}{H_0} \right)$$

$$T_c = 12 \text{ K}$$

$$H_0 = 250 \times 10^3 \text{ A/m}$$

$$H_c = 200 \times 10^3 \text{ A/m}$$

Then,  $T^2 = (12)^2 \left[ 1 - \left( \frac{200}{250} \right)^2 \right]$

$$\therefore T^2 = 144 (1 - 0.64)$$

$$T^2 = 144 \times .36 = 51.84$$

$$T = 7.2 \text{ K.}$$

5. The superconducting transition temperature of tin is 3.7 K. Its critical magnetic field at 0 K is 0.03 Tesla. What is the critical magnetic field at 2.5 K?

**Sol:**  $T_c = 3.7 \text{ K}, \quad T = 2.5 \text{ K}$

$$H_0 = 0.03 \text{ T}, \quad H_c = ?$$

$$H_c = H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right] = 0.03 \left[ 1 - \left( \frac{2.5}{3.7} \right)^2 \right] \text{ Tesla} = 0.0163 \text{ Tesla.}$$

3. What is the frequency of the electromagnetic waves radiated from a Josephson junction, if the voltage drop at the junction is  $650 \mu\text{V}$ ?

**Sol:**  $\nu = ?$

$$V = 650 \times 10^{-6} \text{ V}$$

$$e = 1.6 \times 10^{-19} \text{ C}$$

$$\hbar = 6.625 \times 10^{-34} \text{ JS}$$

$$\nu = \frac{2eV}{\hbar} = \frac{2 \times 1.6 \times 10^{-19} \times 650 \times 10^{-6}}{6.625 \times 10^{-34}} = \frac{2080 \times 10^{-25}}{6.625 \times 10^{-34}}$$

$$= 313.96 \times 10^9 \text{ Hz.}$$

6. A lead super conductor with  $T_C = 7.2$  K has a critical magnetic field of  $6.5 \times 10^3$  Am $^{-1}$  at absolute zero. What would be the value of critical field at 5 K temperature?

**Sol:**  $T_c = 7.2 \text{ K}$

$$H_o = 6.5 \times 10^3 \text{ A/m}$$

$T = 5 \text{ K}$

$$H_C = ?$$

$$H_C = H_0 \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right]$$

$$= 6.5 \times 10^3 \left[ 1 - \left( \frac{5}{7.2} \right)^2 \right] = 6.5 \times 10^3 [1 - 0.482]$$

$$= 3.365 \times 10^3 \text{ A/m.}$$

## Multiple Choice Questions

9. The relation between transition temperature ( $T_c$ ) and isotopic mass ( $M$ ) is. ( )
- (a)  $T_c \propto M^{1/2}$       (b)  $T_c \propto M^{-1/2}$       (c)  $T_c \propto M^{-1}$       (d)  $T_c \propto M$
10. The critical magnetic field ( $H_c$ ) at temperature  $T$  K is.: ( )
- (a)  $H_0 \left[ 1 - \left( \frac{T_c}{T} \right)^2 \right]$       (b)  $H_0 \left[ 1 - \left( \frac{T}{T_c} \right) \right]$       (c)  $H_0 \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right]$       (d)  $H_0 \left[ \left( \frac{T}{T_c} \right)^2 - 1 \right]$
11. The thermal conductivity of a metal in normal and in superconducting state is. ( )
- (a) same      (b) different      (c) both a and b      (d) none
12. Type-I superconductivity is also called as: ( )
- (a) Silsbee effect      (b) Subnikov effect  
 (c) Boltzmann effect      (d) Planck's effect
13. Type-I superconductors can produce magnetic fields of the order of. ( )
- (a) 100 Tesla      (b) 10 Tesla      (c) 1 Tesla      (d) 0.1 Tesla
14. Examples for Type-I superconductors are: ( )
- (a) all elements      (b) alloys  
 (c) ferromagnetic materials      (d) ceramics
15. The distance from the surface of a superconductor to a point in the superconductor at which the intensity of magnetic field is  $(1/e)$  at the surface is called. ( )
- (a) Josephson penetration depth      (b) London penetration depth  
 (c) Maxwell penetration depth      (d) none
16. If  $H_0$  is the intensity of magnetic field on the surface of a material, then the intensity of field at a depth ' $x$ ' from the surface is. ( )
- (a)  $H_0 \exp \left( \frac{x}{\lambda} \right)$       (b)  $H_0 \exp \left( \frac{-x}{\lambda} \right)$       (c)  $H_0 \exp \left( \frac{\lambda}{x} \right)$       (d)  $H_0 \exp \left( \frac{-\lambda}{x} \right)$
17. At temperature  $T (< T_c)$ , the London penetration depth can be expressed as. ( )
- (a)  $\frac{\lambda_0}{\sqrt{1 - \left( \frac{T}{T_c} \right)^4}}$       (b)  $\frac{\lambda_0}{\sqrt{1 - \frac{T}{T_c}}}$       (c)  $\frac{\lambda_0}{1 - \left( \frac{T}{T_c} \right)^4}$       (d)  $\frac{\lambda_0}{\sqrt{1 - \left( \frac{T_c}{T} \right)^3}}$
18. A quantum of magnetic flux in a superconductor is equal to. ( )
- (a)  $\frac{h}{e}$       (b)  $\frac{h}{2e}$       (c)  $\frac{h}{4e}$       (d)  $\frac{h}{5e}$
19. The maintenance cost of superconducting magnets is \_\_\_\_\_ times less than the maintenance cost of electromagnet to produce same magnetic field. ( )
- (a) 10,000      (b) 1000      (c) 100      (d) 10
20. Usually, maglev vehicle is raised above the aluminium path by a height of. ( )
- (a) 10 to 20 cm      (b) 1 to 2 cm      (c) 50 to 70 cm      (d) 70 to 100 cm

21. SQUIDS are used to measure \_\_\_\_\_ associated with brain and chest. ( )  
 (a) power                    (b) energy                    (c) stress                    (d) voltages
22. Superconducting susceptometer is used to detect. ( )  
 (a) epilepsy                (b) haemochromatosis    (c) diabetes                (d) none
23. The electron pairs in a superconductor are called. ( )  
 (a) Cooper pairs            (b) Bardeen pairs          (c) BCS-pairs              (d) Josephson pairs
24. A material changes from normal to superconducting state below \_\_\_\_\_ temperature. ( )  
 (a) Curie                    (b) critical                (c) Weiss                    (d) none
25. The transition temperature of mercury is. ( )  
 (a) 4.2 K                    (b) 7.5 K                    (c) 12 K                    (d) 20 K
26. At transition temperature, the electrical resistance of a material. ( )  
 (a) is large                (b) is less                    (c) vanishes                (d) none
27. For a superconductor, the critical magnetic field \_\_\_\_\_ with decrease of temperature. ( )  
 (a) increases                (b) decreases                (c) will not change        (d) none
28. In superconducting state, we \_\_\_\_\_ pass large current. ( )  
 (a) can                      (b) cannot                    (c) both a & b              (d) none
29. The maximum current that can be passed through a superconductor is called. ( )  
 (a) supercurrent            (b) optimum current        (c) critical current        (d) none
30. Superconductivity is not shown for \_\_\_\_\_. ( )  
 (a) dc current              (b) ac current                (c) saw-tooth current     (d) none
31. A superconductor is in more ordered than \_\_\_\_\_. ( )  
 (a) a normal metal        (b) a semiconductor        (c) a dielectric            (d) none
32. Below transition temperature, the heat capacity of a superconductor. ( )  
 (a) changes with temperature                                    (b) changes with magnetic field  
 (c) changes with electric field                                (d) none
33. The width of superconducting energy gap. ( )  
 (a) increases with temperature                                (b) decreases with increase of temperature  
 (c) will not change with temperature                        (d) none
34. A superconductor is a perfect \_\_\_\_\_ material. ( )  
 (a) diamagnetic            (b) dielectric                (c) insulator                (d) semiconductor
35. In Type-I superconductors, the transition from superconducting to normal state by the application of magnetic field is. ( )  
 (a) erratic                    (b) sharp                    (c) both a & b              (d) none
36. In Type-II superconductors, the transition from superconducting to normal state by the application of magnetic field is. ( )  
 (a) sharp                    (b) not sharp                (c) erratic                    (d) none

37. Type-II superconductors are: ( )  
 (a) alloys (b) transition metals  
 (c) both a & b (d) none
38. The intensity of an applied magnetic field decreases \_\_\_\_\_ with depth from the surface of a superconductor. ( )  
 (a) exponentially (b) linearly (c) logarithmically (d) inversely
39. If dc voltage exists across Josephson junction, then \_\_\_\_\_ current passes across the junction. ( )  
 (a) dc (b) ac (c) pulsating (d) none
40. The material used in the construction of superconducting magnets are: ( )  
 (a) niobium (b) titanium (c) both a & b (d) none
41. Joules heating in superconductors is: ( )  
 (a) present (b) absent (c) both a & b (d) none
42. The core and coil of a cryotron switch is prepared with \_\_\_\_\_ superconducting material. ( )  
 (a) same (b) different (c) both a & b (d) none
43. \_\_\_\_\_ Josephson effect is used to generate and detect electromagnetic waves of frequencies ranging from radiowave to infrared wave. ( )  
 (a) ac (b) dc (c) both a & b (d) none
44. Maglev vehicles are constructed based on \_\_\_\_\_ effect. ( )  
 (a) gravitational (b) electrical (c) Meissner (d) none
45. With the aid of good electronic feedback circuit, SQUIDS can measure magnetic fields that are less than \_\_\_\_\_ of a quantum of magnetic flux. ( )  
 (a) 1/10 (b) 1/100 (c) 1/1000 (d) none

## Answers

1. c	2. b	3. a	4. d	5. b	6. d	7. a	8. b	9. b	10. c
11. b	12. a	13. d	14. a	15. b	16. b	17. a	18. b	19. b	20. a
21. d	22. b	23. a	24. b	25. a	26. c	27. a	28. b	29. c	30. b
31. a	32. a	33. b	34. a	35. b	36. b	37. c	38. a	39. b	40. c
41. b	42. b	43. a	44. c	45. c					

## Review Questions

- Describe the BCS theory of superconductivity. (Set-3–June 2005)
- Write various applications of superconductivity. (Set-3–June 2005)
- Explain dc and ac Josephson's effect. (Set-3–June 2005)
- Write notes on the applications of superconducting materials. (Set-4–May 2008)
- Describe the differences between Type-I and Type-II superconductors. (Set-2–May 2008)

6. Explain the critical parameters and their significance in superconductors. (Set-1–May 2008)
7. Write notes on (i) isotopic effect and (ii) energy gap in superconductors. (Set-1–May 2008)
8. What is Meissner effect? Explain. (Set-2, Set-4–May 2008), (Set-2–May 2007)
9. Explain the following (a) critical magnetic field of a superconductor as a function of temperature, (b) Meissner effect and (c) cryotrons. (Set-4–May 2007)
10. How are superconductors classified? Explain their properties. (Set-4–May 2008), (Set-1–Sept. 2006), (Set-2–May 2006)
11. What is meant by isotopic effect? Explain with suitable example. (Set-2–May 2007)
12. Define the terms of superconductivity: (i) critical temperature, (ii) critical magnetic field and critical current. (Set-3–May 2006)
13. What are Cooper pairs? Explain. (Set-3–May 2006)
14. Write notes on any four applications of superconductors. (Set-3–May 2006)
15. Write notes on the applications of superconducting materials. (Set-4–May 2008), (Set-1–Sept. 2006), (Set-2–May 2006)
16. Explain Meissner effect? (Set-2–May 2007)
17. (a) What is superconductivity?  
(b) Explain the two types of superconductors briefly.
18. Discuss the formation of Cooper pairs and energy gap in superconductors on the basis of BCS theory.
19. Explain the phenomenon of superconductivity and Meissner effect.
20. Briefly describe, how Cooper pairs are formed.
21. Explain flux quantization in superconductivity.
22. Write short notes on Type-I and Type-II superconductors.
23. Explain the origin of energy gap of a superconducting material. How this energy gap differs from that of a normal conductor?
24. Explain the properties of a superconductor in detail.
25. Distinguish between Type-I and Type-II superconductors.
26. What is superconductivity? Describe the effect of: (a) magnetic field (b) frequency and (c) isotopes on superconductors. Mention a few industrial applications of superconductors.
27. What is superconductivity? Explain Meissner effect. What are the possible applications of superconductivity?
28. Explain Type-I and Type-II superconductors. What are Josephson's effects?
29. Mention some important characteristics of superconductivity.
30. Explain the BCS theory of superconductivity.
31. Describe Josephson effect and their applications.
32. Perfect diamagnetism is a more fundamental property than perfect conductivity to assert that a material is in superconducting state. Explain this statement.
33. Explain Meissner effect. How is it used to classify the superconductors?

34. Describe dc and ac Josephson effect in superconductors and prove that the current density across a superconducting junction in the former case varies sinusoidally as the phase difference of state function of Cooper pair on either side of it.
35. Describe the phenomena of flux quantization in superconductors and prove that the current oscillates with a frequency equal to  $\frac{2e}{\hbar}$  times the potential difference across the superconducting junction.
36. Justify that a superconductor can be used as a fuse with the relevant mechanism.
37. Write short notes on Type-II superconductors.
38. Explain the working of a SQUID.
39. Explain BCS theory of superconductors.
40. Describe the Josephson effect underlying a SQUID.
41. Explain Meissner effect. Discuss Type-I and Type-II superconductors. Mention a few applications of superconductors.
42. What are superconductors? Give the qualitative description of the BCS theory.
43. Explain critical temperature, critical field and critical current in a superconductor. Explain BCS theory.

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## CHAPTER

# 10

## Lasers

### 10.1 Introduction

LASER stands for Light Amplification by Stimulated Emission of Radiation. Laser light is different from conventional light. In conventional light sources [such as tube light or electric bulb], there is no coordination among different atoms emitting radiation. Whereas in lasers, all atoms act together and produce highly directional, monochromatic, coherent and stimulated radiation. In conventional light source, different atoms emit radiation at different times and in different directions so that there is no phase relation between the emitted photons. The photons emitted by different atoms of laser are in phase or they maintain constant phase relationship and they move in the same direction. Lasing has been extended upto  $\gamma$ -rays.  $\gamma$ -ray lasers are called Grasers.

### 10.2 Characteristics of laser radiation

Laser radiation has the following important characteristics over ordinary light source. They are: i) monochromaticity, ii) directionality, iii) coherence and iv) brightness.

**(i) Monochromaticity:** A laser beam is more or less in single wavelength. i.e., the line width of laser beams are extremely narrow. The wavelengths spread of conventional light sources is usually 1 in  $10^6$ , whereas in case of laser light it will be 1 in  $10^{15}$ . i.e., if the frequency of radiation is  $10^{15}$  Hz, then the width of line will be 1 Hz. So, laser radiation is said to be highly monochromatic. The degree of non-monochromaticity has been expressed as  $\xi = \frac{d\lambda}{\lambda} = \frac{d\nu}{\nu}$  where  $d\lambda$  or  $d\nu$  is the variation in wavelength or variation in frequency of radiation.

**(ii) Directionality:** Laser beam is highly directional because laser emit light only in one direction. It can travel very long distances without divergence. So, laser communication has been carried between earth and moon.

A laser beam sent from earth to moon was recorded on earth after reflection by moon. The directionality of a laser beam has been expressed in terms of divergence. Suppose  $r_1$  and  $r_2$  are the radii of laser beam at distances  $D_1$  and  $D_2$  from a laser, then we have:

$$\text{The divergence, } \Delta\theta = \frac{r_2 - r_1}{D_2 - D_1}$$

The divergence for a laser beam is 0.01 milliradian whereas in case of search light it is 0.5 radian.

**(iii) Coherence:** Laser beam is spatially and temporally coherent.

**Spatial coherence:** If a wave maintains a constant phase difference or in phase at two different points on the wave over a time ' $t$ ', then the wave is said to have spatial coherence. For He-Ne gas laser, the coherence length ' $L_c$ ' is about 600 Km. Coherence length is defined as the length over which the wave maintains same phase. For sodium lamp light source, the coherent length is 3 cm. There is an inverse relation between non-chromacity and coherent length.

$$\text{non-chromaticity} \propto \frac{1}{L_c}$$

So, laser light has very less non-chromaticity.

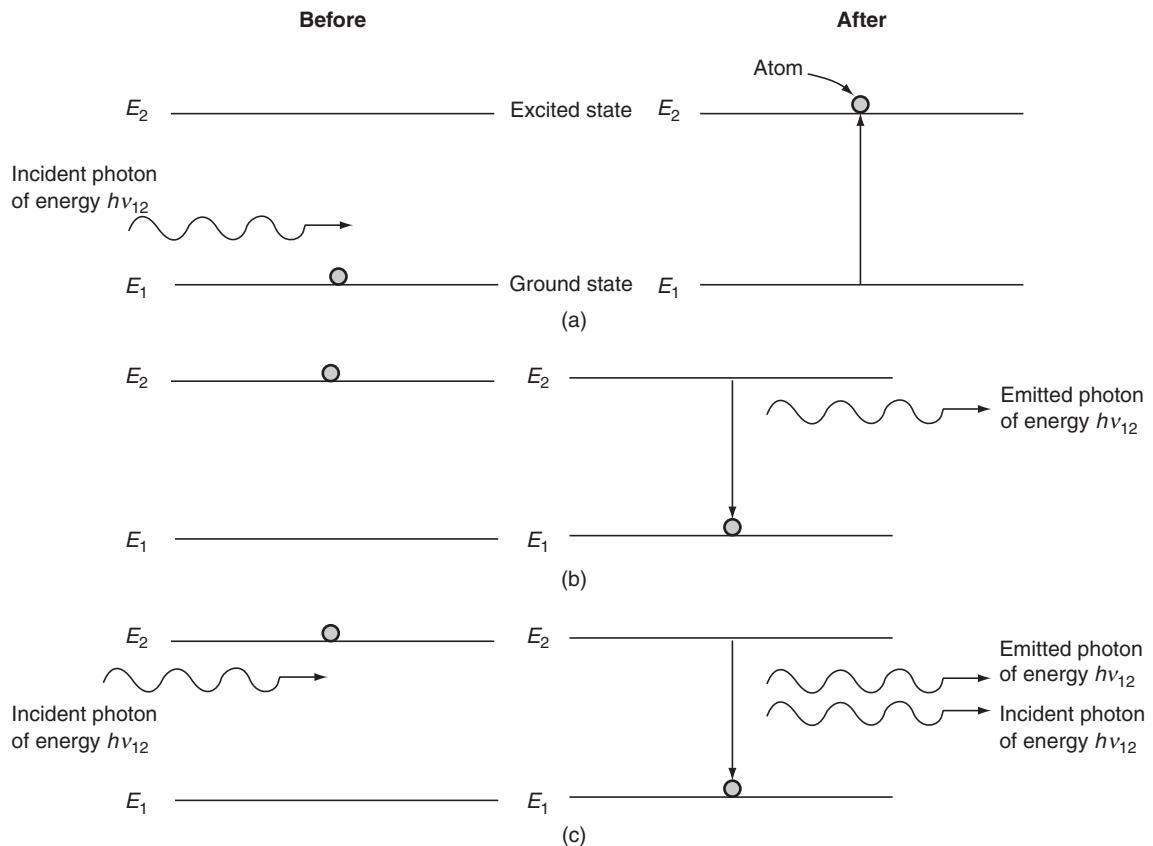
**Temporal coherence:** It refers to the correlation between light fields at different times at a point on the wave. If there is no change in phase over a time ' $t$ ' at a point on the wave, then it is said to be coherent temporally during that time. If the phase changes many times at a point, then it is said to be incoherent. For He-Ne laser, the coherence time is  $2 \times 10^{-3}$  seconds whereas for sodium lamp, it is  $\approx 10^{-10}$  seconds. So, there is no temporal coherence for light from sodium lamp.

**(iv) Brightness:** The laser beam is highly bright (intense) as compared to the conventional light sources because more light energy is concentrated in a small region. The light from an ordinary lamp comes out more or less in all directions. It has been observed that the intensity of 1mV laser light is 10,000 times brighter than the light from the sun at the earth's surface. The number of photons coming out from a laser per second per unit area is about  $10^{22}$  to  $10^{34}$  whereas the number of photons comes out per second per unit area of black body at 1000 K having wavelength ( $\lambda$ ) = 6000 Å is  $\approx 10^{16}$ . Thus, a very hot body cannot generate the number of photons per second per unit area coming out from a laser in the visible region. Laser light is coherent, so at a time many photons are in phase and they superimpose to produce a wave of larger amplitude. The intensity is proportional to the square of amplitude. Hence, the intensity of the resultant laser beam is very high.

## 10.3 Spontaneous and stimulated emission

In lasers, the interaction between matter and light is of three different types. They are: absorption, spontaneous emission and stimulated emission. In these processes, two energy levels of atoms are involved. As shown in Fig. 10.1, Let  $E_1$  and  $E_2$  be ground and excited states of an atom. The dot in Fig. 10.1, represents an atom. Transition between these states involves absorption or emission of a photon of energy  $E_2 - E_1 = h\nu_{12}$ , where ' $h$ ' is Planck's constant. Now, we study these processes in detail.

**Figure 10.1 (a) Absorption; (b) Spontaneous emission; (c) Stimulated emission**



**(a) Absorption:** As shown in Fig. 10.1(a), if a photon of energy  $h\nu_{12}$  ( $= E_2 - E_1$ ) collides with an atom present in the ground state of energy  $E_1$  then the atom completely absorbs the incident photon and makes transition to excited state  $E_2$ .

**(b) Spontaneous emission:** As shown in Fig. 10.1(b), an atom initially present in the excited state makes transition voluntarily on its own, without any aid of external stimulus or an agency to the ground state and emits a photon of energy  $h\nu_{12}$  ( $= E_2 - E_1$ ). This is called spontaneous emission. Different atoms of the medium emit photons at different times and in different directions. Hence, there is no phase relationship among the emitted photons, so they are incoherent. Examples for spontaneous light are glowing tube light, electric bulb, candle flame, etc.

**(c) Stimulated emission:** As shown in Fig. 10.1(c), a photon having energy  $h\nu_{12}$  ( $= E_2 - E_1$ ) impinges (or passes in the vicinity) on an atom present in the excited state and the atom is stimulated to make transition to the ground state and gives off a photon of energy  $h\nu_{12}$ . The emitted photon is in phase with the incident photon. The two photons travel in the same direction and they possess same energy and frequency. They are coherent. This type of emission is known as stimulated emission.

Differences between spontaneous emission and stimulated emission of radiation:

Spontaneous Emission	Stimulated Emission
1. Polychromatic radiation	1. Monochromatic radiation
2. Less intensity	2. High intensity
3. Less directionality, so more angular spread during propagation	3. High directionality, so less angular spread during propagation
4. Spatially and temporally incoherent radiation	4. Spatially and temporally coherent radiation
5. Spontaneous emission takes place when excited atoms make transition to lower energy level voluntarily without any external stimulation.	5. Stimulated emission takes place when a photon of energy equal to $h\nu (= E_2 - E_1)$ stimulates an excited atom to make transition to lower energy level.

## 10.4 Einstein's coefficients

To illustrate a laser, the idea of stimulated emission is essential. This can be understood in the following way: atoms absorb photons and emits photons of different frequencies. The emission may be spontaneous or stimulated. To obtain an expression that represents the ratio of spontaneous emission to stimulated emission, we consider a container having atoms and radiation. Some of the atoms present in the ground state absorb photons of energy  $h\nu_{12}$  and raised to excited state ( $E_2$ ) and they make spontaneous or stimulated emissions.

In steady state, let  $n_1$  and  $n_2$  be the number of atoms in ground state ( $E_1$ ) and in excited state ( $E_2$ ) per unit volume of the material. The ratio of  $n_1$  and  $n_2$  can be represented using Boltzmann distribution law, as:

$$\frac{n_1}{n_2} = \exp\left[\frac{E_2 - E_1}{K_B T}\right] = \exp\left[\frac{hf}{K_B T}\right] \quad (10.1)$$

where  $K_B$  is Boltzmann constant,  $f$  is the frequency of radiation and  $T$  is the absolute temperature of the atoms. Inside the container, radiation is present so, the number of photons per unit volume having frequencies around ' $f$ ' in unit range [ i.e., radiation density] is represented as  $\sigma(f)$  and is given by Planck's black body radiation law as:

$$\sigma(f) = \frac{8\pi hf^3}{c^3 \left[ \exp\left(\frac{hf}{K_B T}\right) - 1 \right]} \quad (10.2)$$

where ' $b$ ' is Planck's constant and  $c$  is the velocity of light. An atom in the lower energy state  $E_1$  gets excited to  $E_2$  state by absorbing radiation of frequency,

$$f = \frac{E_2 - E_1}{h} \quad (10.3)$$

The number of such absorptions in unit volume of the material per unit time is proportional to  $n_1$  and radiation density  $\sigma(f)$ . Hence, we have:

$$\text{The absorption rate} = B_{12} n_1 \sigma(f) \quad (10.4)$$

where  $B_{12}$  is the absorption proportionality constant. The atoms in the excited state are unstable, they make transition from excited state to ground state by making spontaneous and stimulated emissions. The number of spontaneous emissions in unit volume of the material per unit time is proportional to  $n_2$ . Hence, we have:

$$\text{The spontaneous emission rate} = A_{21} n_2 \quad (10.5)$$

where  $A_{21}$  is the spontaneous emission proportionality constant. Similarly, the number of stimulated emissions in unit volume of the material per unit time is proportional to  $n_2$  and radiation density,  $\sigma(f)$ . Hence, we have:

$$\text{The stimulated emission rate} = B_{21} n_2 \sigma(f) \quad (10.6)$$

where  $B_{21}$  = stimulated emission proportionality constant.

In steady state,

$\therefore$  From Equations (10.4), (10.5) and (10.6) we write:

$$B_{12} n_1 \sigma(f) = A_{21} n_2 + B_{21} n_2 \sigma(f)$$

$$(or) \quad \sigma(f) [B_{12} n_1 - B_{21} n_2] = A_{21} n_2 \quad (10.7)$$

$$\begin{aligned} \sigma(f) &= \frac{A_{21} n_2}{B_{12} n_1 - B_{21} n_2} = \frac{A_{21} n_2}{n_2 B_{21} \left[ \frac{B_{12} n_1}{B_{21} n_2} - 1 \right]} \\ &= \frac{A_{21}/B_{21}}{\frac{B_{12}}{B_{21}} \frac{n_1}{n_2} - 1} \quad (10.8) \end{aligned}$$

Substituting Equation (10.1) in (10.8) for  $n_1/n_2$ , we have:

$$\sigma(f) = \frac{A_{21}/B_{21}}{\frac{B_{12}}{B_{21}} \exp \frac{hf}{K_B T} - 1} \quad (10.9)$$

In thermal equilibrium state, Equations (10.2) and (10.9) are equal.  
so,

$$\frac{8\pi hf^3}{c^3 \left[ \exp \left( \frac{hf}{K_B T} \right) - 1 \right]} = \frac{A_{21}/B_{21}}{\frac{B_{12}}{B_{21}} \exp \left( \frac{hf}{K_B T} \right) - 1} \quad (10.10)$$

Under stimulated emission, the probability of upward transitions and probability of downward transitions are equal, so:

$$B_{12} = B_{21} = B \text{ and } A_{21} = A \text{ (say).}$$

Then, Equation (10.10) becomes:

$$\frac{A_{21}}{B_{21}} = \frac{A}{B} = \frac{8\pi hf^3}{c^3} \quad \text{--- (10.11)}$$

The proportionality constants  $A_{21}$ ,  $B_{12}$  and  $B_{21}$  are called Einstein's  $A$  and  $B$  coefficients. From Equations (10.5) and (10.6), the ratio of spontaneous emission rate to stimulated emission rate is:

$$\frac{A_{21} n_2}{B_{21} n_2 \sigma(f)} = \frac{A_{21}}{B_{21} \sigma(f)} = \frac{A/B}{\sigma(f)} \quad \text{--- (10.12)}$$

Substituting Equations (10.2) and (10.11) in (10.12) gives:

$$= \frac{8\pi hf^3}{c^3} \left/ \frac{8\pi hf^3}{c^3 \left[ \exp\left(\frac{hf}{K_B T}\right) - 1 \right]} \right. = \exp\left(\frac{hf}{K_B T}\right) - 1 \quad \text{--- (10.13)}$$

This ratio works out to be  $10^{10}$ , thus at optical frequencies, the emission is predominantly spontaneous. So, the conventional light sources emit incoherent radiation.

## 10.5 Population inversion

Usually in a system the number of atoms ( $N_1$ ) present in the ground state ( $E_1$ ) is larger than the number of atoms ( $N_2$ ) present in the higher energy state. The process of making  $N_2 > N_1$  is called population inversion. Population inversion can be explained with three energy levels  $E_1$ ,  $E_2$  and  $E_3$  of a system. Let  $E_1$ ,  $E_2$  and  $E_3$  be ground state, metastable state and excited states of energies of the system respectively such that  $E_1 < E_2 < E_3$ . In a system, the population of atoms ( $N$ ) in an energy level  $E$ , at absolute temperature  $T$  has been expressed in terms of the population ( $N_1$ ) in the ground state using Boltzmann's distribution law

$$N = N_1 \exp(-E/K_B T) \quad \text{where } K_B = \text{Boltzmann's constant}$$

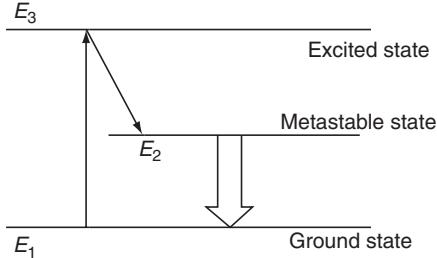
Graphically this has been shown in Fig. 10.2(b). As shown in Fig. 10.2(a), let the atoms in the system be excited from  $E_1$  state to  $E_3$  state by supplying energy equal to  $E_3 - E_1$  ( $= h\nu$ ) from an external source. The atoms in  $E_3$  state are unstable, they make downward transition in a time approximately  $10^{-8}$  seconds to  $E_2$  state. In  $E_2$  state, the atoms stay over a very long duration of the order of milliseconds. So, the population of  $E_2$  state increases steadily. As atoms in  $E_1$  state are continuously excited to  $E_3$  so, the population in  $E_1$  energy level goes on decreasing. A stage will reach at which the population in  $E_2$  state exceeds as that present in  $E_1$  state (i.e.,  $N_2 > N_1$ ). This situation is known as population inversion. Graphically the population inversion has been shown in Fig. 10.2(c).

Conditions for population inversion are:

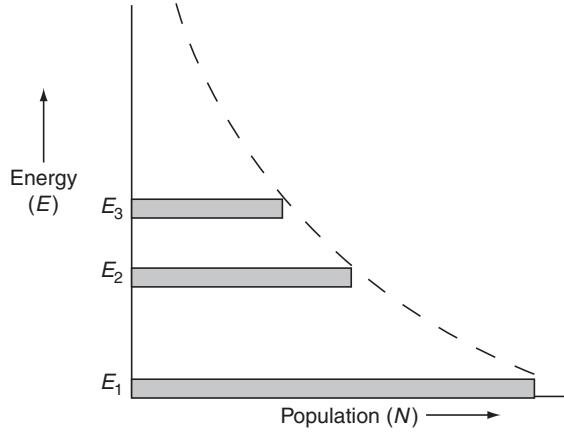
- The system should possess at least a pair of energy levels ( $E_2 > E_1$ ), separated by an energy equal to the energy of a photon ( $h\nu$ ).
- There should be a continuous supply of energy to the system such that the atoms must be raised continuously to the excited state.

Figure 10.2

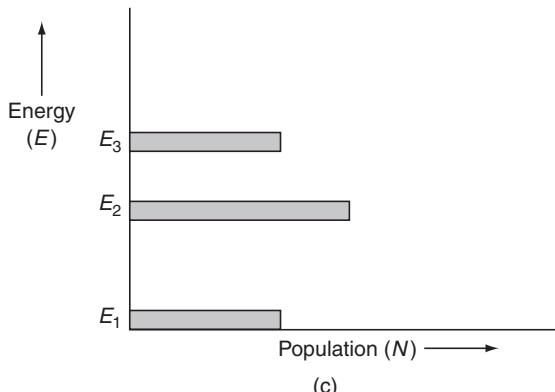
(a) Population inversion between  $E_1$  and  $E_2$  energy levels; (b) Population under thermal equilibrium; (c) Population inversion of  $E_2$  with respect to  $E_1$



(a)



(b)



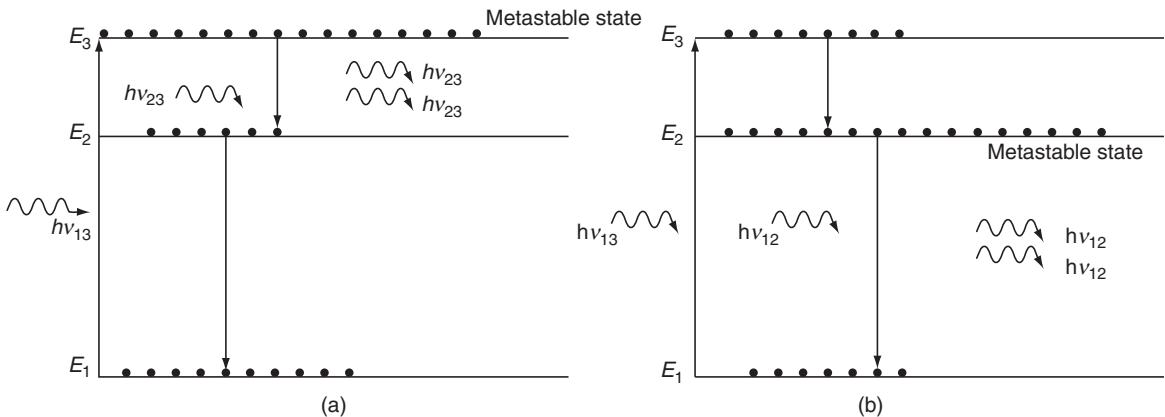
(c)

Population inversion can be achieved by a number of ways. Some of them are: (i) optical pumping (ii) electrical discharge (iii) inelastic collision of atoms (iv) chemical reaction and (v) direct conversion.

In a laser, if the active medium is a transparent dielectric, then optical pumping method is used. If the active medium is conductive, then electric field is used to produce population inversion. Few of the above pumping methods are explained below.

**Optical Pumping:** To explain optical pumping, we consider the three energy levels of atoms as shown in Fig. 10.3(a) & 10.3(b).

The transitions of atoms in these energy levels and laser emission has been explained in two ways. (i) As shown in Fig. 10.3(a), an atom present in the ground state ( $E_1$  energy level) absorbs a photon of energy equal to  $\hbar\nu_{13}$  and occupies  $E_3$  energy level.

**Figure 10.3 Three-level laser energy levels**

If the atoms makes transition from  $E_3$  to  $E_2$  energy level slowly and  $E_2$  to  $E_1$  fastly, then the number of atoms in  $E_3$  energy level will be more than in  $E_2$  energy level. i.e., population inversion ( $N_3 > N_2$ ) exists between  $E_3$  and  $E_2$  energy levels. The energy level  $E_3$  is called metastable state. An external photon of energy  $h\nu_{23}$  ( $=E_3 - E_2$ ) stimulates an atom in  $E_3$  level and hence stimulated emission takes place. So, the photon of energy  $h\nu_{23}$  acts as a laser light. The atoms present in  $E_2$  energy level makes non-radiative transition to  $E_1$  energy level.

(ii) As shown in Fig. 10.3(b), an atom present in the ground state ( $E_1$  energy level) absorbs a photon of energy  $h\nu_{13}$  and excited to  $E_3$  energy level. The atoms will remain very short duration ( $<10^{-8}$  sec) in  $E_3$  energy level and makes transition to  $E_2$  energy. This transition is non-radiative. In  $E_2$  energy level, the atoms will remain for longer duration than in  $E_3$  energy level. By continuous supply of energy  $h\nu_{13}$ , the number of atoms in  $E_2$  energy level go on increasing and the number of atoms in  $E_1$  energy level is reduced. Hence, population inversion exists between  $E_2$  and  $E_1$  energy levels i.e.,  $N_2 > N_1$ . Now, an external photon of energy  $h\nu_{12}$  can make stimulated emission. Hence, a laser beam of photon energy  $h\nu$  is obtained.

In electrical pumping, the applied electric field caused ionization of the medium and raises to the excited state. This has been used in gas lasers.

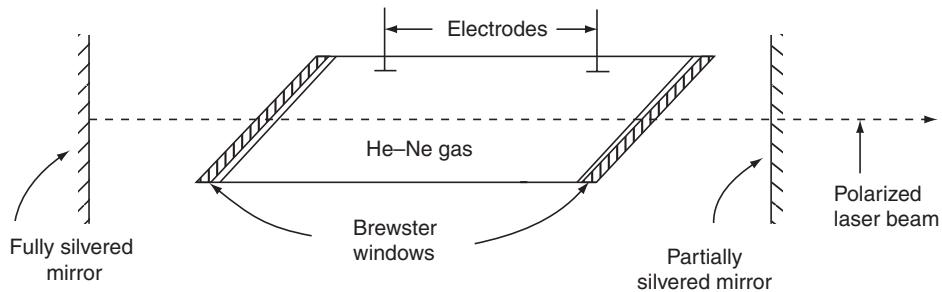
Direct conversion of electric energy into light energy has been used in semiconductor lasers.

## 10.6 Helium–Neon gas [He–Ne] laser

Helium–Neon gas laser is a continuous four level gas laser. It consists of a long, narrow cylindrical tube made up of fused quartz. The diameter of the tube will vary from 2 to 8 mm and length will vary from 10 to 100 cm. Flat quartz plates are sealed at the ends of the tube, the plates are sealed at Brewster angle with the axis of the tube to obtain polarized laser light as shown in Fig. 10.4. So, the plates are called Brewster windows. The tube is filled with helium and neon gases in the ratio of 10:1. The partial pressure of helium gas is 1 mm of Hg and neon gas is 0.1 mm of Hg, so that the pressure of the mixture of gases inside the tube is nearly 1 mm of Hg.

Laser action is due to the neon atoms. Helium is used for selective pumping of neon atoms to upper energy levels. Two electrodes are fixed near the ends of the tube to pass electric discharge through the gas. Two optically plane mirrors are fixed at the two ends of the tube normal to its axis. One of the mirrors is

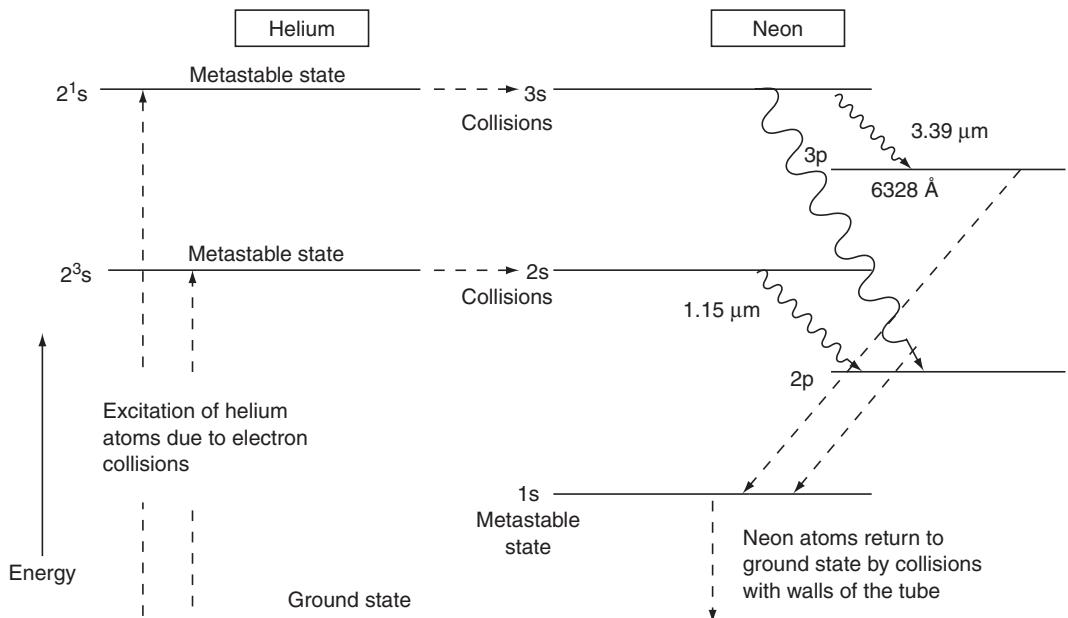
**Figure 10.4** Helium–Neon gas laser



fully silvered so that nearly 100% reflection takes place and the other is partially silvered so that 1% of the light incident on it will be transmitted. Optical resonance column is formed between these mirrors.

**Working:** When a voltage of about 1000 V is applied between the electrodes, then electric discharge takes place through the gas in the tube. The free electrons accelerate towards the positive electrode. In their journey, some of these electrons collide with the majority helium gaseous atoms in the tube. When a fast-moving electron collides with a ground state He atoms then the helium atoms are pumped to two metastable energy levels  $2^1s$  and  $2^3s$  of helium as shown in Fig. 10.5. In the metastable state, the atoms remain relatively long time. So, more number of helium atoms will be present in metastable state than in ground state, which leads to an increase of population in each of these metastable states.

**Figure 10.5** He–Ne energy level diagram



Inside the tube, the helium atoms present in metastable states may make collisions with the neon atoms present in the ground state and excite them to 2s and 3s levels. During collisions, the metastable helium atoms transfer their energy to ground state neon atoms and the helium atoms come back to the ground state. During collision, resonance transfer of energy from He to Ne atoms takes place because the 2<sup>1</sup>s and 2<sup>3</sup>s energy levels of helium atoms are very close with 3s and 2s energy levels of neon. Thus, the population inversion in neon atoms takes place. The excited neon atoms transit to ground state in three different ways leading to three lasers of different wavelengths. They are: (a) transition from 3s level to 3p level gives rise to radiation of wavelength 3.39  $\mu\text{m}$ , this lies in the infrared region (b) transition from 3s level to 2p level gives rise to visible radiation of wavelength 6328  $\text{\AA}$ , this lies in red region and (c) the transition from 2s level to 2p level gives rise to a wavelength of 1.15  $\mu\text{m}$ , this again lies in the infrared region. The atoms in 3p and 2p level undergo spontaneous transitions to 1s level, this is a metastable state [3s and 2s levels are not metastable states]. The photons emitted by the atoms coming down from 3p or 2p level to 1s level are likely to excite the 1s atoms back to 3p or 2p levels. This affects the population inversion in 3s and 2s levels. The atoms in 1s level return back to the ground level mainly by collisions with the walls of the discharge tube. This effect makes the gain of He-Ne laser to be inversely proportional to the diameter of the discharge tube, so the discharge tubes are made only to a few millimetres of diameter. The mirrors placed outside the tube produces optical pumping in the resonance column inside the tube, which enhances stimulated emissions. Red laser light comes out of the partially silvered mirror.

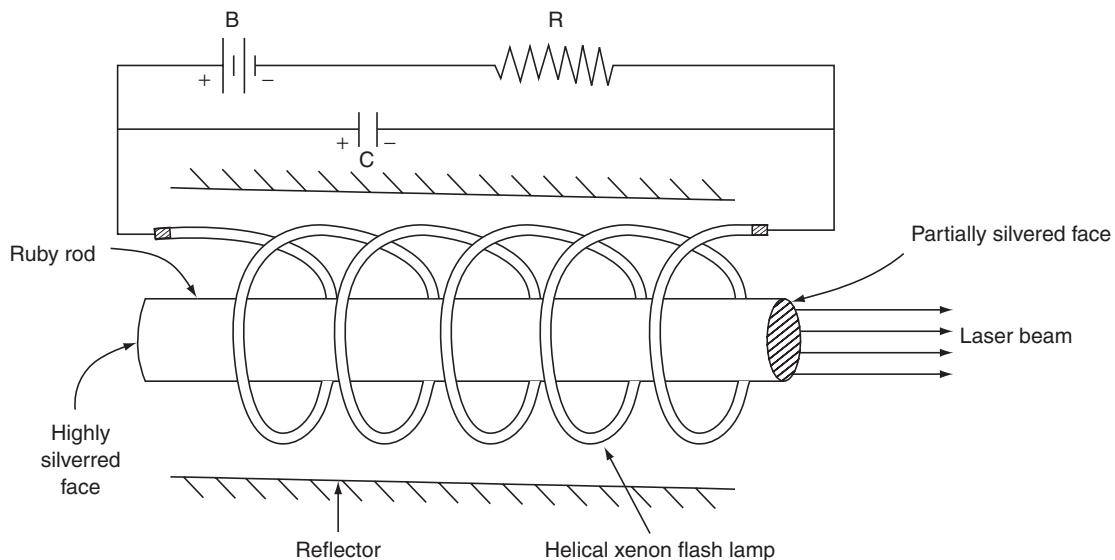
## 10.7 Ruby laser

Ruby laser is a solid state pulsed, three-level laser. It consists of a cylindrical-shaped ruby crystal rod of length varying from 2 to 20 cms and diameter varying from 0.1 to 2 cms. The end faces of the rod are highly flat and parallel. One of the faces is highly silvered and the other face is partially silvered so that it transmits 10 to 25% of incident light and reflects the rest so as to make the rod-resonant cavity. Basically, ruby crystal is aluminium oxide [ $\text{Al}_2\text{O}_3$ ] doped with 0.05 to 0.5% of chromium atoms. These chromium atoms serve as activators. Due to the presence of 0.05% of chromium, the ruby crystal appears in pink colour. The ruby crystal is placed along the axis of a helical Xenon or Krypton flash lamp of high intensity. This is surrounded by a reflector as shown in Fig. 10.6. The ends of the flash lamp are connected to a pulsed high-voltage source, so that the lamp gives flashes of an intense light.

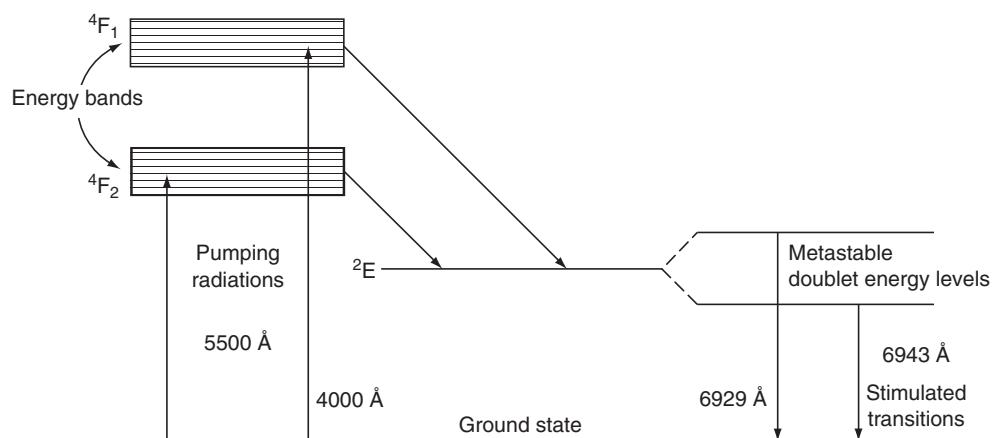
Each flash of light lasts for several milliseconds. The ruby rod absorbs the flashes of light to excite chromium ions [ $\text{Cr}^{3+}$ ] to higher energy levels. During the course of flash, enormous amount of heat is produced. The ruby rod is protected from the heat by enclosing it in a hollow tube through which cold water is circulated [not shown in the Figure]. The chromium ions are responsible for the stimulated emission of radiations whereas aluminium and oxygen ions are passive.

The emission of radiations by chromium atoms can be explained with the help of energy level diagram as shown in Fig. 10.7. The energy level diagram of a solid consists of energy bands. As large number of the chromium ions absorb the radiations of wavelength around 5500  $\text{\AA}$  and 4000  $\text{\AA}$  emitted by the flash lamp and get excited to  $^4\text{F}_1$  and  $^4\text{F}_2$  energy levels from ground state. The chromium ions remain for about  $10^{-8}$  to  $10^{-9}$  seconds in these energy levels and makes non-radiative transition to the metastable state  $^2\text{E}$ , consisting of a pair of energy levels. In metastable state, the chromium ions remain for longer duration of the order of milliseconds. So, population inversion takes place between metastable and ground state. As a result, stimulated emission takes place and the chromium ions translate from metastable to ground state. The transitions give rise to the emission of light of wave lengths 6929  $\text{\AA}$  and 6943  $\text{\AA}$ , respectively. In these 6929  $\text{\AA}$ , wavelength radiation is

**Figure 10.6 Ruby laser**



**Figure 10.7 Energy level diagram of chromium ions in a ruby crystal**



very weak in intensity and the laser radiation is mostly due to 6943 Å wavelength radiation. The spontaneously emitted initial photons would travel in all directions, of these, those travelling parallel to the axis of the rod would be reflected at the ends and pass many times through the amplifying medium and stimulates the atoms in metastable state. The output of this laser consists of a series of laser pulses for a duration of microseconds or less.

## 10.8 Semiconductor lasers

A highly doped p-n junction diode made up of direct band gap semiconductor material under forward bias emits photons from the junction due to the recombination of conduction band electrons and valence band holes. Example for direct band gap semiconductor is GaAs. During recombination a conduction band electron crosses the energy gap ( $E_g$ ) and combines with a hole present in the valence band. A photon of energy,  $\hbar\nu$  equal to  $E_g$  is released. Hence  $E_g = \hbar\nu = \frac{hc}{\lambda}$ . Where  $\hbar$  = Planck's constant =  $6.63 \times 10^{-34}$  J-S;  $C$  = velocity of light =  $3 \times 10^8$  m/s and  $\lambda$  = wavelength of emitted photon. In semiconductors, p-n junction is the active region to produce laser radiation. To produce laser radiation two conditions must be satisfied: (1) population inversion and (2) optical feedback. Population inversion means there must be a region of the device in which large density of free electrons in the bottom energy levels of conduction band and large density of holes in the top energy levels of valence band exists. This is obtained with high doping concentration. Optical feedback is obtained by clearing or by polishing the ends of p-n junction at right angles to the junction layer. Forward-biased current is slowly increased through the junction. At low current densities, spontaneous emission takes place. Above threshold current density-stimulated emission takes place.

**Homo- and Heterostructure lasers:** If the energy gap width of the semiconductor material on one side of p-n junction is the same as that on the other side of the junction, then such a semiconductor laser is known as homostructure laser. On the other hand, if the energy gap width of the semiconductor material on one side of p-n junction is different from that on the other side of the junction, then such a semiconductor laser is known as heterostructure laser. The basic structure of a p-n junction laser is shown in Fig. 10.8.

A pair of opposite parallel faces of the p-n junction laser are polished to provide optical feedback and the other two opposite faces are roughened to eliminate lasing in that direction.

The band diagram of a heavily doped homostructure p-n junction laser is shown in Fig. 10.9(a). In the  $n^+$  region, the Fermi level lies within the conduction band and in the  $P^+$  region, the Fermi level lies in the valence band. The junction is forward-biased such that the biasing voltage is equal to the energy gap voltage ( $E_g/e$ ), then the electrons and holes are injected across the junction and population inversion takes place in the active region.

**Figure 10.8** Semiconductor p-n junction laser

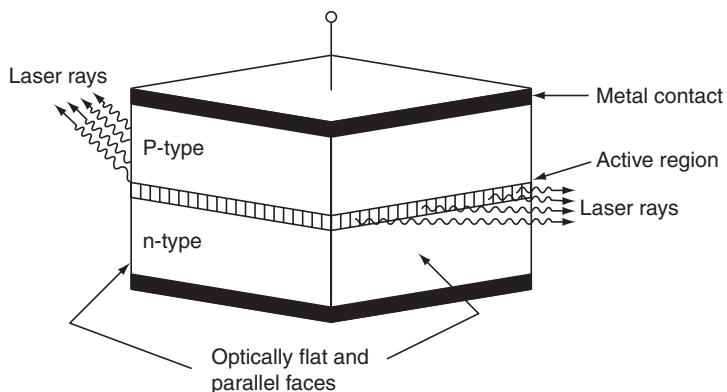
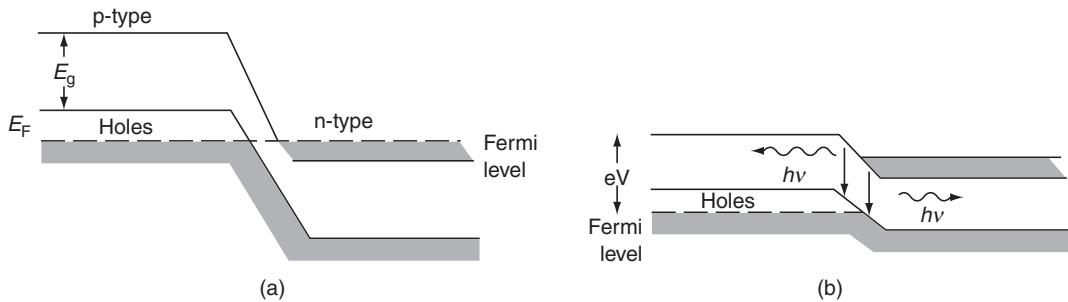


Figure 10.9

- (a) Band diagram of a heavily doped p-n junction in equilibrium  
 (b) Band diagram of a heavily doped p-n junction with forward bias



The band diagram after forward biasing is shown in Fig. 10.9(b).

When the biasing current is low, then spontaneous emission takes place in all directions. As the biasing current reaches threshold value, then stimulated emission occurs and a monochromatic and highly directional beam of light is emitted from the junction.

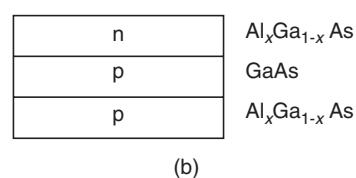
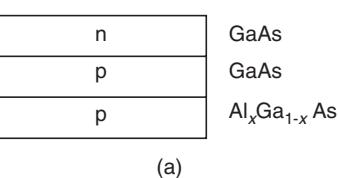
In case of homojunction lasers [for example GaAs p-n junction], the threshold current density ( $J_{th}$ ) increases rapidly with raise of temperature. At room temperature [300K], the threshold current density is about  $5.0 \times 10^4 \text{ A/cm}^2$ . This large current density leads to serious difficulties in operating the laser continuously at room temperature. Threshold current densities are of the order of  $10^3 \text{ A/cm}^2$  in heterojunction lasers. These lasers are built using epitaxial techniques as shown in Fig. 10.10.

In the structure shown in Fig. 10.10(a), there is only one heterojunction and that shown in Fig. 10.10(b), there are two heterojunctions. In  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ,  $x$  represents mole fraction.

The variation of threshold current density with temperature is very much less in double heterostructure laser when compared to homostructure and single heterostructure laser. The above semiconductor lasers are broad area lasers. Because, in the complete area of p-n junction, lasing action takes place. To reduce the operating currents to a large extent, heterostructure strip geometry lasers are used. Figure 10.11 shows two such strip geometries.

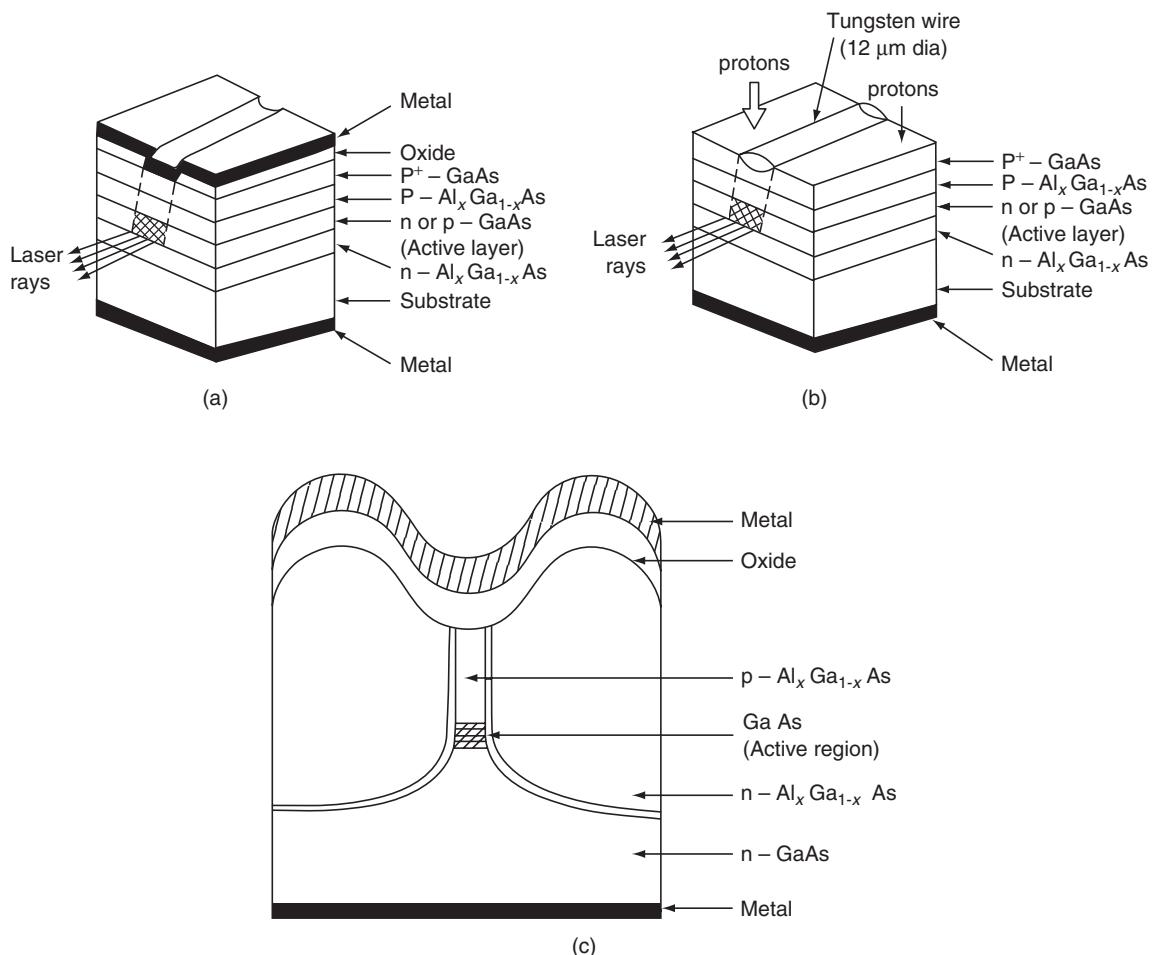
The various layers shown in the above structures are fabricated by epitaxial growth. The oxide layer in the structure shown in Fig. 10.11(a) is an insulating layer. A thin strip of oxide layer at the centre has been removed by chemical etching techniques and a metal layer was deposited. On biasing, current passes under the strip contact only, because the oxide layer insulates the remaining region. Lasing takes place under the strip in the active layer. Instead of an oxide layer, proton bombardment is carried at the top surface of the structure as shown in Fig. 10.11(b). Proton bombardment produces high resistance;

Figure 10.10



(a) Single heterostructure laser; (b) Double heterostructure laser

**Figure 10.11** (a) Oxide-coated heterostructure strip geometry laser;  
 (b) Proton-bombarding heterostructure strip geometry laser;  
 (c) Buried heterostructure laser



this bombardment has been carried except along a stripe at the centre of active layer. The strip widths vary from 5 to 30  $\mu\text{m}$ . The advantages of stripe geometry are: (1) reduction of operating current and (2) improve response time due to small junction capacitance.

Lasing action can be obtained with extremely small currents by using buried heterostructure laser shown in Fig. 10.11(c). The active region in this structure is completely surrounded by higher band gap, lower refractive index material so, all those photons which are produced in the active region and whose energies are less than energy gap of the surrounding material are transmitted without absorption. Due to lower refractive index of the surrounding material, the rays bend less when come out of the device. The cross-sectional area of the active region is as small as 1  $\mu\text{m}^2$ . So, the threshold current is as low as 15 mA.

## 10.9 Carbon dioxide laser

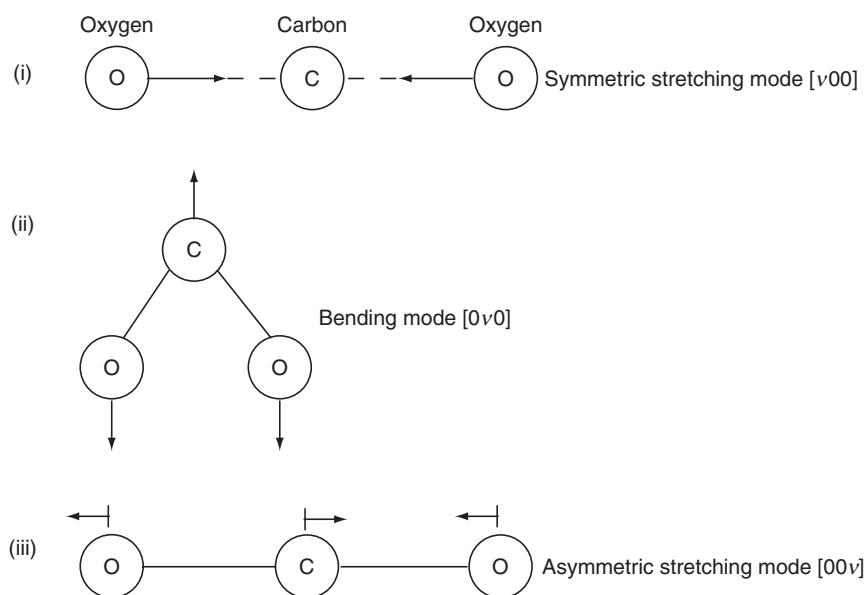
**(i) Introduction:** The carbon dioxide laser was invented by C. Kumar. N. Patel in the year 1963. This laser uses a mixture of carbon dioxide [ $\text{CO}_2$ ], Nitrogen [ $\text{N}_2$ ] and Helium [ $\text{He}$ ] gases in the active medium of laser. The lasing action is from carbon dioxide molecules. They are the active molecules in the laser. The  $\text{CO}_2$  molecule is a linear symmetric molecule with carbon atom at the centre and oxygen atoms are on each side of the carbon atom. The lasing is due to the transitions of  $\text{CO}_2$  molecules in between vibrational-rotational levels. The  $\text{CO}_2$  molecules possess three different types of vibrational modes and each vibrational mode possesses a number of rotational modes. The vibrational modes are described as shown in Fig. 10.12.

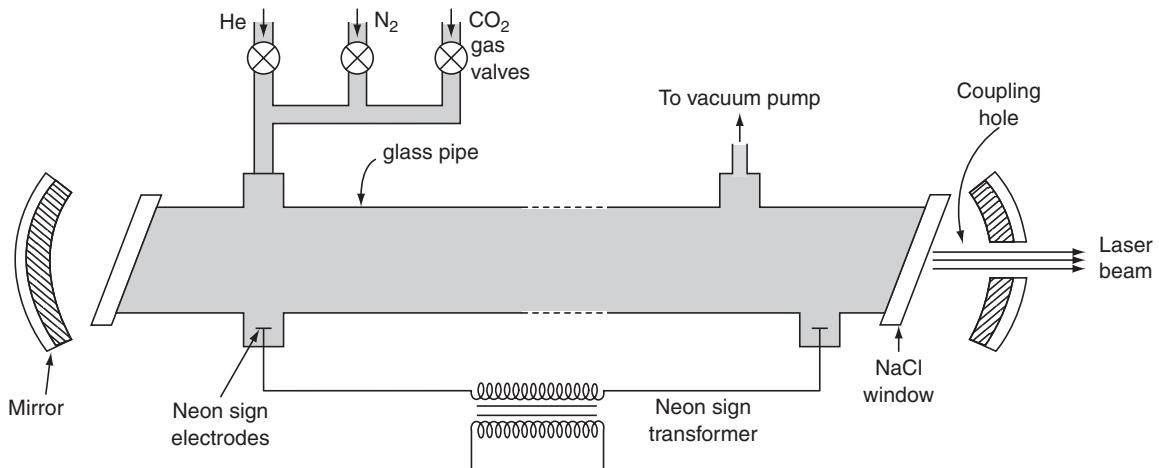
In symmetric stretching mode, the carbon atom is stationary and the oxygen atoms symmetrically move away or approaches the carbon atom.

In bending mode, some atoms (not all) move perpendicular to the molecular axis. In asymmetric stretching mode, both the oxygens move in one direction along the molecular axis and carbon move in opposite direction. [The state of a vibrating molecule is represented by a set of three vibrational quantum numbers, labeled as  $(nm'l)$ , where  $n$  is the frequency of the photon emitted due to symmetric stretch,  $m$  is the frequency of the photon emitted due to bending and  $l$  is the frequency of the photon emitted due to asymmetric stretch. The bending vibration is doubly degenerate, i.e., it can occur both in the plane of the figure and the plane perpendicular to it. The superscript  $l$  represents the angular momentum of this vibration with respect to molecular axis. For example,  $(02^0)$  shows the two vibrations combine to give an angular momentum  $l = 0$ ]

**(ii) Construction:** As shown in Fig. 10.13, one of the  $\text{CO}_2$  laser consists of a long tube of about 5 m long and 2.5 cm diameter. The output power of this laser is approximately proportional to the length of the tube. The ends of the tube is closed with alkali halide [ $\text{NaCl}$ ] Brewster windows. Outside the ends of the tube,

**Figure 10.12 Fundamental modes of vibration of  $\text{CO}_2$  molecule**



**Figure 10.13** CO<sub>2</sub> laser

confocal silicon mirrors coated with aluminium are arranged. This forms the resonant cavity. The gases CO<sub>2</sub>, N<sub>2</sub> and He are allowed into the tube through gas valves. Inside the tube, these gases combine and continuously pass through it. During discharge, the gases may dissociate and contaminate the laser, so continuous flow of gases is maintained in the tube.

The pressures of the gases in the tube are  $P_{\text{He}} \approx 7$  torr;  $P_{\text{N}_2} \approx 1.2$  torr and  $P_{\text{CO}_2} \approx 0.33$  torr.

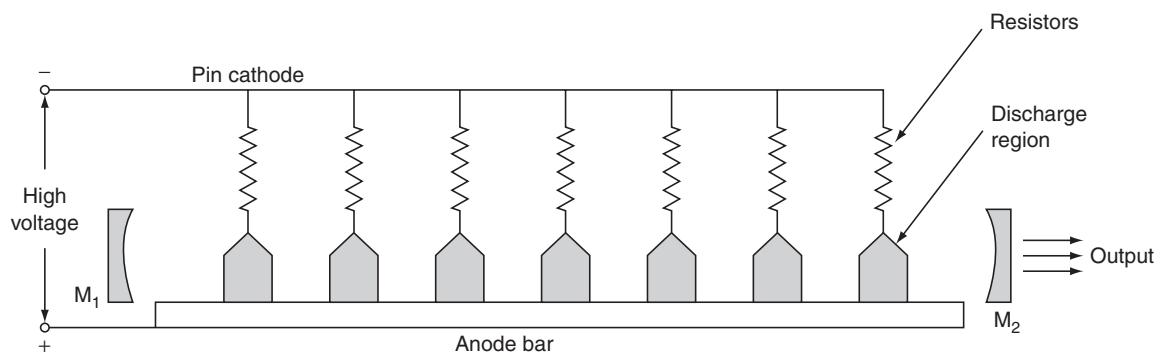
The optimum value of pressure tube diameter product is around 33 torr mm. The purpose of N<sub>2</sub> gas in the tube is to produce high population inversion in CO<sub>2</sub> molecules. Here, resonance transfer of energy from N<sub>2</sub> gas molecules to CO<sub>2</sub> gas molecules takes place in the tube. To avoid population in the lower laser levels by thermal excitation, it is necessary that the temperature of CO<sub>2</sub> should be low. For this purpose, helium gas is passed through the tube along CO<sub>2</sub> and N<sub>2</sub> gases, because helium gas possesses high thermal conductivity and helps to conduct heat away to the walls, keeping CO<sub>2</sub> temperature low. Thus N<sub>2</sub> helps to increase the population of upper level and helium helps to depopulate the lower level.

**(iii) Working:** Sufficiently high voltage of the order of 8 KV per metre length of the tube must be maintained to get discharge. Two different configurations are available for high output power. They are TEA and Gas dynamic laser.

**(a) TEA [Transverse Excitation Atmospheric] CO<sub>2</sub> laser:** The output power of the laser can be increased by increasing gas pressure. At atmospheric pressure, to initiate and maintain electric discharge, 12 KV per cm is required. In longitudinal configuration with 1 m or above length tubes, it is not possible to apply such high electric fields. In TEA laser, the discharge is arranged to take place at a number of points in a direction transverse to laser cavity, as shown in Fig. 10.14.

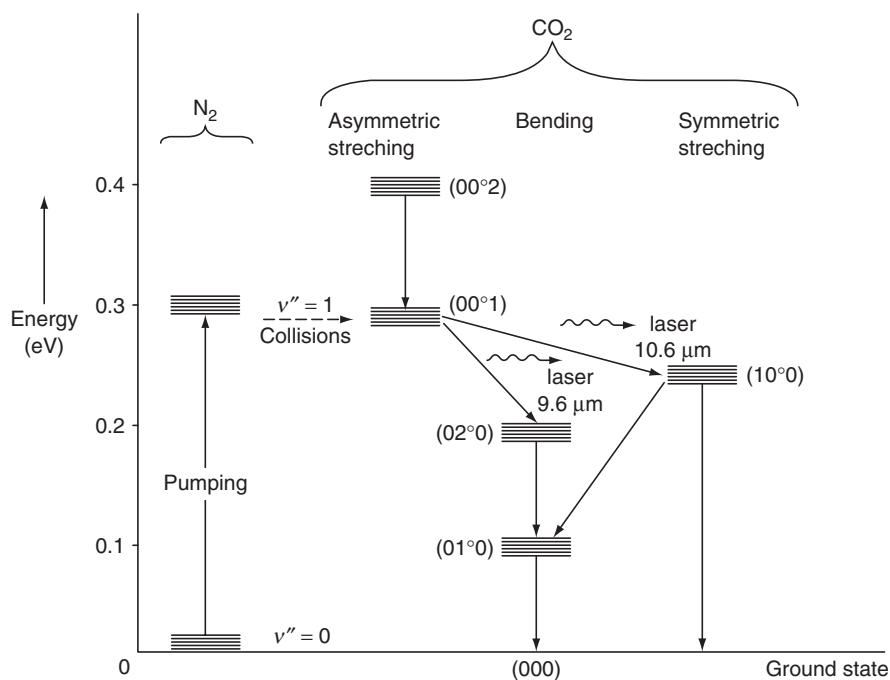
**(b) Gas dynamic laser:** In this laser, population inversion is obtained through thermodynamic principles rather than discharge. The gas mixture containing N<sub>2</sub> and CO<sub>2</sub> is heated, compressed and allow to expand into low-pressure region. At high temperatures, the N<sub>2</sub> molecules reaches to the higher vibrational levels and after expansion into low-pressure region, the N<sub>2</sub> molecules makes resonant collisions with CO<sub>2</sub> molecules. Then, the CO<sub>2</sub> molecules makes transition to (001) state and produce population inversion. This laser produce output powers in excess of 100 KW.

Figure 10.14 TEA laser



The emission of laser radiation from  $\text{CO}_2$  molecules has been explained with the help of vibrational-rotational energy levels in the following way.

The electric discharge in  $\text{CO}_2$  laser may excite  $\text{CO}_2$  and  $\text{N}_2$  molecules to higher vibrational rotational levels by electron impacts. The electronic collision cross-section of  $\text{CO}_2$  for the excitation to the level

Figure 10.15  $\text{CO}_2$  laser energy levels

(00°1) is very large, this is the metastable state. This level is populated by: (i) non-radiative transition from the upper excited levels such as (00°2) of CO<sub>2</sub> and (ii) the collision of N<sub>2</sub> molecules present in ν'' = 1 level with CO<sub>2</sub> molecules lead to resonance transfer of energy. Because the ν'' = 1 level of N<sub>2</sub> molecules and (00°1) levels of CO<sub>2</sub> are nearly at the same energy and the lifetime of ν'' = 1 is quite large [0.1 s at 1 torr]. Population inversion exists between (00°1) and (10°0), (02°0) levels. Two laser transitions takes place between these levels: (i) (00°1) to (10°0) gives laser radiation of wavelength 10.6 μm and (ii) (00°1) to (02°0) gives laser radiation of wavelength 9.6 μm. Of these 10.6 μm waves are intense, its power output is of 10 KW, efficiency being 30%, this is quite large and 9.6 μm waves are weak. The lower levels (10°0), (02°0) and (01°0) are very close. The CO<sub>2</sub> molecules present in (10°0), (02°0) and (01°0) levels may make non-radiative transition to the ground state quickly by colliding with He atoms (Fig. 10.15). In this process, energy dissipation takes place in the form of heat.

## 10.10 Applications of lasers

Lasers find applications in various fields of science and technology. They are described below:

### (1) In communications:

- (a) Lasers are used in optical fibre communications. In optical fibre communications, lasers are used as light source to transmit audio, video signals and data to long distances without attenuation and distortion.
- (b) The narrow angular spread of laser beam recommends that laser beam can be used for the communication between earth and moon or to other satellites.
- (c) As laser radiation is not absorbed by water, so laser beam can be used in under water [inside sea] communication networks.

### (2) Industrial applications:

Lasers are used in metal cutting, welding, surface treatment and hole drilling.

- (a) When a laser beam is focussed on a very small area, then laser light energy is converted into heat energy, so, the material may be heated, melted and evaporated. Using these techniques, holes can be drilled in steel, ceramics, diamond and alloys. Using lasers, controlled orifices and aerosol nozzles are drilled with controlled precision. Holes of micron order can be easily drilled using lasers. These techniques are used in cutting materials such as metal sheets and cloths. In mass production of stitched clothes, the cutting in the desired dimension is done by stock filing a large number of cloth material and cutting them all at once by exposing a laser beam.

Using lasers, cutting can be obtained to any desired shape and the cutted surface is very smooth.

- (b) Welding has been carried by using laser beam. A laser beam is exposed to the place where welding has to be done, at that place the material melts due to the heat produced by the beam and on cooling the material makes a stronger joint.
- (c) Dissimilar metals can be welded and microwelding is done with great ease.
- (d) Laser beam is used in selective heat treatment for tempering the desired parts in automobile industry.
- (e) Lasers are widely used in electronic industry in trimming the components of ICs.

### (3) Medical applications:

- (a) Lasers are used in eye surgery, especially in detached retina. Under certain abnormal conditions, the retina may get detached from the choroid, this results blindness at the detached part of the retina. The

retina can be attached to the choroid by heating it over a number of spots almost of the size of tissues. The heating can be achieved by focusing a laser beam of predetermined intensity on to the retina. The laser beam reaches the right spot where the welding of the retina to the choroid occurs. The flash of laser beam last in short time (1 millisecond). The patient does not feel any pain, so anaesthesia is not required.

- (b) Lasers are used for treatments such as plastic surgery, skin injuries and to remove moles and tumours developed in skin tissue.
- (c) Lasers are used in stomatology—the study of mouth and its disease. Where a laser beam is used for selective destroying, the part of the tooth affected by caries. Mouth ulcers can be cured by exposing it to a laser beam.
- (d) Laser radiation is sent through optical fibre to open the blocked artery region, here the laser rays burn the excess growth in the blocked region and regulates blood flow without any requirement for bypass surgery.
- (e) Lasers are used to destroy kidney stones and gall stones. The laser pulses are sent through optical fibres to the stoned region. The laser pulses break the stones into small pieces.
- (f) Lasers are used in cancer diagnosis and therapy.
- (g) Lasers are used in blood loss less surgery. During operation, the cutted blood veins are fused at their tips by exposing to infrared laser light, so that there is no blood loss.
- (h) Lasers are used to control haemorrhage.
- (i) Using organ and CO<sub>2</sub> lasers, liver and lung treatment can be carried out.
- (j) Lasers are used in endoscopes to detect hidden parts.
- (k) Laser doppler velocimetry is used to measure blood velocity in the blood vessels.

**(4) Military applications:** The various military applications are:

- (a) Death rays: By focusing high-energetic laser beam for few seconds to aircraft, missile, etc. can be destroyed. So, these rays are called death rays or war weapons.
- (b) Laser gun: The vital part of enemy body can be evaporated at short range by focusing a highly convergent laser beam from a laser gun.
- (c) LIDAR [Light Detecting And Ranging]: In place of RADAR, we can use LIDAR to estimate the size and shape of distant objects or war weapons. The difference between RADAR and LIDAR is that, in case of RADAR, radio waves are used whereas in case of LIDAR light is used.

**(5) In computers:** By using lasers, a large amount of information or data can be stored in CD-ROM or their storage capacity can be increased. Lasers are also used in computer printers.

**(6) In thermonuclear fusion:** To initiate nuclear fusion reaction, very high temperature and pressure is required. This can be created by concentrating large amount of laser energy in a small volume. In the fusion of deuterium and tritium, irradiation with a high-energy laser beam pulse of 1 nanosecond duration develops a temperature of 10<sup>17</sup> °C, this temperature is sufficient to initiate nuclear fusion reaction.

**(7) In scientific research:**

- (a) Laser beam can initiate or fasten chemical reactions. Laser beam helps us to study the nature of chemical bonds. An intense laser beam can break molecules.
- (b) Lasers are used in counting of atoms in isotope separation and to separate isotopes of uranium.
- (c) Lasers are used to estimate the size and shape of biological cells such as erythrocytes.
- (d) Lasers can be used in air pollution, to find the size of dust particles.

- (e) Lasers are used in holography for recording and reconstruction of a hologram. Using holograms, the three-dimensional images of objects can be recorded.
- (f) To measure the constantly changing distance between moon and earth by astronomers. This gives the day-to-day changes in the rotation of earth about its axis and slight wobbles.
- (g) In plastic industries, polymers are obtained by irradiating monomers. During laser irradiation, the monomers are united to form polymers.
- (h) By using lasers, the stimulated Raman spectrum is obtained for small biological samples.
- (i) Lasers are used to develop hidden finger prints and to clean delicate pieces of art.

## Formula

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$$1. \frac{\text{Spontaneous emission}}{\text{Stimulated emission}} = \frac{A/B}{\sigma(f)} = \exp\left(\frac{hf}{K_B T}\right) - 1$$

## Solved Problems

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1. A semiconductor diode laser has a peak emission wavelength of  $1.55 \mu\text{m}$ . Find its band gap in eV.

(Set-2–May 2008)

**Sol:** Energy gap of semiconductor,  $E_g$  = energy of emitted photon,  $h\nu$

$$E_g = h\nu = \frac{hc}{\lambda} \quad \text{where } c = \text{velocity of light} = 3 \times 10^8 \text{ m/s}$$

$$\text{Wavelength, } \lambda = 1.55 \mu\text{m} = 1.55 \times 10^{-6} \text{ m}$$

$$\text{Energy gap, } E_g = ?$$

$$\begin{aligned} E_g &= \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.55 \times 10^{-6}} \text{ J} \\ &= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.55 \times 10^{-6} \times 1.6 \times 10^{-19}} \text{ eV} = 0.8 \text{ eV} \end{aligned}$$

2. Calculate the wavelength of emitted radiation from GaAs which has a band gap of  $1.44 \text{ eV}$ .

(Set-3–May 2008)

**Sol:** Energy gap of semiconductor,  $E_g = h\nu$

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

$$E_g = h\nu = \frac{hc}{\lambda} \quad \text{or} \quad \lambda = \frac{hc}{E_g}$$

$$E_g = 1.44 \text{ eV} = 1.44 \times 1.6 \times 10^{-19} \text{ J}$$

$$= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.44 \times 1.6 \times 10^{-19}} = 8633 \times 10^{-10} \text{ m} = 8633 \text{ \AA}$$

## Multiple Choice Questions

1. Laser action is found in \_\_\_\_\_ semiconductor. ( )  
(a) direct band gap (b) indirect band gap  
(c) germanium (d) silicon

2. In computer, printers \_\_\_\_\_ laser is used. ( )  
(a) He-Ne gas (b) ruby  
(c) semiconductor (d)  $\text{CO}_2$

3. Laser radiation is: ( )  
(a) highly monochromatic (b) partially monochromatic  
(c) white light (d) none

4. Under population inversion, the number of atoms in the higher energy state is \_\_\_\_\_ than in the lower energy state. ( )  
(a) lesser (b) larger (c) both a and b (d) none

5. Laser radiation is: ( )  
(a) highly directional (b) monochromatic  
(c) coherent and stimulated (d) all

6. In conventional light sources, ( )  
(a) different atoms emit radiation at different times  
(b) there is no phase relation between the emitted photons  
(c) different atoms emit photons in different directions  
(d) all

7. In laser sources, ( )  
(a) photons emitted by different atoms are in phase or maintain constant phase relationship  
(b) different atoms emit photons in the same direction  
(c) both a and b  
(d) none

8. In spontaneous emissions, ( )  
(a) atoms are initially in the excited state  
(b) transitions are without any aid of an external agency  
(c) both a and b  
(d) none

9. In conventional light sources, the ratio of spontaneous emission rate to stimulated emission rate is nearly: ( )  
(a)  $10^{10}$  (b)  $10^{20}$  (c)  $10^5$  (d)  $10^3$

10. In excited states, the atoms will remain for a time of: ( )  
(a)  $10^8$  s (b)  $10^{-8}$  s (c)  $10^{-3}$  s (d)  $10^{-5}$  s

11. He-Ne gas laser is a: ( )  
(a) continuous laser (b) pulsed laser  
(c) both a and b (d) none

12. The ratio of the Helium and Neon gaseous atoms are: ( )  
(a) 1:10 (b) 10:1 (c) 1:1 (d) 1:20



26. He-Ne laser gives \_\_\_\_\_ coloured laser light. ( )  
(a) pink (b) red (c) green (d) orange

27. In ruby laser, chromium ions are responsible for stimulated emission of radiations whereas \_\_\_\_\_ ions are passive. ( )  
(a) oxygen (b) aluminium (c) both a & b (d) none

28. Mostly, the wavelength of laser radiation from ruby laser is \_\_\_\_\_. ( )  
(a) 6943 Å (b) 6929 Å (c) 6328 Å (d) 1.15 nm

29. In homostructure semiconductor laser, the energy gap on one side of P-N junction is \_\_\_\_\_ on the other side of the junction. ( )  
(a) different as that (b) same as that  
(c) both a & b (d) none of the above

30. In heterostructure semiconductor laser, the energy gap on one side of the P-N junction is \_\_\_\_\_ on the other side of the junction. ( )  
(a) different as that (b) same as that (c) both a & b (d) none

31. At room temperature (300K), the threshold current density of homostructure laser is about: ( )  
(a)  $5.0 \times 10^5 \text{ A/cm}^2$  (b)  $5.0 \times 10^4 \text{ A/cm}^2$   
(c)  $5.0 \times 10^{-4} \text{ A/cm}^2$  (d)  $5.0 \times 10^{-5} \text{ A/cm}^2$

32. To reduce the operating currents to a large extent, heterostructure \_\_\_\_\_ geometry lasers are used. ( )  
(a) strip (b) rectangular (c) helical (d) parabolic

33. Basically, a ruby crystal is aluminium oxide doped with 0.05 to \_\_\_\_\_ % of chromium atoms. ( )  
(a) 5 (b) 10 (c) 15 (d) 0.5

34. Lasing action can be obtained with extremely small currents by using \_\_\_\_\_ structure lasers. ( )  
(a) homo (b) hetero  
(c) buried homo (d) buried hetero

35. The threshold current in buried heterostructure is as low as \_\_\_\_\_. ( )  
(a) 5 mA (b) 10 mA (c) 15 mA (d) 15 A

36. Because of narrow angular spread, laser beam can be used for the communication between \_\_\_\_\_ and moon or other satellites. ( )  
(a) earth (b) sun (c) both a & b (d) none

37. Lasers are used in \_\_\_\_\_ the components of IC's. ( )  
(a) fabricating (b) trimming (c) both a & b (d) none

## Answers

## Review Questions

1. Explain the principle, construction and working of a semiconductor laser. (Set-3–June 2005)
2. Explain the purpose of an active medium in a gas laser. (Set-3–Nov. 2004)
3. State the applications of lasers. (Set-1–Nov. 2003), (Set-2–Nov. 2003), (Set-3–Nov. 2003)
4. Derive the relation between the probabilities of spontaneous emission and stimulated emission in terms of Einstein's coefficients. (Set-4–Sept. 2007), (Set-1, Set-3–May 2007), (Set-2–Nov. 2004)
5. Explain the characteristics of a laser. (Set-1–May 2008), (Set-2, Set-3–Sept. 2007), (Set-2–Sept. 2006), (Set-1–Nov. 2004)
6. With the help of suitable diagrams, explain the principle, construction and working of a ruby laser. (Set-4–Nov. 2004)
7. What do you understand by population inversion? How it is achieved? (Set-4–Sept. 2007), (Set-1, Set-3–May 2007), (Set-2–Nov. 2004)
8. Mention any two applications of laser, each in the field of scientific research, engineering and medicine. (Set-2–June 2005), (Set-1–Nov. 2004), (Set-1–May 2003)
9. Explain the characteristics of laser beam. (Set-2, Set-3–Sept. 2007), (Set-2–Sept. 2006), (Set-2–June 2005), (Set-1–Nov. 2004), (Set-1–May 2003)
10. Explain the need of a cavity resonator in a laser, with the help of suitable diagrams explain the principle, construction and working of a ruby laser. (Set-1–Sept. 2006), (Set-4–May 2003)
11. Explain the purpose of an active medium in a gas laser. With the help of suitable diagrams, explain the principle, construction and working of a Helium–Neon laser. (Set-3–Nov. 2004), (Set-3–May 2003)
12. What do you understand by population inversion? How it is achieved? Derive the relation between the probabilities of spontaneous emission and stimulated emission in terms of Einstein's coefficients. (Set-2–May 2003)
13. With neat diagram, explain the construction and working of He–Ne gas laser. (Set-1–Nov. 2003)
14. Describe the construction and working of a ruby laser. (Set-1–May 2008), (Set-3–Sept. 2007), (Set-2–June 2005), (Set-1–Nov. 2004), (Set-1–May 2003)
15. Write the applications of lasers. (Set-4–Sept. 2006), (Set-4–May 2006), (Set-3–June 2005)
16. Describe the principle, construction and working of He–Ne laser. (Set-2–Nov. 2003)
17. Describe the principle, construction and working of a semiconductor laser. (Set-4–May 2006), (Set-3–Nov. 2003)
18. Distinguish between spontaneous emission and stimulated emission of the light. (Set-2, Set-3–May 2008), (Set-1–May 2006)
19. With the help of a suitable diagram, explain the principle, construction and working of a semiconductor laser. (Set-4–May 2008)
20. Write any four applications of laser. (Set-1–May 2008), (Set-2–Sept. 2008)
21. Distinguish between homo-junction semiconductor laser and hetero-junction semiconductor laser. (Set-2, Set-3–May 2008), (Set-4–Sept. 2008)

22. Describe the various methods to achieve population inversion relating to lasers.  
(Set-4-May 2008), (Set-3-Sept. 2008)
23. Explain the terms (i) absorption, (ii) spontaneous emission, (iii) stimulated emission, (iv) pumping mechanism, (v) population inversion and (vi) optical cavity.  
(Set-2-May 2007)
24. Mention the medical applications of laser.  
(Set-2-May 2007)
25. With neat sketch explain the construction and working of a ruby laser.  
(Set-2-Sept. 2007), (Set-2-Sept. 2006)
26. Explain the following typical characteristics of a laser (i) coherence, (ii) divergence and monochromaticity.  
(Set-3-May 2006), (Set-3-Sept. 2006)
27. Explain the principle and working of a ruby laser.  
(Set-3-May 2006), (Set-3-Sept. 2006)
28. What is population inversion.  
(Set-2-Sept. 2007), (Set-2-Sept. 2006)
29. With neat diagrams, describe the construction and action of ruby laser.  
(Set-4-Sept. 2006)
30. Explain the following (i) life time of an energy level, (ii) optical pumping process and (iii) metastable states.  
(Set-1-May 2006)
31. Discuss briefly the different methods of producing laser light.  
(Set-1-May 2006)
32. Explain with a neat diagram (i) absorption, (ii) spontaneous emission and (iii) stimulated emission of radiation.  
(Set-4-May 2007)
33. With necessary theory and energy level diagram, explain the working of a He-Ne gas laser.  
(Set-1-Sept. 2007), (Set-2-May 2006)
34. Mention some important applications of lasers.  
(Set-1-Sept. 2007), (Set-2-May 2006)
35. What is population inversion? How it is achieved by optical pumping.  
(Set-4-May 2007)
36. Discuss, how lasers are helpful in induced fusion and isotope separation process.  
(Set-3-Sept. 2007)
37. What is population inversion relating to laser action? Explain.  
(Set-1, Set-4-Sept. 2008)
38. Show that the ratio of Einstein's coefficient of spontaneous emission to Einstein's Coefficient of absorption is proportional to the cube of the frequency of the incident photon.  
(Set-1-Sept. 2008).
39. With the help of a suitable diagram, explain the principle, construction and working of a helium-neon laser.  
(Set-3-Sept. 2008)
40. Describe the construction and working of a semiconductor laser.  
(Set-2-Sept. 2008)
41. What are the important characteristics of laser radiation?
42. Explain the phenomenon of absorption, spontaneous and stimulated emission of radiation with two energy levels of an atom.
43. Explain the construction and working of a semiconductor laser.
44. Explain the various applications of lasers.
45. Write short notes on population inversion and Einstein's coefficients.
46. Describe semiconductor laser. Give the applications of lasers.
47. Explain the basic principle for producing laser beam. Write the medical applications of lasers.
48. What is population inversion in a laser? How it is achieved? What are the advantages of lasers in communication?

10-26 | **Applied Physics**

49. Describe He–Ne laser.
50. What are Einstein's coefficients?
51. Explain the terms: stimulated emission and population inversion. Mention the applications of lasers in the field of communication and medicine.
52. Explain in detail the working of a semiconductor laser.
53. Explain the principle and working of a semiconductor laser.
54. Write short notes on energy level diagram of He–Ne laser.
55. Write briefly on Einstein's coefficients.
56. Write short notes on stimulated emission.
57. Write short notes on semiconductor laser.



## CHAPTER

# 11

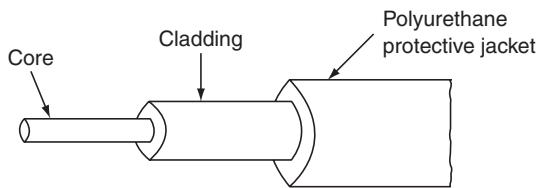
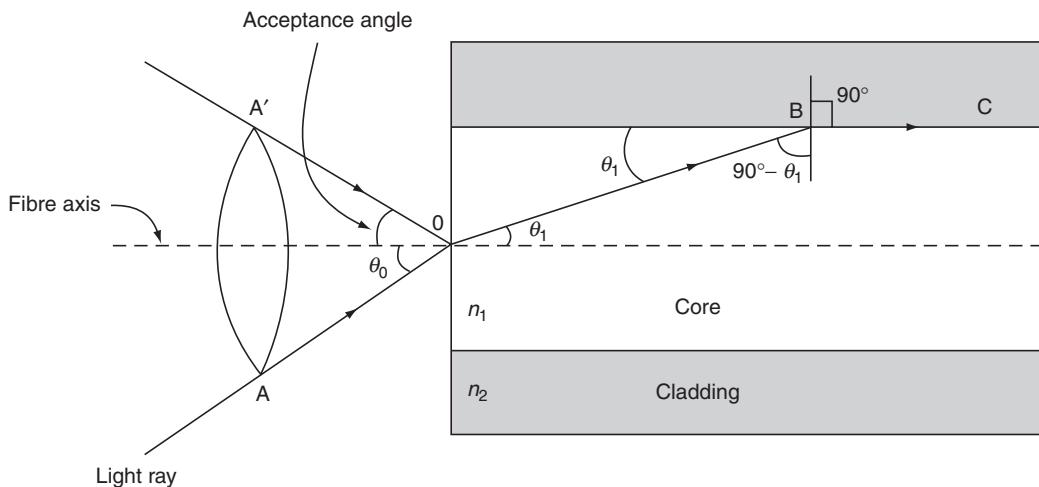
## Fibre Optics

### 11.1 Introduction

Optical fibre is a long, thin transparent dielectric material made up of glass or plastic, which carries electromagnetic waves of optical frequencies [visible to infrared] from one end of the fibre to the other by means of multiple total internal reflections. Thus, optical fibres work as wave guides in optical communication systems. An optical fibre consists of an inner cylindrical material made up of glass or plastic called core. The core is surrounded by a cylindrical shell of glass or plastic called the cladding. The refractive index of core ( $n_1$ ) is slightly larger than the refractive index of cladding ( $n_2$ ), [i.e.,  $n_1 > n_2$ ]. Typical refractive index values are  $n_1 = 1.48$  and  $n_2 = 1.46$ . The core diameter is  $\approx 50 \mu\text{m}$  and the thickness of cladding is  $\approx 1$  or  $2$  wavelengths of light propagate through the fibre. The cladding is enclosed in a polyurethane jacket as shown in Fig. 11.1. This layer protects the fibre from the surrounding atmosphere. Many fibres are grouped to form a cable. A cable may contain one to several hundred such fibres.

### 11.2 Principle of optical fibre, acceptance angle and acceptance cone

**Principle:** Once light rays enter into core, they propagate by means of multiple total internal reflections at the core-cladding interface, so that the rays travel from one end of the optical fibre to the other. The phenomenon of total internal reflection in a straight optical fibre is explained in the following way. Let the refractive index of the core is  $n_1$  and that of the cladding is  $n_2$  such that  $n_1 > n_2$ . As shown in Fig. 11.2, a ray of light AO is incident at 'O' on the end face of core; let this ray makes an angle of incidence  $\theta_0$  with the axis of the fibre. This ray is refracted into the core and passes along OB, the angle of refraction in the core is, say  $\theta_1$ . The ray OB is incident on the core-cladding interface with an angle of incidence,  $90^\circ - \theta_1$ . Suppose this angle of incidence is equal to the critical angle [ $\theta_c = 90^\circ - \theta_1$ ] in core at the core-cladding interface, then the angle of refraction in cladding is  $90^\circ$ , so that the ray (BC) passes along the interface between core and cladding. If the angle of incidence for a ray at the end face is less than  $\theta_0$ , then the angle of refraction is less than  $\theta_1$  and angle of incidence at the core-cladding interface is larger than critical angle, so the ray suffers total internal reflection at the

**Figure 11.1** Optical fibre**Figure 11.2** Light propagation in an optical fibre

core-cladding interface. If the angle of incidence for a ray at the end face is larger than  $\theta_0$ , then the angle of refraction is larger than  $\theta_1$  and the angle of incidence at the core-cladding interface is less than critical angle so that the ray will be refracted into the cladding and get lost in it due to absorption.

So, all those rays which enter the core at an angle of incidence less than  $\theta_0$  will have refracting angles less than  $\theta_1$ . As a result, their angles of incidence at the interface between core and cladding will be more than critical angle. As a consequence, they will be totally reflected in core and travel by multiple total internal reflections.

**Acceptance angle and acceptance cone:** As shown in Fig. 11.2, if the ray AO is rotated around the fibre axis keeping the angle of incidence  $\theta_0$  constant, it results in a conical surface. As such, only those rays which are within this cone suffer total internal reflections so that they confine to the core for propagation. If a ray falls at the end face of the optical fibre at an angle greater than  $\theta_0$  or out of the cone, that ray does not undergo total internal reflection at the core-cladding interface, it enters into cladding material and gets lost in the cladding material. Thus, for light rays to propagate through the optical fibre by total internal reflection, they must be incident on the fibre core within the angle  $\theta_0$ . This angle is known as acceptance angle. Acceptance angle is defined as the maximum angle of incidence at the end face of an optical fibre for which the ray can be propagated in the optical fibre. This angle is also called acceptance cone half-angle.

A cone obtained by rotating a ray at the end face of an optical fibre, around the fibre axis with acceptance angle is known as acceptance cone. Expression for acceptance angle is obtained by applying Snell's law at points B and 0°.

Snell's law at 'B' is:

$$n_1 \sin (90^\circ - \theta_1) = n_2 \sin 90^\circ$$

$$n_1 \cos \theta_1 = n_2$$

$$\cos \theta_1 = \frac{n_2}{n_1}$$

$$\begin{aligned} \text{or } \sin \theta_1 &= \sqrt{1 - \cos^2 \theta_1} \\ &= \sqrt{1 - \frac{n_2^2}{n_1^2}} \end{aligned} \quad (11.1)$$

Snell's law at 'O'

$$n_0 \sin \theta_0 = n_1 \sin \theta_1$$

$$\text{or } \sin \theta_0 = \frac{n_1}{n_0} \sin \theta_1 \quad (11.2)$$

Substitute Equation 11.1 in Equation 11.2

$$\sin \theta_0 = \frac{n_1}{n_0} \sqrt{1 - \frac{n_2^2}{n_1^2}} = \frac{\sqrt{n_1^2 - n_2^2}}{n_0} \quad (11.3)$$

As the fibre is in air.

So, the refractive index  $n_0 = 1$

The Equation (11.3) becomes:

$$\sin \theta_0 = \sqrt{n_1^2 - n_2^2} \quad (11.4)$$

This is the equation for acceptance angle.

## 11.3 Numerical aperture (NA)

Numerical aperture represents the light-gathering capacity of an optical fibre. Light-gathering capacity is proportional to the acceptance angle,  $\theta_0$ . So, numerical aperture can be represented by the sine of acceptance angle of the fibre i.e.,  $\sin \theta_0$ .

**Expression for numerical aperture (NA):** Expression for numerical aperture can be obtained by applying Snell's law at 'O' and at 'B' in Fig. 11.2. Let  $n_1$ ,  $n_2$  and  $n_0$  be the refractive indices of core, cladding and the surrounding medium (air), respectively. Applying Snell's law at the point of entry of the ray [i.e., at 'O'],

We have:

$$n_0 \sin \theta_0 = n_1 \sin \theta_1 \quad (11.5)$$

At point 'B' on the core-cladding interface, the angle of incidence =  $90^\circ - \theta_1$ . Applying Snell's law at 'B', we have:

$$n_1 \sin (90^\circ - \theta_1) = n_2 \sin 90^\circ$$

## 11-4 | Applied Physics

$$n_1 \cos \theta_1 = n_2$$

$$\cos \theta_1 = \frac{n_2}{n_1} \quad (\text{or})$$

$$\sin \theta_1 = \sqrt{1 - \cos^2 \theta_1} = \sqrt{1 - \frac{n_2^2}{n_1^2}} \quad (11.6)$$

Substituting Equation (11.6) in (11.5), we have:

$$\begin{aligned} n_0 \sin \theta_0 &= n_1 \sqrt{1 - \frac{n_2^2}{n_1^2}} \\ \sin \theta_0 &= \frac{n_1}{n_0} \sqrt{\frac{n_1^2 - n_2^2}{n_1^2}} \\ \sin \theta_0 &= \frac{\sqrt{n_1^2 - n_2^2}}{n_0} \end{aligned} \quad (11.7)$$

If the surrounding medium of the fibre is air, then  $n_0 = 1$ .

$$\text{So, } \sin \theta_0 = \sqrt{n_1^2 - n_2^2}$$

According to the definition for numerical aperture (NA),

$$\text{NA} = \sin \theta_0 = \sqrt{n_1^2 - n_2^2} \quad (11.8)$$

Let the fractional change in the refractive index ( $\Delta$ ) be the ratio between the difference in refractive indices of core and cladding to the refractive index of core.

$$\text{i.e., } \Delta = \frac{n_1 - n_2}{n_1} \quad (11.9)$$

$$(\text{or}) \quad n_1 - n_2 = \Delta n_1 \quad (11.10)$$

Equation (11.10) can be written as:

$$\text{NA} = \sqrt{n_1^2 - n_2^2} = \sqrt{(n_1 - n_2)(n_1 + n_2)} \quad (11.11)$$

Substituting Equation (11.10) in (11.11), we have:

$$\text{NA} = \sqrt{\Delta n_1 (n_1 + n_2)}$$

Since  $n_1 \approx n_2$ ; so,  $n_1 + n_2 \approx 2n_1$

$$\therefore \text{NA} = \sqrt{2\Delta n_1^2} = n_1 \sqrt{2\Delta} \quad (11.12)$$

Numerical aperture can be increased by increasing ' $\Delta$ ' and thus enhances the light-gathering capacity of the fibre. We cannot increase  $\Delta$  to a very large value because it leads to intermodal dispersion, which causes signal distortion.

**Condition for light propagation in the fibre:** If  $\theta_i$  is the angle of incidence of an incident ray at the end of optical fibre, then the ray will propagate if  $\theta_i < \theta_0$

$$(\text{or}) \quad \sin \theta_i < \sin \theta_0$$

$$(or) \quad \sin \theta_i < \sqrt{n_1^2 - n_2^2}$$

(or)  $\sin \theta_i < \text{NA}$  is the condition for propagation of light within the fibre.

## 11.4 Step index fibres and graded index fibres—transmission of signals in them

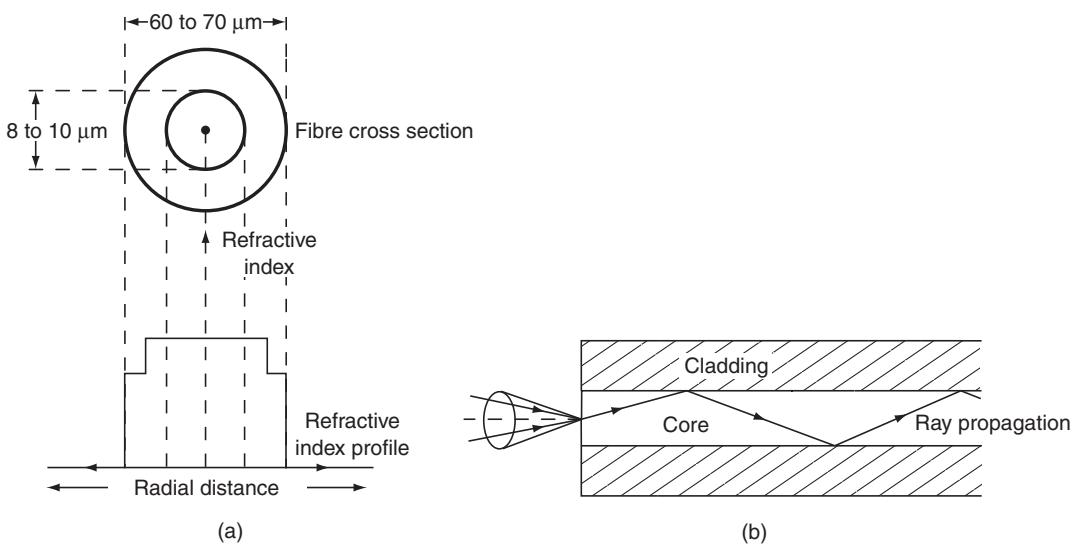
Based on the variation of refractive index of core, optical fibres are divided into: (1) step index and (2) graded index fibres. Again based on the mode of propagation, all these fibres are divided into: (1) single mode and multimode fibres. In all optical fibres, the refractive index of cladding material is uniform. Now, we will see the construction, refractive index of core and cladding with radial distance of fibre, ray propagation and applications of the above optical fibres.

**(1) Step index fibre:** The refractive index is uniform throughout the core of this fibre. As we go radially in this fibre, the refractive index undergoes a step change at the core-cladding interface. Based on the mode of propagation of light rays, step index fibres are of two types: (a) single mode step index fibres and (b) multimode step index fibres. Mode means, the number of paths available for light propagation in a fibre. We describe the different types of fibres below.

**(a) Single mode step index fibre:** The core diameter of this fibre is about 8 to 10  $\mu\text{m}$  and outer diameter of cladding is 60 to 70  $\mu\text{m}$ . There is only one path for ray propagation, so, it is called single mode fibre. The cross sectional view, refractive index profile and ray propagation are shown in Fig. 11.3. In this fibre, the transmission of light is by successive total internal reflections. i.e., it is a reflective type fibre. Nearly 80% of the fibres manufactured today in the world are single mode fibres. So, they are extensively used. Lasers are used as light source in these fibres. These fibres are mainly used in submarine cable system.

Figure 11.3

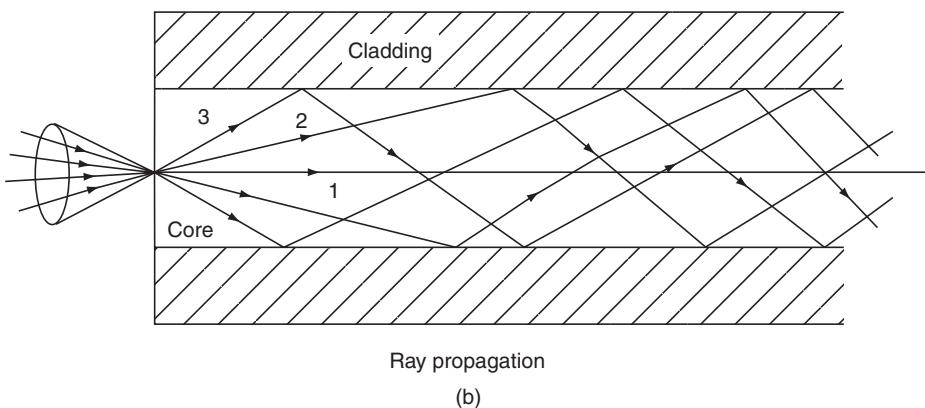
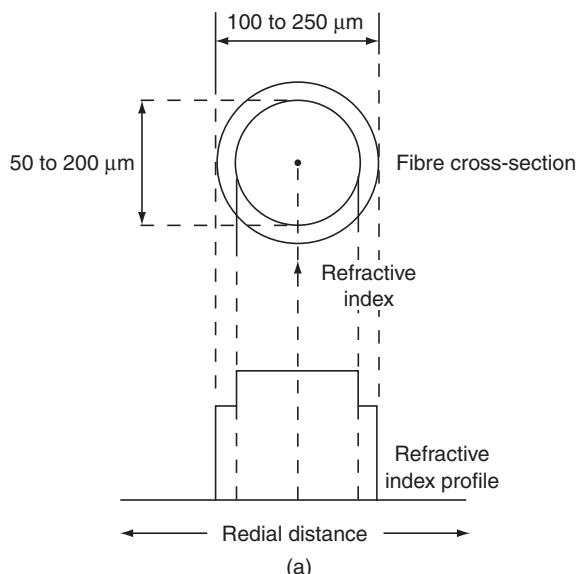
Single mode step index fibre: (a) Cross sectional view and refractive index profile; (b) Ray propagation



**(b) Multimode step index fibre:** The construction of multimode step index fibre is similar to single mode step index fibre except that its core and cladding diameters are much larger to have many paths for light propagation. The core diameter of this fibre varies from 50 to 200  $\mu\text{m}$  and the outer diameter of cladding varies from 100 to 250  $\mu\text{m}$ . The cross-sectional view, refractive index profile and ray propagation are shown in Fig. 11.4. Light propagation in this fibre is by multiple total internal reflections. i.e., it is a reflective type fibre. It is used in data links which have lower bandwidth requirements.

**(c) Transmission of signal in step index fibre:** Generally, the signal is transmitted through the fibre in digital form i.e., in the form of 1's and 0's. The propagation of pulses through multimode fibre is shown in Fig. 11.4(b). The pulse which travels along path 1 (straight) will reach first at the other end of fibre. Next, the pulse that travels along path 2 (zig-zag) reaches the other end with some time delay. Lastly, the pulse that travels along path 3 reaches the other end. Hence, the pulsed signal received at the other end is broadened. This is known as

**Figure 11.4** Multimode step index fibre: (a) Cross sectional view and refractive index profile; (b) Ray propagation

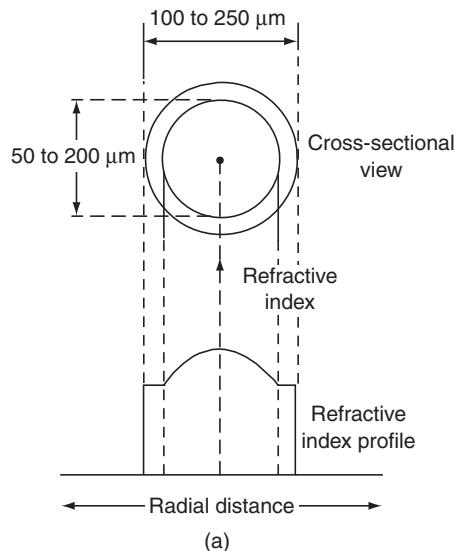


intermodal dispersion. This imposes limitation on the separation between pulses and reduces the transmission rate and capacity. To overcome this problem, graded index fibres are used.

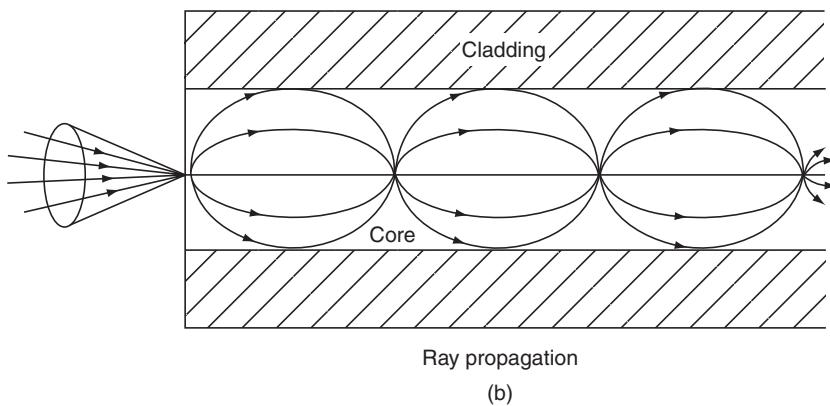
**(2) Graded index fibre:** In this fibre, the refractive index decreases continuously from centre radially to the surface of the core. The refractive index is maximum at the centre and minimum at the surface of core. This fibre can be single mode or multimode fibre. The cross-sectional view, refractive index profile and ray propagation of multimode graded index fibre are shown in Fig. 11.5(a). The diameter of core varies from 50 to 200  $\mu\text{m}$  and outer diameter of cladding varies from 100 to 250  $\mu\text{m}$ .

The refractive index profile is circularly symmetric. As refractive index changes continuously radially in core, the light rays suffer continuous refraction in core. The propagation of light rays is not due to total internal reflection but by refraction as shown in Fig. 11.5(b). In graded index fibre, light rays travel at different speeds in different parts of the fibre. Near the surface of core, the refractive index is lower, so rays near the outer surface travel faster than the rays travel at the centre. Because of this, all the rays arrive at

**Figure 11.5** Multimode graded index fibre: (a) Cross sectional view and refractive index profile; (b) Ray propagation



(a)



Ray propagation

(b)

the receiving end of the fibre approximately at the same time. This fibre is costly. Either laser or LED is used as light source. Its typical applications is in the telephone trunk between central offices.

**Transmission of signal in graded index fibre:** In multimode graded index fibre, large number of paths are available for light ray propagation. To discuss about intermodal dispersion, we consider ray path 1 along the axis of fibre as shown in Fig. 11.5(b) and another ray path 2. Along the axis of fibre, the refractive index of core is maximum, so the speed of ray along path 1 is less. Path 2 is sinusoidal and it is longer; along this path refractive index varies. The ray mostly travels in low refractive index region, so the ray 2 moves slightly faster. Hence, the pulses of signals that travel along path 1 and path 2 reach other end of fibre simultaneously. Thus, the problem of intermodal dispersion can be reduced to a large extent using graded index fibres.

## 11.5 Differences between step index fibres and graded index fibres

Step Index Fibre	Graded Index Fibre
1. The refractive index of the core is uniform and step or abrupt change in refractive index takes place at the interface of core and cladding in step index fibres.	1. The refractive index of core is non-uniform, the refractive index of core decreases parabolically from the axis of the fibre to its surface.
2. The light rays propagate in zig-zag manner inside the core. The rays travel in the fibre as meridional rays and they cross the fibre axis for every reflection.	2. The light rays propagate in the form of skew rays or helical rays. They will not cross the fibre axis.
3. Signal distortion is more in case of high-angle rays in multimode step index fibre. In single mode step index fibre, there is no distortion.	3. Signal distortion is very low even though the rays travel with different speeds inside the fibre.
4. The bandwidth is about 50 MHz km for multimode step index fibre whereas it is more than 1000 MHz Km in case of single mode step index fibre.	4. The bandwidth of the fibre lies in between 200 MHz Km to 600 MHz Km even though theoretically it has an infinite bandwidth.
5. Attenuation of light rays is more in multimode step index fibres but for single mode step index fibres, it is very less.	5. Attenuation of light rays is less in graded index fibres.
6. NA of multimode step index fibre is more whereas in single mode step index fibres, it is very less.	6. NA of graded index fibres is less.

## 11.6 Differences between single mode fibres and multimode fibres

Single Mode Fibres	Multimode Fibres
1. In single mode fibres there is only one path for ray propagation.	1. In multimode fibres, large number of paths are available for light ray propagation.
2. Single mode step index fibres have less core diameter ( $<10 \mu\text{m}$ ) and the difference between the refractive indices of core and cladding is very small.	2. Multimode step index fibres have larger core diameter (50 to $200 \mu\text{m}$ ) and the difference between the refractive indices of core and cladding is large.

3. In single mode fibres, there is no dispersion.	3. There is signal distortion and dispersion takes place in multimode fibres.
4. Signal transmission capacity is less but the single mode fibres are suitable for long distance communication.	4. Signal transmission capacity is more in multimode fibres. Because of large dispersion and attenuation, they are less suitable for long distance transmission.
5. Launching of light into single mode fibres is difficult.	5. Launching of light into multi mode fibres is easy.
6. Fabrication cost is very high.	6. Fabrication cost is less.
7. The V-number of a fibre $V = \frac{2\pi}{\lambda} n_1 r \sqrt{2\Delta}$ is less than 2.405 for single mode fibre. $n_1, r$ are the refractive index and radius of core respectively, $\lambda$ = wavelength of light that propagates through the fibre.	7. The V-number of a multimode fibre is greater than 2.405.

## 11.7 Attenuation in optical fibres

A very important parameter of an optical fibre is the attenuation of light signal in the fibre. Attenuation decreases light transmittance. Usually, the power of light at the output end of optical fibre is less than the power launched at the input end, then the signal is said to be attenuated. The signal attenuation is defined as the ratio of the input optical power ( $P_i$ ) into the fibre to the power of light coming out at the output end ( $P_o$ ). The attenuation coefficient is given as:

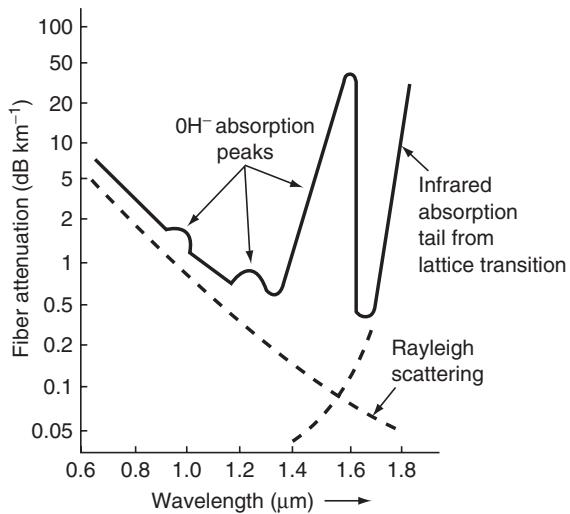
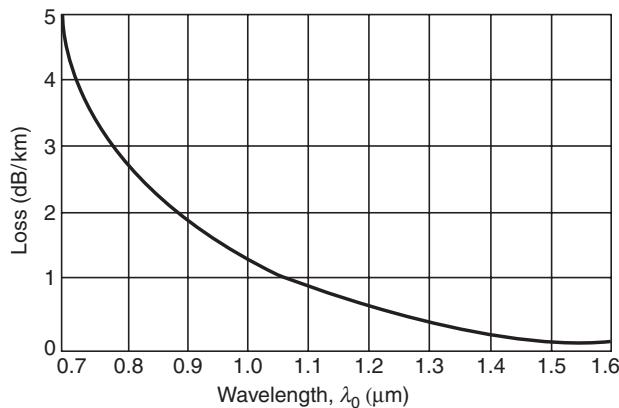
$$\alpha = \frac{10}{L} \log_{10} \frac{P_i}{P_o} \text{ dB/Km} \quad \text{where } L \text{ is the length of the fibre}$$

The causes of attenuation are numerous, some of them are waveguide structure, material compositions, material dispersion, material scattering, microbending losses, mode coupling radiation losses, etc. The attenuation is the function of wavelength and material. Optical communication wavelengths are 0.8, 1.3 and 1.55  $\mu\text{m}$ . The attenuation is mainly due to: (i) absorption and (ii) scattering.

**(i) Absorption losses:** In glass fibres, three different absorptions take place. They are ultraviolet absorption, infrared absorption and ion resonance absorption. Ion resonance absorption losses in pure fused silica are shown in Fig.11.6.

Absorption of uv radiation around 0.14  $\mu\text{m}$  results in the ionization of valence electrons. Absorption of IR photons by atoms within the glass molecules causes heating. This gives absorption peak at 8  $\mu\text{m}$ , also minor peaks at 3.2, 3.8 and 4.4  $\mu\text{m}$ . The  $\text{OH}^-$  ions of water trapped during manufacturing causes absorption at 0.95, 1.25 and 1.39  $\mu\text{m}$  as shown in Fig. 11.6. The presence of other impurities such as iron, copper and chromium also causes absorption. All these absorptions results in absorption loss in the fibre.

**(ii) Scattering losses:** The molten glass, when drawn into a very thin fibre under proper tension causes sub-microscopic variation in the density of glass in the fibre takes place. The dopants added to glass to vary the refractive index also leads to inhomogeneities in the fibre. The microscopic variation of density and inhomogeneities acts as reflecting and refracting facets, these scatter a small portion of light passing through the glass. Thus, the scattering losses. If the size of density-fluctuating regions is of the order of  $\lambda/10$  or less then they act as point source scattering centre. This kind of scattering is known as Rayleigh scattering. The scattering losses is proportional to  $1/\lambda^4$ . On this basis, the scattering losses at a wavelength of 1.3  $\mu\text{m}$  is about 0.3 dB/Km whereas at a wavelength of 0.7  $\mu\text{m}$  it is about 5 dB/Km. The Rayleigh scattering losses for silica is shown in Fig. 11.7.

**Figure 11.6** Ion resonance absorption loss effects in fused silica glass fibres**Figure 11.7** Rayleigh scattering losses in silica fibres

**(iii) Bending Losses:** In a bent fibre, there is loss in power of the transmitted signal called bending losses. Einstein explained the bending losses. According to Einstein's theory of relativity, the part of the ray that enters into cladding will travel faster. The energy associated with this part of the ray is lost. This loss can be represented by absorption coefficient ( $\alpha$ )

$$\alpha = C \exp\left(\frac{-R}{R_c}\right) \quad \text{where } C \text{ is constant}$$

$$R = \text{radius of curvature of fibre bend} \text{ and } R_c = \frac{r}{(\text{NA})^2}$$

$r$  = radius of the fibre. The bends with radius of curvature is of magnitude of the fibre radius gives rises to heavy losses.

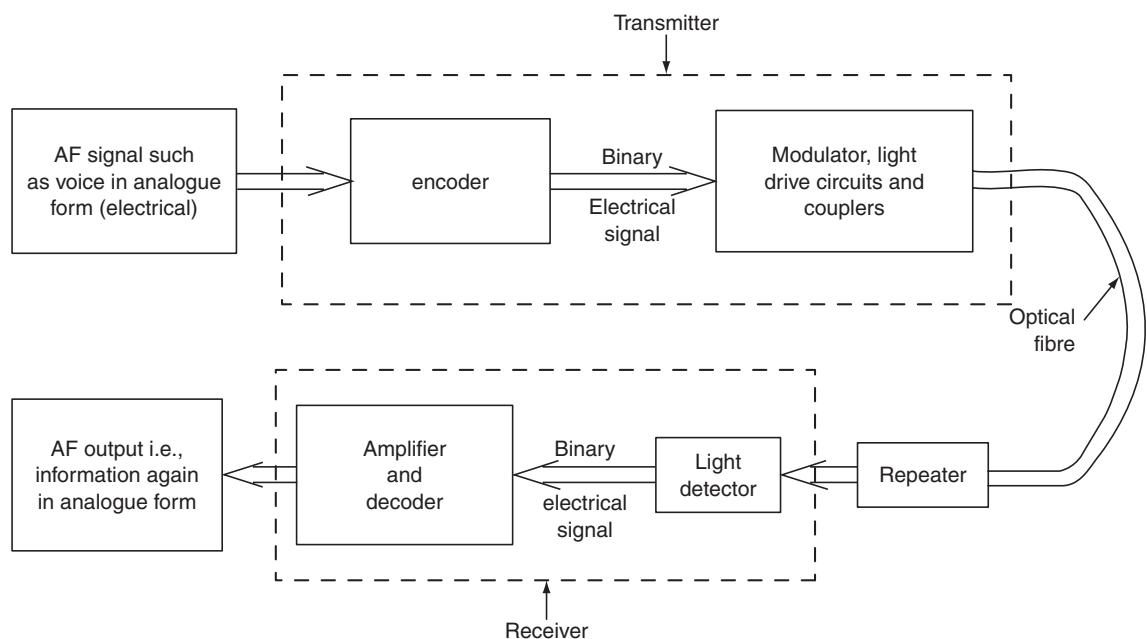
(iv) **Microbending and wave guide losses:** A large number of small bends present in the fibre causes large attenuation in the signal transmission. This is known as microbending loss. Usually, microbends are formed when an unsheathed fibre is wound in tension on a drum during manufacture. These bends will be more if the surface of drum is non-uniform.

During manufacturing, if proper care is not taken, then a continuous small variation in the fibre diameter or circularity is formed. This gives scattering loss, known as waveguide losses.

## 11.8 Optical fibres in communication

Fibre optics essentially deals with the communication [including voice signals, video signals or digital data] by transmission of light through optical fibres. Optical fibre communication system essentially consists of three parts: (a) transmitter (b) optical fibre and (c) receiver (Fig. 11.8). The transmitter includes modulator, encoder, light source, drive circuits and couplers. The light source can be a light emitting diode [LED] or a semiconductor laser diode. Basically, a fibre optic system simply converts an electrical signal [corresponds to analogue information such as voice] to binary data by an encoder and this binary data comes out as a stream of electrical pulses and these electrical pulses are converted into pulses of optical power by modulating the light emitted by the light source. That means the laser drive circuit directly modulates the intensity of the semiconductor

**Figure 11.8** Block diagram represents optical fibre communication system



laser light with the encoded digital signal. This digital optical signal is launched into the optical fibre cable. The transmitter also has couplers to couple the transmitted light signals with the fibre. Fibres might require connectors to increase the length of the fibre medium. To transmit signals to long distances, repeaters are used after certain lengths in the optical fibre.

As the signal propagates in the fibre, it is subjected to attenuation and delay distortion. Attenuation is the loss of optical power due to absorption and scattering of photons. Even the leakage of light due to fibre bends adds to the attenuation effect. Delay distortion is because of spreading of pulses with time. The pulse spreading is mainly due to the variation in velocity of various spectral components of the pulse during its propagation in the fibre. When the attenuation and pulse spreading reaches beyond a limiting stage, then it may not be possible to retrieve the information from the light signal. Just at this threshold stage, a repeater is needed in the transmission path.

An optical repeater consists of a receiver and a transmitter arranged adjacently. The receiver section converts the optical signal into corresponding electrical signal, further this electrical signal is amplified and recast in the original form by means of an electrical regenerator i.e., reshape the signal and this signal is sent into an optical transmitter section, where the electrical signal is again converted back to optical signal and fed into an optical fibre.

Finally, at the end of optical fibre the signal is fed to the receiver. The receiver contains light detector. This can be either an Avalanche Photo Diode [APD] or a Positive Intrinsic Negative [PIN] diode. In the photodetector, the signal is converted into pulses of electrical current, which is then fed to the decoder, which converts the sequence of binary data stream into an analogue signal as that fed at the transmitting end.

## 11.9 Advantages of optical fibres in communication

The following are the advantages of optical fibres in communication:

- (i) Extremely wide band: The rate at which information can be transmitted is directly related to signal frequency. Light has very high frequency in the range of  $10^{14}$  to  $10^{15}$  Hz, as compared to radio frequencies  $\sim 10^6$  Hz and microwave frequencies  $10^8$ – $10^{10}$  Hz. So, light can transmit information at a higher rate than systems that operate at radio frequencies or microwave frequencies.
- (ii) Smaller diameter and light weight: Optical fibres are light-weight, smaller diameter and flexible; so, they can be handled more easily than copper cables.
- (iii) Lack of cross-talk between parallel fibres: In copper cable communication circuits, signals often stray from one circuit to another, resulting in other calls being heard in the background.

This cross talk is negligible in optical fibres even when many fibres are cabled together.

- (iv) Longer life-span: The life-span of optical fibres is expected to be 20–30 years as compared to copper cables, which have a life-span of 12–15 years.
- (v) Temperature resistant: In contrast to copper cables, they have high tolerance to temperature extremes.
- (vi) Easy maintenance: Optical cables are more reliable and easy to maintain than copper cables.
- (vii) Much safer than copper cables: This is because only light and not electricity is being conducted.
- (viii) Potential of delivering signals at low cost, because fibres are made up of silica, which is available in abundance in nature.
- (ix) They possess low transmission loss and noise-free transmission is obtained as compared to copper cables. Since the transmission loss in optical fibres is as low as 0.2 dB/Km.
- (x) Ruggedness and flexibility: Optical fibre cables are flexible, compact and extremely rugged.

## 11.10 Fibre optic sensing applications

Fibre optic sensors are used to monitor displacement, liquid level, flow, temperature and pressure, chemical composition etc. Optic fibre sensors can be divided into two types, they are:

- (a) Intrinsic sensors/active sensors and (b) extrinsic sensors/pассивные сенсоры.

**The Active sensors:** In active sensors, the quantity to be measured acts directly on the fibre and modifies the radiation passing down the fibre.

The various active sensors are:

- (i) Intensity modulated sensors:** These are based on the change in refractive index, temperature, absorption, etc
- (ii) Phase-modulated sensors:** These involve the interference between the signal and reference in the interferometer. This leads to a shift in the interference fringes by the variable.
- (iii) Polarization-modulated sensors:** In this, a change in polarization state of the guided signal by the variable takes place.
- (iv) Wavelength-modulated sensors:** In this, the spectral dependent variation of absorption and emission by the variable takes place.

**The passive sensors:** In passive sensors, the modulation takes place outside the fibre. The fibre acts merely as a convenient transmission channel for light. The passive sensors has a sensor head and the sensed optical signal is transmitted to a remote point for signal processing. The table below gives the physical parameter to be measured using passive sensor and the modulation effects in the fibre.

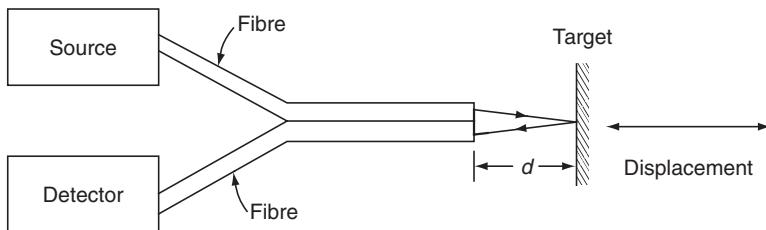
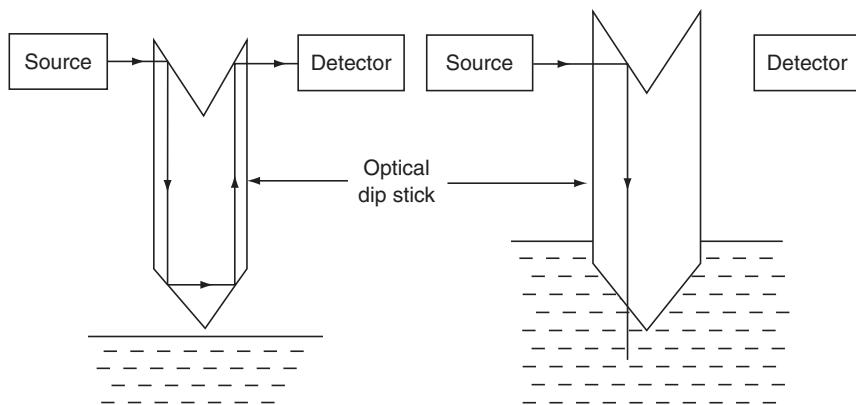
Physical Quantity to be Measured	Modulation Effects in the Fibres
1. Temperature	Thermoluminescence
2. Pressure	Piezo optic effect
3. Density	Triboluminescence
4. Mechanical force	Stress birefringence
5. Electric field	Electro optic effect
6. Magnetic field	Magneto optic effect
7. Electric current	Electro luminescence
8. Nuclear radiation	Radiation-induced luminescence

Now, we study some sensors in detail.

### (a) Displacement sensors

Intensity modulation of the transmitted light beam is utilized in this sensor. Figure 11.9 shows the displacement sensor.

Light from the source passes through one optical fibre and incident on the target. The reflected light reaches the detector through another optical fibre. Light reflected from the target and collected by the detector

**Figure 11.9 Displacement sensor****Figure 11.10 Fluid level detector**

is a function of the distance between the fibre ends and the target. Hence, the position or displacement of the target may be registered at the optical detector. Further, the sensitivity of this sensor may be improved by placing the axis of the feed and return fibre at an angle to one another and to the target.

### (b) Liquid level sensor

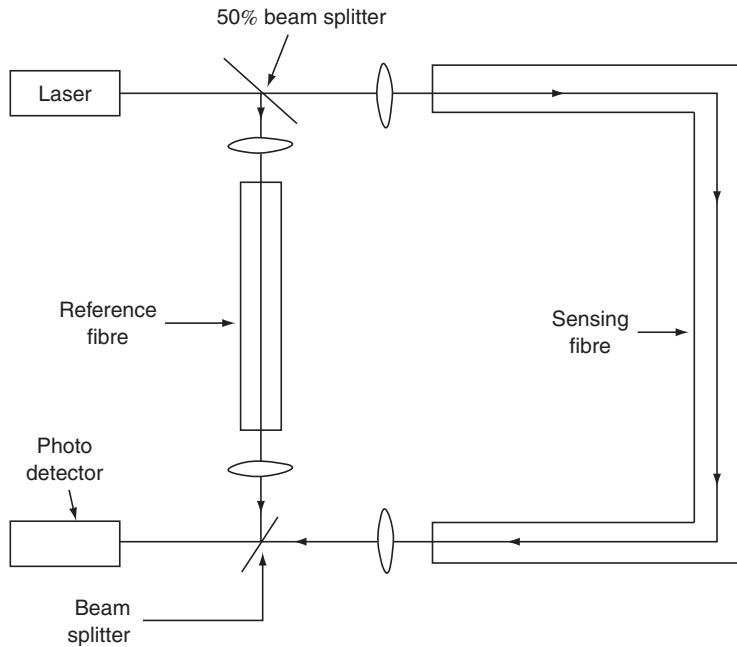
Figure 11.10 shows the operation of a simple optical fluid level switch. If the level of liquid is below the optical dipstick, due to total internal reflection, light from the source reaches the detector. If the level of liquid is above the camfered end of the dipstick, then the light is transmitted into the fluid and the detector ceases to get light.

### (c) Temperature and pressure sensor

When a single optical fibre is subjected to temperature or pressure variations, then its length and refractive index changes. This causes change in phase of light at the end of fibre. The change in phase of light is proportional to magnitude of the change in temperature or pressure. The phase changes can be measured by an interferometer method shown in Fig. 11.11.

Here, the light from a laser source is split into two beams of approximately equal amplitude by a 50% beam splitter. One beam is passed through sensing fibre, which is subjected to temperature or pressure variations and

**Figure 11.11 Measurement of phase changes by interferometer method**



the other beam through reference fibre, which is not subjected to any changes and is used for comparison. Light from these two fibres is superimposed using another beam splitter. Interference of these two waves gives fringes. The intensity of the fringe depends on the phase relation between the two waves. If the waves are in phase, then the intensity is maximum; this happens when the sensing fibre is not disturbed. The intensity is minimum if the waves are out of phase due to  $\lambda/2$  change in length of sensing fibre. The intensity of interference fringes can be measured with a photodetector and temperature or pressure changes can be measured.

#### (d) Chemical sensors

Here, the sensing element is a modified fibre, and this sensing element senses the concentration of a chemical in terms of the phase change of the light wave. For example, in hydrogen sensor, palladium wire is fixed to the sensor. Hydrogen absorption changes the dimensions of the wire. This change produces strain in the optical fibre. This strain in the fibre changes the path length of light in the fibre. So, the concentration of hydrogen is proportional to the change in path length of light.

### 11.11 Applications of optical fibres in medical field

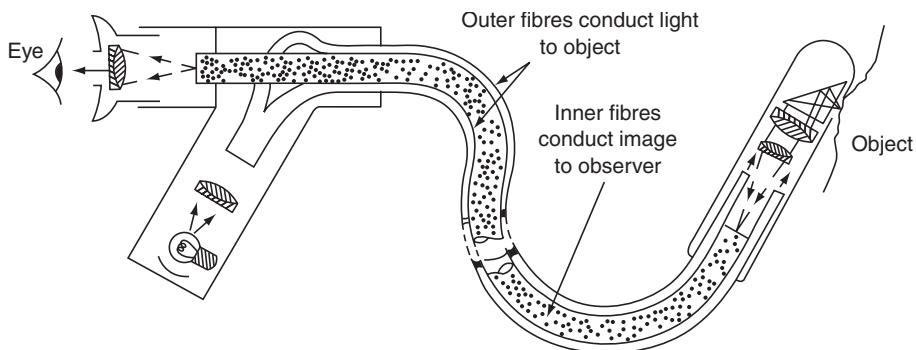
Optical fibre medical instruments may contain bundles of optical fibres. An optical fibre instrument used to see the internal parts of human body is endoscope. The endoscope facilitates the physicians to see the internal parts of body without performing surgery. The main part in endoscope is fibrescope. Based on application, the endoscopes are classified into:

- (i) **Gastroscope** is used to examine the stomach. A gastroscope can be fitted with various parts to photograph tumours and ulcers. Laser-used gastroscope is used to remove objects that have been swallowed. Gastroscope can also guide a laser, used to destroy tumours.
- (ii) **Bronchoscope** is used to see upper passages of lungs.
- (iii) **Orthoscope** is used to see the small spaces within joints.
- (iv) **Couldoscope** is used to test female pelvic organs.
- (v) **Peritoneoscope** is used to test the abdominal cavity, lower parts of liver and gall bladder.

Also in ophthalmology, laser guided by the fibres is used to reattach the detached retina and to correct the defects in the vision.

The fabrication of fibrescope is used in endoscope. Fibrescope is shown in Fig. 11.12 below.

**Figure 11.12 Flexible fibrescope**



The fibrescope is also useful in industry. It could be used to examine welds, nozzles and combustion chambers inside the aircraft engines. These are not easily accessible for observation otherwise.

## Formulae

1.  $NA = \sin \theta_0 = \sqrt{n_1^2 - n_2^2}$
2.  $\Delta = \frac{n_1 - n_2}{n_1}$
3.  $NA = n_1 \sqrt{2\Delta}$

## Solved Problems

1. The refractive indices of core and cladding materials of a step index fibre are 1.48 and 1.45, respectively. Calculate: (i) numerical aperture, (ii) acceptance angle, and (iii) the critical angle at the core-cladding interface and (iv) fractional refractive indices change.

(Set-1–May 2006)

**Sol:** Let the refractive index of core,  $n_1 = 1.48$

and the refractive index of cladding,  $n_2 = 1.45$

(i) Numerical aperture (NA) =  $\sqrt{n_1^2 - n_2^2}$

$$= \sqrt{(1.48)^2 - (1.45)^2} = \sqrt{2.1904 - 2.1025} = \sqrt{0.0879} = 0.2965$$

(ii) Let  $\theta_0$  be the acceptance angle

Then,  $\sin \theta_0 = \text{NA} = \sqrt{n_1^2 - n_2^2}$

$$\theta_0 = \sin^{-1} \sqrt{n_1^2 - n_2^2} = \sin^{-1}(0.2965) = 17^\circ 15'$$

(iii)  $n_2 \sin 90 = n_1 \sin \theta_c$  [  $\theta_c$  = critical angle]

$$\sin \theta_c = \frac{n_2}{n_1}$$

$$\theta_c = \sin^{-1} \frac{n_2}{n_1} = \sin^{-1} \left( \frac{1.45}{1.48} \right) = 78^\circ 26'$$

(iv) The fractional refractive indices change,  $\Delta = \frac{n_1 - n_2}{n_1} = \frac{1.48 - 1.45}{1.48} = 0.02$

2. Calculate the angle of acceptance of a given optical fibre, if the refractive indices of the core and cladding are 1.563 and 1.498, respectively.

(Set-3–Sept. 2008), (Set-1–May 2004)

**Sol:** Refractive index of core,  $n_1 = 1.563$

Refractive index of cladding,  $n_2 = 1.498$

Numerical aperture, NA =  $\sqrt{n_1^2 - n_2^2} = \sqrt{1.563^2 - 1.498^2} = 0.446$

Acceptance angle,  $\theta_0 = \sin^{-1}(\text{NA}) = \sin^{-1}(0.446) = 26^\circ 30'$ .

3. Calculate the fractional index change for a given optical fibre if the refractive indices of the core and cladding are 1.563 and 1.498, respectively.

(Set-1–Sept. 2007), (Set-4–May 2004)

**Sol:** Refractive index of the core,  $n_1 = 1.563$

Refractive index of cladding,  $n_2 = 1.498$

The fractional refractive indices change,  $\Delta = \frac{n_1 - n_2}{n_1} = \frac{1.563 - 1.498}{1.563} = 0.0416$ .

4. An optical fibre has a core material of refractive index 1.55 and cladding material of refractive index 1.50. The light is launched into it in air. Calculate its numerical aperture.

(Set-4–May 2006), (Set-2–May 2004)

**Sol:** Refractive index of core,  $n_1 = 1.55$

Refractive index of cladding,  $n_2 = 1.50$

Numerical aperture, NA =  $\sqrt{n_1^2 - n_2^2}$

$$= \sqrt{1.55^2 - 1.50^2} = 0.3905$$

5. The numerical aperture of an optical fibre is 0.39. If the difference in the refractive indices of the material of its core and the cladding is 0.05, calculate the refractive index of material of the core.

(Set-1-May 2008), (Set-3-May 2004)

**Sol:** Numerical aperture, NA = 0.39

$$\text{The difference in refractive indices} = n_1 - n_2 = 0.05 \quad \dots \quad (1)$$

Refractive index of the core,  $n_1 = ?$

From Equation (1)

$$n_1 = n_2 + 0.05 \quad \dots \quad (2)$$

$$\text{NA} = \sqrt{n_1^2 - n_2^2} = \sqrt{(n_1 - n_2)(n_1 + n_2)}$$

$$0.39 = \sqrt{0.05 \times (n_1 + n_2)}$$

$$\frac{0.39^2}{0.05} = n_1 + n_2 = 3.042 \quad \dots \quad (3)$$

Substituting Equation (2) in (3), we get:

$$3.042 = n_2 + 0.05 + n_2 = 2n_2 + 0.05$$

$$n_2 = 1.496$$

$$\therefore n_1 = n_2 + 0.05 = 1.496 + 0.05 = 1.546.$$

6. An optical fibre has a core material of refractive index 1.55 and cladding material of refractive index 1.50. The light is launched into it in air. Calculate its numerical aperture.

(Set-4-May 2006), (Set-1-June 2005)

**Sol:** Refractive index of core,  $n_1 = 1.55$

Refractive index of cladding,  $n_2 = 1.50$

$$\text{Numerical aperture, NA} = \sqrt{n_1^2 - n_2^2} = \sqrt{1.55^2 - 1.50^2} = 0.3905$$

7. Calculate the numerical aperture and acceptance angle for an optical fibre with core and cladding refractive indices being 1.48 and 1.45, respectively.

(Set-4-May 2007), (Set-4-June 2005)

**Sol:** Refractive index of core,  $n_1 = 1.48$

Refractive index of cladding,  $n_2 = 1.45$

Numerical aperture, NA = ?

acceptance angle,  $\theta_0 = ?$

$$\text{NA} = \sqrt{n_1^2 - n_2^2} = \sqrt{1.48^2 - 1.45^2} = 0.2965$$

$$\theta_0 = \sin^{-1} \sqrt{n_1^2 - n_2^2} = \sin^{-1} 0.2965 = 17^\circ 15'.$$

8. Calculate the refractive indices of core and cladding of an optical fibre with a numerical aperture of 0.33 and their fractional difference of refractive indices being 0.02.

(Set-2–May 2006)

**Sol:** Refractive index of core,  $n_1 = ?$

Refractive index of cladding,  $n_2 = ?$

Numerical aperture, NA = 0.33

Fractional difference of refractive index,  $\Delta = 0.02$

$$\Delta = \frac{n_1 - n_2}{n_1} \quad \text{or} \quad 0.02n_1 = n_1 - n_2$$

$$n_2 = (1 - .02)$$

$$n_1 = 0.98n_1$$

$$\text{NA} = \sqrt{n_1^2 - n_2^2}$$

$$0.33 = \sqrt{n_1^2 - (0.98n_1)^2}$$

$$0.33 = n_1 \times 0.198997$$

$$n_1 = 1.6583$$

$$n_2 = 0.98 \times 1.6583 = 1.625$$

9. An optical fibre has a numerical aperture of 0.20 and a cladding refractive index of 1.59. Find the acceptance angle for the fibre in water which has a refractive index of 1.33.

(Set-3–May 2006), (Set-1, Set-2, Set-4–Sept. 2006), (Set-2–May 2007), (Set-2–Sept. 2007)

**Sol:** Numerical aperture of the fibre, NA = 0.20

Refractive index of cladding,  $n_2 = 1.59$

Refractive index of water,  $n_0 = 1.33$

Acceptance angle of fibre in water,  $\theta_0 = ?$

$$\text{NA} = \sqrt{n_1^2 - n_2^2}$$

$$\text{NA}^2 = n_1^2 - n_2^2$$

$$0.04 = n_1^2 - (1.59)^2$$

$$n_1^2 = 0.04 + (1.59)^2$$

$$= 2.5681$$

$$n_1 = 1.60253$$

$$\sin \theta_0 = \frac{\sqrt{n_1^2 - n_2^2}}{n_0}$$

$$= \frac{\sqrt{(1.60253)^2 - (1.59)^2}}{1.33}$$

$$= \frac{\sqrt{2.5681 - 2.5281}}{1.33} = \frac{0.2}{1.33}$$

$$= 0.15037$$

$$\theta_0 = \sin^{-1}[0.15037]$$

$$= 8^\circ 38' 56''$$

10. A fibre has the core and cladding refractive indices 1.45 and 1.44 respectively. Find the relative refractive index difference.  
(Set-4-Sept. 2007)

**Sol:** Refractive index of core ( $n_1$ ) = 1.45

Refractive index of cladding ( $n_2$ ) = 1.44

Relative refractive index difference ( $\Delta$ )

$$= \frac{n_1 - n_2}{n_1} = \frac{1.45 - 1.44}{1.45} = 6.896 \times 10^{-3}$$

11. The refractive index of core of step index fibre is 1.50 and the fractional change in refractive index is 4%. Estimate:  
(i) refractive index of cladding, (ii) numerical aperture, (iii) acceptance angle in air and (iv) the critical angle at the core-cladding interface.

**Sol:** (i) The refractive index of the core,  $n_1 = 1.50$

$$\text{The fractional change in refractive index, } \Delta = \frac{n_1 - n_2}{n_1} = \frac{4}{100}$$

where  $n_2$  = refractive index of cladding

$$\therefore \frac{n_1 - n_2}{n_1} = 0.04$$

$$n_1 - n_2 = 0.04 \times 1.5 = 0.06$$

$$1.5 - n_2 = 0.06$$

$$\therefore n_2 = 1.44$$

$$(ii) \text{ Numerical aperture, } \text{NA} = \sqrt{n_1^2 - n_2^2}$$

$$= \sqrt{(1.5)^2 - (1.44)^2} = \sqrt{2.25 - 2.0736} = \sqrt{0.1764} = 0.42$$

$$(iii) \text{ Acceptance angle, } \theta_0 = \sin^{-1}(\text{NA})$$

$$= \sin^{-1}(0.42) = 24^\circ 50'$$

$$(iv) \text{ Critical angle, } \theta_c = \sin^{-1} \frac{n_2}{n_1}$$

$$\sin^{-1} \frac{1.44}{1.50} = \sin^{-1} 0.96 = 73^\circ 44'$$

12. The refractive indices of core and cladding of a step index optical fibre are 1.563 and 1.498, respectively. Calculate: (i) numerical aperture and (ii) angle of acceptance in air.

**Sol:** Refractive index of core ( $n_1$ ) = 1.563

Refractive index of cladding ( $n_2$ ) = 1.498

(i) Numerical aperture (NA) = ?

$$\text{NA} = \sqrt{n_1^2 - n_2^2}$$

$$= \sqrt{1.563^2 - 1.498^2} = 0.446$$

(ii) Acceptance angle ( $\theta_0$ ) = ?

$$\theta_0 = \sin^{-1}(NA)$$

$$= \sin^{-1}(0.446)$$

$$= 26^\circ 30'$$

## Multiple Choice Questions

- The light sources used in fibre optic communication are. ( )  
(a) LEDs (b) semiconductor lasers  
(c) phototransistors (d) both a and b
  - Acceptance angle is defined as the \_\_\_\_\_ angle of incidence at the endface of an optical fibre, for which the ray can be propagated in the optical fibre is. ( )  
(a) maximum (b) minimum  
(c) Either a or b (d) none of the above
  - The core diameter of single mode step index fibre is about: ( )  
(a) 60 to 70  $\mu\text{m}$  (b) 8 to 10  $\mu\text{m}$   
(c) 100 to 250  $\mu\text{m}$  (d) 50 to 200  $\mu\text{m}$
  - In multimode graded index fibre, light rays travel \_\_\_\_\_ in different parts of the fibre. ( )  
(a) at different speeds (b) with same speed  
(c) both a and b (d) none of the above
  - In optical communication system, the light detector is: ( )  
(a) Avalanche Photo Diode (APD) (b) Positive Intrinsic Negative (PIN) diode  
(c) phototransistor (d) Either a or b
  - Optical fibres guides light waves by: ( )  
(a) interference of waves (b) diffraction of waves  
(c) polarization of waves (d) by total internal reflection of waves

7. In an optical fibre, if  $n_1$  and  $n_2$  are the refractive indices of core and cladding, the condition for light propagation through fibre is: ( )
- (a)  $n_1 = n_2$
  - (b)  $n_1 > n_2$
  - (c)  $n_1 < n_2$
  - (d) none of the above
8. Loss of intensity of light in optical fibre is due to: ( )
- (a) absorption
  - (b) scattering
  - (c) reflection
  - (d) both a and b
9. If  $n_1$  and  $n_2$  are the refractive indices of core and cladding, then numerical aperture (NA) of the fibre is: ( )
- (a)  $n_1^2 - n_2^2$
  - (b)  $n_2^2 - n_1^2$
  - (c)  $\sqrt{n_1^2 - n_2^2}$
  - (d)  $\sqrt{n_1^2 + n_2^2}$
10. By increasing the refractive index of core material, the number of modes of propagation in an optical fibre \_\_\_\_\_ . ( )
- (a) increases
  - (b) decreases
  - (c) remains same
  - (d) none of the above
11. The life span of optical fibres is expected to be: ( )
- (a) 40 to 50 years
  - (b) about 100 years
  - (c) 20 to 30 years
  - (d) less than 10 years
12. Fibre optic sensors are used to monitor: ( )
- (a) displacement and flow
  - (b) temperature
  - (c) pressure
  - (d) all the above
13. Total internal reflection takes place when the angle of incidence is \_\_\_\_\_ the critical angle. ( )
- (a) greater than
  - (b) less than
  - (c) equal to
  - (d) both a and b
14. Numerical aperture represents \_\_\_\_\_ capacity of a optical fibre. ( )
- (a) light gathering
  - (b) light dissipation
  - (c) heat dissipation
  - (d) magnetic lines gathering
15. In optical fibres, mode means \_\_\_\_\_ available for light rays to propagate in the fibre. ( )
- (a) the number of paths
  - (b) the number of fibre in optical fibre cable
  - (c) the change in refractive index
  - (d) none of the above
16. In multimode step index fibres, the core diameter is \_\_\_\_\_. ( )
- (a) 8 to 10  $\mu\text{m}$
  - (b) 10 to 30  $\mu\text{m}$
  - (c) 50 to 200  $\mu\text{m}$
  - (d) 100 to 250  $\mu\text{m}$
17. In multimode graded index fibre, the core refractive index profile is \_\_\_\_\_. ( )
- (a) circularly symmetric
  - (b) non-linear
  - (c) step index
  - (d) none of the above
18. The widely used optical fibre in the world is: ( )
- (a) multimode step index fibre
  - (b) multimode graded index
  - (c) single mode step index
  - (d) none of the above

19. The acceptance angle is maximum if the critical angle is \_\_\_\_\_. ( )  
 (a) minimum      (b) maximum      (c) both a & b      (d) none
20. In multimode optical fibre, the core diameter is \_\_\_\_\_ in single mode fibre. ( )  
 (a) lesser than      (b) larger than      (c) equal to      (d) none
21. Optical fibres are made up with \_\_\_\_\_ materials. ( )  
 (a) semiconductors      (b) metals  
 (c) conductors      (d) dielectrics
22. In a reflective type optical fibre, the light rays pass from one end of the fibre to the other end by means of \_\_\_\_\_. ( )  
 (a) multiple total internal reflections      (b) refraction  
 (c) diffraction      (d) polarization
23. If the angle of incidence for a ray at the end face of an optical fibre is larger than acceptance angle, then the ray \_\_\_\_\_. ( )  
 (a) will not propagate in the fibre      (b) will propagate in the fibre  
 (c) both a & b      (d) none of the above
24. All the light rays which enter at a time into the multimode graded index fibre may arrive at \_\_\_\_\_. ( )  
 (a) different times at the other end of the fibre  
 (b) same time at the other end of the fibre  
 (c) both a & b  
 (d) none of the above
25. Delay distortion of light pulses in optical fibre is because of: ( )  
 (a) spreading of pulses with time  
 (b) spreading of pulses with wavelength  
 (c) spreading of pulses with refractive index  
 (d) none of the above
26. Optical fibres carry very large information compared to copper cables because of: ( )  
 (a) large thickness of fibre      (b) extremely wide bandwidth  
 (c) extremely less band width      (d) none

## Answers

1. d	2. a	3. b	4. a	5. d	6. d	7. b	8. d	9. c	10. a
11. c	12. d	13. a	14. a	15. a	16. c	17. a	18. c	19. a	20. b
21. d	22. a	23. a	24. b	25. a	26. b				

## Review Questions

1. Explain the advantages of optical fibres in communication. (Set-3–May 2004)
2. Explain the terms numerical aperture and acceptance angle.  
 (Set-4–May 2006), (Set-1–June 2005), (Set-2–May 2004)

3. Define acceptance angle and numerical aperture. Obtain an expression for numerical aperture of an optical fibre.  
(Set-4-May 2007), (Set-1-May 2006), (Set-4-June 2005)
4. What are the advantages of an optical fibre communication system over the conventional ones?  
(Set-4-Sept. 2007), (Set-4-Nov. 2003)
5. Describe the basic elements of a fibre optics communication system with a block diagram. (Set-4-Nov. 2003)
6. Write a note on the applications of optical fibres. (Set-1-Sept. 2007), (Set-4-May 2004)
7. Explain how the optical fibres are classified. (Set-3-Sept. 2008), (Set-1-May 2004)
8. Describe the construction of a typical optical fibre and give the dimensions of the various parts.  
(Set-4-May 2007), (Set-1-May 2006), (Set-4-June 2005)
9. With the help of a suitable diagram, explain the principle, construction and working of an optical fibre as a waveguide.  
(Set-4-May 2006), (Set-1-June 2005), (Set-2-May 2004)
10. Explain the principle of an optical fibre. (Set-3-Sept. 2008), (Set-1-May 2004)
11. Derive expressions for the numerical aperture and the fractional change of an optical fibre.  
(Set-1-Sept. 2007), (Set-3, Set-4-May 2004)
12. Describe the graded index optical fibres and explain the transmission of signal through it. (Set-3-Sept. 2007)
13. Derive an expression for the numerical aperture of an optical fibre. (Set-1-May 2008), (Set-3-Sept. 2006)
14. Explain the advantages of optical communication system. (Set-1-May 2008)
15. Derive the expressions for (i) acceptance angle and (ii) numerical aperture of an optical fibre.  
(Set-2-May 2008), (Set-4-Sept. 2008), (Set-3-Sept. 2006)
16. Describe different types of fibres by giving the refractive index profiles and propagation details.  
(Set-2-May 2008), (Set-4-Sept. 2008)
17. What are important features of optical fibres? (Set-3-May 2008)
18. Describe the communication process using optical fibres. (Set-3-May 2008)
19. Write the uses of fibre optics in different fields. (Set-3-May 2008)
20. Distinguish between light propagation in (i) step index optical fibre and graded index optical fibre.  
(Set-4-May 2008), (Set-2-May 2006)
21. Write a note on fibre optic medical endoscopy. (Set-4-May 2008)
22. Define the relative refractive index difference of an optical fibre. Show how it is related to numerical aperture.  
(Set-1, Set-3-May 2007)
23. Draw the block diagram of an optical fibre communication system and explain the function of each block.  
(Set-1, Set-3-May 2007)
24. Discuss the various advantages of communication with optical fibres over the conventional coaxial cables.  
(Set-2-May 2006)
25. Explain the principle behind the functioning of an optical fibre.  
(Set-2-Sept. 2007), (Set-2-May 2007), (Set-1, Set-4-Sept. 2006), (Set-3-May 2006)
26. Derive an expression for acceptance angle for an optical fibre. How it is related to numerical aperture?  
(Set-2-Sept. 2007), (Set-2-May 2007), (Set-1, Set-4-Sept. 2006), (Set-3-May 2006)
27. What is meant by an acceptance angle and numerical aperture; obtain mathematical expressions for acceptance angle and numerical aperture.  
(Set-2-Sept. 2006)

28. What is the principle of optical fibre communication? Explain. (Set-3–Sept. 2006)
29. Explain the basic principle of an optical fibre. (Set-3–Sept. 2007), (Set-1–Sept. 2008)
30. What are different losses in optical fibres? Write brief notes on each. (Set-3–Sept. 2007)
31. Explain the difference between a step index fibre and graded index fibre. (Set-4–Sept. 2007)
32. Write the applications of fibre optics in medicine and industry. (Set-1–Sept. 2008)
33. Describe the structure of an optical fibre. (Set-1–Sept. 2008)
34. Describe the step index fibre and explain the transmission of signal through it.
35. Write short notes on acceptance angle in a fibre.
36. Explain the propagation of light waves through an optical fibre.
37. Draw the block diagram of fibre optic communication system and explain the function of each element in the system.
38. Describe the structure of different types of optical fibres with ray paths.
39. Explain the terms: numerical aperture and acceptance angle of a fibre. Derive expressions for them.
40. Explain the transmission of signal in step index and graded index fibres.
41. Describe optical fibres in communication system.
42. What is the principle of optical fibre? Describe various types of optical fibres.
43. Distinguish between step index and graded index fibres with the help of refractive index profile.
44. What is mode in optical fibre? Distinguish between single mode and multimode step index fibres.
45. Describe the various fibre optic sensor applications.
46. Explain the advantages of optical fibre communications.
47. Write briefly on step and graded index optical fibres and numerical aperture of optical fibres.
48. Write briefly on numerical aperture of optical fibre, step and graded index optical fibres.
49. Write short notes on acceptance angle in optical fibres.
50. Write short notes on refractive index profiles of step-graded index fibres.

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## CHAPTER

# 12

## Holography

### 12.1 Introduction

The conventional photography records only the intensities of light coming from an object. It fails to record the phases of the waves that come from the objects. Hence, they show two-dimensional images of three-dimensional objects. In 1948, Dennis Gabor, a British scientist, developed a method of recording and producing three-dimensional images of objects through interference phenomena of coherent light known as holography. In Greek, 'holo' means 'whole' or 'complete', 'holography' means 'complete recording' i.e., the intensities and phase of the waves that come from the objects are recorded. In 1971, he received noble prize for his efforts.

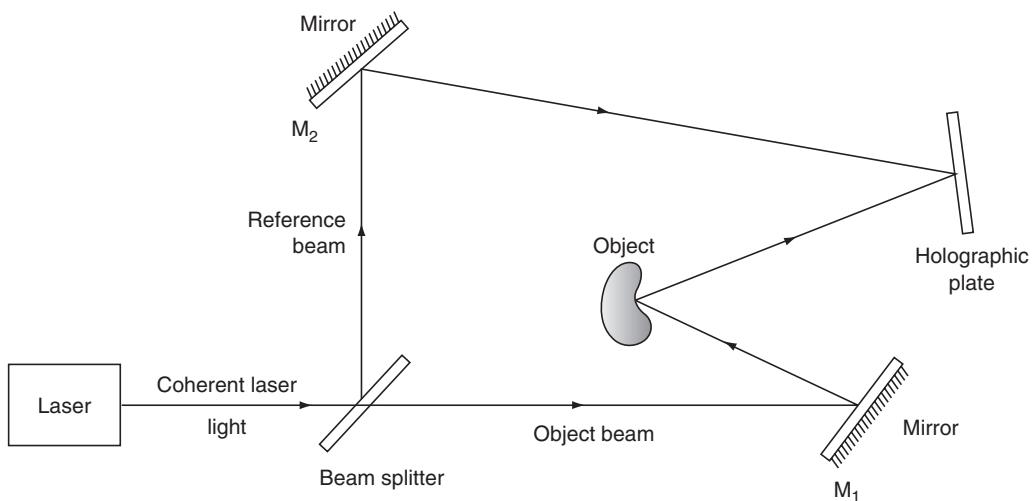
### 12.2 Basic principle of holography

An object is illuminated with a beam of coherent light [object beam]. Then every point on the surface of the object acts as a source of secondary waves. These secondary waves spread in all directions. Some of these waves are allowed to fall on a recording plate [holographic plate]. Simultaneously, another beam of same coherent light [reference beam] is allowed to fall on this holographic plate. In the holographic plate, both the beams combine and interference pattern will be formed. This interference pattern is recorded on the holographic plate. The three-dimensional image of the object can be seen by exposing the recorded holographic plate [hologram] to coherent light. This is the principle of holography.

### 12.3 Recording of image on a holographic plate

Figure 12.1 shows the method of recording a image on a holographic plate. The monochromatic light from a laser has been passed through a 50% beam splitter so that the amplitude division of the incident beam into two beams takes place. One beam falls on mirror  $M_1$  and the light reflected from  $M_1$  falls on the object. This beam is known as an object beam.

**Figure 12.1 Recording of hologram**

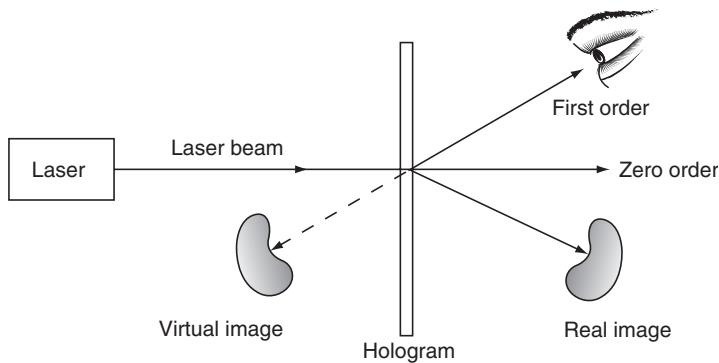


The object scatters this beam in all directions, so that a part of the scattered beam falls on the holographic plate. The other beam is reflected by mirror  $M_2$  and falls on the holographic plate. This beam is known as reference beam. Superposition of the scattered rays from the object and the reference beam takes place on the plane of the holographic plate, so that interference pattern is formed on the plate and it is recorded. The recorded interference pattern contains all the information of the scattered rays i.e., the phases and intensities of the scattered rays. For proper recording, the holographic plate has to be exposed to the interference pattern for a few seconds. After exposing, the holographic plate is to be developed and fixed as like in the case of ordinary photograph. The recorded holographic plate is known as hologram or Gabor zone plate. The hologram does not contain a distinct image of the object. It contains information in the form of interference pattern.

## 12.4 Reconstruction of image from a hologram

As shown in Fig. 12.2, the hologram is exposed to the laser beam [that used during construction or identical to the reference beam used for construction] from one side and it can be viewed from the other side. This beam is known as reconstruction beam. The reconstruction beam illuminates the hologram at the same angle as the reference beam. The hologram acts as a diffraction grating, so constructive interference takes place in some directions and destructive interference takes place in other directions. A real image is formed in front of the hologram and a virtual image is formed behind the hologram. It is identical to the object and hence it appears as if the object is present. The three-dimensional effect in the image can be seen by moving the head of the observer. During recording, the secondary waves from every point of the object reach complete plate. So, each bit of the plate contains complete information of the object. Hence, image can be constructed using a small piece of hologram.

**Figure 12.2** Image reconstruction



## 12.5 Applications of holography

1. The three-dimensional images produced by holograms have been used in various fields, such as technical, educational also in advertising, artistic display etc.
2. Holographic diffraction gratings: The interference of two plane wavefronts of laser beams on the surface of holographic plate produces holographic diffraction grating. The lines in this grating are more uniform than in case of conventional grating.
3. Hologram is a reliable object for data storage, because even a small broken piece of hologram contains complete data or information about the object with reduced clarity.
4. The information-holding capacity of a hologram is very high because many objects can be recorded in a single hologram, by slightly changing the angle between reference beam and holographic plate. For each different angle, different images can be stored.
5. In hospitals holography can be used to view the working of inner organs three dimensionally. i.e., the beating of the heart, the foetus of the pregnant lady and flowing blood based on motion holography.
6. Holographic interferometry is used in non-destructive testing of materials to find flaws in structural parts and minute distortions due to stress or vibrations, etc. in the objects.
7. Holography is used in information coding.

### Multiple Choice Questions

1. Holography records \_\_\_\_\_ of light coming from an object. ( )
 

(a) intensities	(b) phases
(c) both a and b	(d) none of the above
2. Holography was discovered by ( )
 

(a) Dennis Gabor	(b) Einstein
(c) Newton	(d) Curie brothers

## 12-4 | Applied Physics

3. Through holography we can produce \_\_\_\_\_ dimensional images of objects. ( )  
(a) one (b) two  
(c) three (d) none of the above
4. Holography produces ( )  
(a) real images (b) virtual images  
(c) both a and b (d) none of the above
5. A recorded holographic plate contains information in the \_\_\_\_\_ pattern. ( )  
(a) interference (b) diffraction  
(c) both a and b (d) none of the above
6. In holography interference pattern is produced from ( )  
(a) object beam (b) reference beam  
(c) both a and b (d) none of the above
7. If a hologram breaks into pieces, then each piece can produce ( )  
(a) part of image (b) complete image  
(c) no image (d) none of the above
8. In the reconstruction of images from hologram, we get ( )  
(a) one real and one virtual image (b) two real images  
(c) two virtual images (d) large number of real and virtual images
9. The recorded holographic plate is known as ( )  
(a) hologram (b) Gabor zone plate  
(c) both a and b (d) none of the above
10. A hologram acts as a \_\_\_\_\_. ( )  
(a) diffraction grating (b) polariser  
(c) analyser (d) mirror
11. Holography has been used in ( )  
(a) to view the working of the inner organs of body in three dimensionally  
(b) in non-destructive testing of materials to find flaws  
(c) data storage  
(d) all the above
12. Information holding capacity of a hologram is ( )  
(a) limited (b) large (c) less (d) none of the above

### Answers

1. c      2. a      3. c      4. c      5. a      6. c      7. b      8. a      9. c      10. a      11. d      12. b

### Review Questions

1. What is the basic principle of holography? Explain. (Set-2–Sept. 2008)
2. How does one construct and reconstruct a hologram? (Set-2–Sept. 2008)



## CHAPTER

# 13

## Acoustics of Buildings and Acoustic Quieting

### 13.1 Introduction to acoustics of buildings

Acoustics deals with the origin, propagation and hearing of sound. Architectural acoustics deals with the design and construction of acoustically good buildings, music halls, sound recording rooms and movie theatres where the audience receive the best sound quality. In 1911, Wallace C. Sabine, professor of physics at Harvard university laid the foundations of acoustic engineering. Here, we see some definitions of sound:

- (i) *Tone*: A sound having a well-defined frequency is called tone. Suppose a fundamental tone has frequency  $f$ , then the frequencies  $2f, 3f, 4f\dots$  are called overtones or harmonics.
- (ii) *Pitch*: It is a physiological quantity, which produces a mental sensation that varies with frequency. The sound appears shrill at high frequencies and hoarse at low frequencies. Pitch will not depend on loudness or quality.
- (iii) *Timbre/quality*: It is the ability to distinguish between different sounds of the same frequency.
- (iv) *Intensity/loudness of sound*: It is a sensation perceived by the ear. It is measured by the amount of sound energy flowing through unit area of a section kept perpendicular to the direction of propagation of sound.
- (v) *Echo and reverberation*: These are reflected sound waves. A reflected sound wave that reaches the ear at least 100 ms later than the direct sound is called an echo. A reflected sound that reaches the ear within 60 ms after the original sound due to prolonged reflections, is called a reverberation.

### 13.2 Reverberation and time of reverberation

A sound produced inside a hall will propagate in all directions. Sound waves incident on the surfaces of walls, floor, ceiling and furniture inside a hall will be multiply reflected. A listener inside the hall will receive the sound waves directly from the source, as well as the reflected waves. As the source of sound is turned off, the

listener hears the sound with gradually reducing intensity for some time due to the persistence of sound by multiple reflections at different places in the room. The persistence of audible sound even after the source of sound is turned off is called reverberation.

The time taken by the sound intensity to fall to one millionth  $\left(\frac{1}{10^6}\right)$  of its initial intensity i.e., the intensity just before the source of sound is turned off, is called reverberation time.

### 13.3 Sabine's empirical formula for reverberation time

The following are Sabine's conclusions:

- The reverberation time is directly proportional to the volume ( $V$ ) of the hall.
- The reverberation time is inversely proportional to the coefficient of absorption of different materials and surfaces inside the hall.
- Reverberation time depends on the frequency of the sound waves, because absorption coefficient for most of the materials increases with frequency.

$$\therefore \text{Reverberation time, } T \propto \frac{\text{Volume of the hall, } V}{\text{Absorption of sound, } A}$$

$$\text{or } T = \frac{KV}{A} \text{ where } K = \text{proportionality constant, the value of } K \text{ is 0.161.}$$

$$\therefore T = 0.161 \frac{V}{A}$$

$$\text{where } A = \sum_1^n a_i S_i = a_1 s_1 + a_2 s_2 + \dots + a_n s_n,$$

where  $s_1, s_2, s_3, \dots, s_n$  are surface areas of different materials and  $a_1, a_2, a_3, \dots, a_n$  are their absorption coefficients respectively.

### 13.4 Sabine's reverberation theory for reverberation time

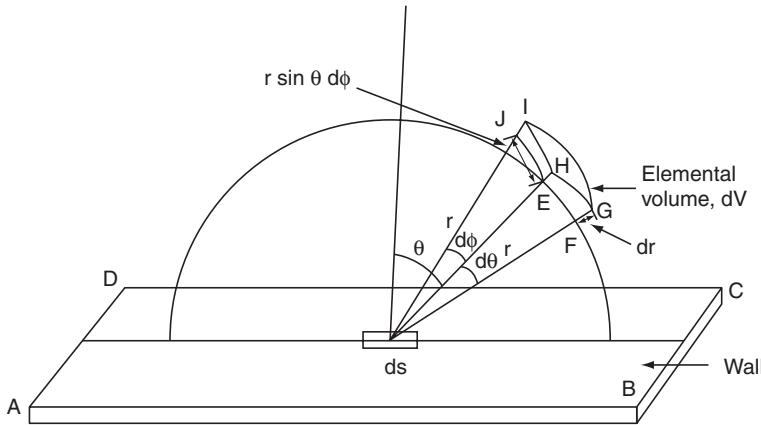
Sabine derived a mathematical equation for reverberation time by measuring the rise and decay of sound energy inside a closed hall. The following assumptions are considered in the derivation.

- The enclosure is a big one so that sound energy is uniformly distributed in it.
- Sound travels uniformly in all directions from the source.
- Absorption of sound energy by air is negligible.
- Standing wave formation is negligible.

When sound is produced inside a hall, the sound energy is spread uniformly inside the hall. As shown in Fig. 13.1, let us consider a small element of area as on the surface of a wall  $ABCD$ , on which sound energy is incident from different elemental volumes of the hall.

First, we consider the elemental volume  $EFGH$  of volume  $dV$ , on the surface of a hemisphere of radius  $r$ .

**Figure 13.1** Volume element at a distance  $r$  from  $ds$  on the surface of wall ABCD



The origin of the hemisphere is at the centre of  $ds$ . The rate of sound energy absorbed by  $ds$  due to  $dV$  is determined as follows:

Let the arc length  $EF$  of elemental volume  $dV$  be  $rd\theta$  and its thickness  $FG$  be  $dr$  as shown in Fig. 13.1. The face  $EFGH$  of area  $rd\theta dr$  is rotated about the normal (along  $E$  to  $J$ ) through an angle  $d\phi$ . The distance moved by this area will be the circumferential length  $r \sin \theta d\phi$ .

$\therefore$  The volume of the element,  $dV = \text{Area of face } EFGH \times \text{length } EJ$  (approximately)

$$= (rd\theta dr) \times (r \sin \theta d\phi) = r^2 \sin \theta d\theta dr d\phi \quad (13.1)$$

If  $E$  is the energy per unit volume of the hall (i.e. energy density) then the energy in the element,

$$dv = Er^2 \sin \theta d\theta dr d\phi \quad (13.2)$$

This energy travels equally in all directions.

$$\text{The energy that travels per unit solid angle} = \frac{Er^2 \sin \theta d\theta dr d\phi}{4\pi} \quad (13.3)$$

$$\text{The solid angle subtended by } ds \text{ at } dV = \frac{ds \cos \theta}{r^2} \quad (13.4)$$

Therefore the sound energy that is received by

$$ds \text{ from } dv = \frac{Er^2 \sin \theta d\theta dr d\phi}{4\pi} \times \frac{ds \cos \theta}{r^2} = \frac{Eds}{4\pi} \sin \theta \cos \theta d\theta dr d\phi \quad (13.5)$$

In one second, the sound travels a distance of  $v$  equal to its velocity. So  $r = v$ . The amount of energy that reaches  $ds$  in unit time is obtained by integrating equation (13.5).

$$\begin{aligned} \text{Energy received at } ds &= \frac{Eds}{4\pi} \int_0^{2\pi} d\phi \int_0^v dr \int_0^{\pi/2} \cos \theta \sin \theta d\theta \\ &= \frac{Evds}{4\pi} \times 2\pi \times v \times \frac{1}{2} = \frac{Evds}{4} \end{aligned} \quad (13.6)$$

## 13-4 | Applied Physics

If  $\alpha$  is the absorption coefficient of the surface of wall, then the sound energy absorbed per second by  $ds$  is

$$= \frac{Evads}{4}$$

$\therefore$  The total energy absorbed by all surfaces in the hall

$$= \frac{Ev}{4} \sum \alpha ds = \frac{EvA}{4} \quad \text{_____ (13.7)}$$

Where  $A$  = Total absorption =  $\sum ads$

Again, to total energy in the room =  $EV$  where  $E$  = energy density

This total energy increases continuously as the source gives off energy continuously.

$$\therefore \text{The rate of growth of energy in the hall} = \frac{d}{dt}(EV) = V \frac{dE}{dt} \quad \text{_____ (13.8)}$$

### **Sound energy build up in the Hall:**

At any instant,

$$\left\{ \begin{array}{l} \text{The rate of growth} \\ \text{of energy in the hall} \end{array} \right\} = \left\{ \begin{array}{l} \text{Rate of supply of} \\ \text{energy by the source} \end{array} \right\} - \left\{ \begin{array}{l} \text{Rate of absorption} \\ \text{of energy by all} \\ \text{surfaces in the hall} \end{array} \right\}$$

$$\therefore \frac{VdE}{dt} = P - \frac{EvA}{4} \quad \text{_____ (13.9)} \quad (\text{where } P = \text{power of sound source})$$

$$\text{or } \frac{VdE}{dt} + \frac{VAE}{4} = P$$

$$\text{or } \frac{dE}{dt} + \frac{VA}{4V} E = \frac{P}{V} \quad \text{_____ (13.10)}$$

$$\text{Let } \alpha = \frac{vA}{4V} \quad \text{_____ (13.11)}$$

Equation (13.10) becomes

$$\frac{dE}{dt} + \alpha E = \frac{P}{V}$$

$$\text{or } \frac{dE}{dt} + \alpha E = \frac{4\alpha}{vA} P = \frac{4P\alpha}{vA} \quad \text{_____ (13.12)} \quad (\text{using equation (13.11)})$$

Multiplying both sides of equation (13.12) with  $e^{\alpha t}$

$$\left( \frac{dE}{dt} + \alpha E \right) e^{\alpha t} = \frac{4P}{vA} \alpha e^{\alpha t}$$

$$\frac{d}{dt} \left( E e^{\alpha t} \right) = \frac{4P}{vA} \alpha e^{\alpha t} \quad \text{_____ (13.13)}$$

Integrating equation (13.13) we have

$$E e^{\alpha t} = \frac{4P}{vA} e^{\alpha t} + K \quad (13.14)$$

where  $K$  is the constant of integration.

Using initial conditions,  $K$  can be extracted.

When  $t = 0, E = 0$

$$\text{So } 0 = \frac{4P}{vA} + K$$

$$\text{or } K = -\frac{4P}{vA} \quad (13.15)$$

Substituting (13.15) in (13.14)

$$E e^{\alpha t} = \frac{4P}{vA} e^{\alpha t} - \frac{4P}{vA}$$

Dividing throughout with  $e^{\alpha t}$ , we have

$$E = \frac{4P}{vA} - \frac{4P}{vA} e^{-\alpha t}$$

$$\text{or } E = \frac{4P}{vA} (1 - e^{-\alpha t})$$

$$\text{or } E = E_m (1 - e^{-\alpha t}) \quad (13.16)$$

$$\text{where } E_m = \frac{4P}{vA}$$

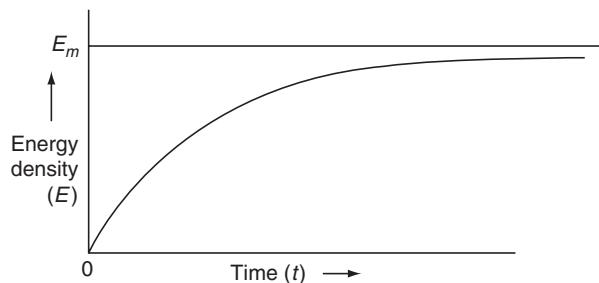
The growth of sound energy density  $E$  with time is shown in Fig. 13.2.

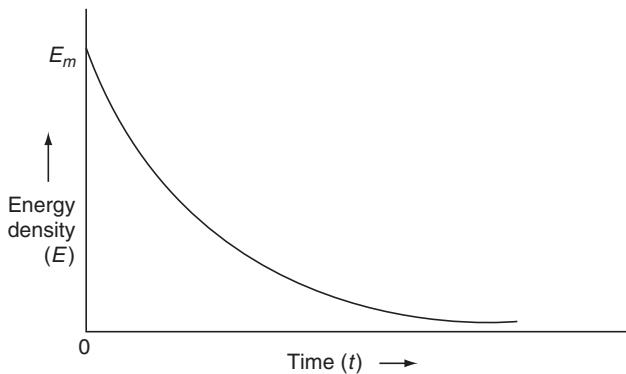
#### **Decay of sound energy in the hall:**

At steady state  $E = E_m$ . If the source of sound is cut off, then  $t = 0$  and  $p = 0$ . Equation (13.14) then becomes

$$E_m = 0 + K \quad \text{or} \quad K = E_m \quad (13.17)$$

**Figure 13.2 Growth of sound energy density in a hall**



**Figure 13.3 Decay of sound energy density**

Substituting equation (13.17) in equation (13.14), we have

$$Ee^{\alpha t} = E_m \quad \text{since } P = 0$$

$$\text{or } E = E_m e^{-\alpha t} \quad \text{_____ (13.18)}$$

The above equation shows the decay of sound energy density with time when the source of sound is turned off. A graph can be plotted between the sound density versus time as shown in Fig. 13.3.

#### *Sabine's formula*

According to the definition of reverberation time,  $T$ , we have

$$\frac{E}{E_m} = 10^{-6} \quad \text{at } t = T$$

From equation (13.18) we can write

$$\frac{E}{E_m} = e^{-\alpha t} = 10^{-6} \quad \text{at } t = T$$

Taking logarithms on both sides of above equation

$$\alpha T = 6 \log 10 = 6 \times 2.3026$$

$$\text{Substituting } \alpha = \frac{vA}{4V}$$

$$\alpha T = \frac{vA}{4V} T = 6 \times 2.3026$$

Taking  $v$  = Velocity of sound in air = 344 m/s

$$T = \frac{4 \times 6 \times 2.3026 V}{344 \times A}$$

$$\text{or } T = \frac{0.161 V}{A} \quad \text{_____ (13.19)}$$

This is Sabine's formula for reverberation time.

Equation (13.19) is applicable for large halls; when the average absorption coefficient is less than 0.2. Eyring's formula gives correct results for all values of  $a$ . It is given as  $T = \frac{0.161 V}{S \ln(1-a)^{-1}}$

For a dead room (where  $a = 1$ )

$$\text{we have } T = \frac{0.161 V}{S \ln(1-1)^{-1}} = \frac{0.161 V}{S \ln(\alpha)} = 0$$

## 13.5 Absorption coefficient of sound and its measurement

The absorption coefficient ( $a$ ) of a material is defined as the ratio of sound energy absorbed by its surface to that of the total sound energy incident on the surface.

$$\text{i.e Absorption coefficient } (a) = \frac{\text{Sound energy absorbed by the surface}}{\text{Sound energy incident on the surface}}$$

An open window is considered as an ideal absorber of sound. The unit of sound absorption is open window unit or Sabin. A  $1\text{m}^2$  Sabine is equal to the amount of sound energy that is absorbed or passed through one square metre area of open window. Table 13.1 given below shows the absorption coefficients of different materials.

### Measurement

The reverberation time inside a room are measured without and with a standard large sample of material. Let the reverberation time be  $T_1$  and  $T_2$  respectively. By using Sabine's formula we have

$$\frac{1}{T_1} = \frac{A}{0.161 V} = \frac{\Sigma aS}{0.161 V} \quad \text{and} \quad \frac{1}{T_2} = \frac{\Sigma aS + a_s S_s}{0.161 V}$$

**Table 13.1: Sound Absorption Coefficient of Different Materials**

Material	Absorption coefficient per $\text{m}^2 500 \text{ Hz}$
Open window	1.00
Fibre glass	0.75
Human body	0.50
Fibre board	0.55
Heavy curtains	0.50
Carpet	0.30
Straw board	0.30
Asbestos	0.26
Cork	0.23
Concrete	0.17
Marble	0.01

Where  $\alpha_s$  is the absorption coefficient of the sample and  $S_s$  is the surface area of the sample. From the above equations we have,

$$\frac{1}{T_2} = \frac{1}{T_1} = \frac{\alpha_s S_s}{0.161V} \quad \text{or} \quad \frac{0.161V}{S_s} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)$$

Using the above equation,  $\alpha_s$  can be determined.

## 13.6 Basic requirements of an acoustically good hall

The following are the conditions for an acoustically good hall:

- (i) The speech or music carried on the dias should be clearly audible to all the participants.
- (ii) The syllables should be clear without overlap.
- (iii) The loudness, intensity and quality of sound should be uniform and sufficiently high throughout the hall.
- (iv) The boundaries should be sufficiently provided with sound proofs to exclude the sounds produced outside the theatre or auditorium.
- (v) Echoes, interference, resonance and echelon effects should not occur in the hall.
- (vi) Proper reverberation time should be maintained. For music the reverberation time should be 1 to 2 seconds and for speech it should be 0.5 to 1 second.
- (vii) Whether the hall is fully or partially filled with audience, the quality of music heard should be unchanged.
- (viii) The hall must be full of audience.
- (ix) Sound should not be concentrated towards any part of the hall.

## 13.7 Factors affecting architectural acoustics and their remedies

In an acoustically good hall, every syllable or musical note reaches an audible level of loudness at every point in the hall and then quickly dies away to make place for the next syllable. Any deviation from this makes the hall acoustically defective. Architectural acoustics depends on the volume of the hall and the surface materials such as chairs and curtains that are present inside. Some of the factors that affect the architectural acoustics are given below.

- (i) Reverberation:** Large reverberation causes overlapping of successive sounds, this causes loss in clarity of hearing. On the other hand, low reverberation causes inadequate loudness. Reverberation determines the speed of sound decay in a hall. A very short reverberation time makes a room dead. Thus the time of reverberation for a hall should neither be too large nor too small, it must have a definite value that satisfies the speaker and the audience. This is known as optimum reverberation. Practically, it was found that the time of reverberation depends on size of the hall, loudness of sound and the type of sound [speech or music] in the hall. For music, reverberation adds to the fullness of tone, blended sound and richness of bass frequencies. The optimum reverberation time at a frequency of 512 Hz for a small hall will be between 1 and 1.5 seconds, while for large halls it will be upto 2.3 seconds. A reverberation time of 0.5 seconds is acceptable for speeches and lectures. Reverberation can be controlled by the following factors:

- (a) By closing or opening doors, windows and ventilators, the time of reverberation can be made optimum.
- (b) By using heavy curtains with folds.
- (c) By covering the walls of the hall with sound-absorbing materials such as glass wool, thermocole, fibre board, card board and felt. The sound absorbing materials should have porous structure and a rough surface.
- (d) By covering the floor with carpets.
- (e) By having a full-capacity audience, since audience also contribute to the absorption of sound.

**(ii) Adequate loudness:** A short reverberation time achieved by using large absorbing materials will minimise the chances of confusion between different syllables of sound. However the loudness of the sound will drop below the level of hearing. Sufficient loudness should be perceived at every portion of the hall for satisfactory hearing by the audience. Loudness can be increased in the following ways:

- (a) By providing good quality loud speakers.
- (b) By using large polished reflecting surfaces and sounding board, behind the speaker and facing the audience.
- (c) Low ceilings are also help in reflecting sound towards the audience.

**(iii) Focusing due to walls and ceilings:** Inside the hall, if there are any focusing surfaces (curved surfaces), such as concave, spherical, cylindrical or parabolic surfaces on the walls, ceilings or on the floor of the hall, then sound is concentrated at their focus regions. Hence, no sound reaches the other regions of the hall, causing poor audibility. There should be no interference of direct and reflected waves, because it produces maximum sound at some places and minimum sound at other places. This non-uniform distribution of sound intensity is unwanted and hence correction is required. For uniform distribution of sound energy the following points are to be taken into account.

- (a) No curved surfaces should be present inside the hall. If they are present, they should be covered with absorbent material.
- (b) A paraboloidal surface behind the speaker may send uniform reflected sound across the hall.
- (c) The ceiling should be low.

**(iv) Echoes:** Echo is a reflected sound, coming from a long distance, so that it reaches the listener later than  $\frac{1}{7}$  second of direct sound wave from the source. The echoes causes confusion. These can be avoided by covering the long distant walls and high ceiling with absorbent material. The surface of the wall should be roughened but not polished.

**(v) Echelon effect:** A musical note produced due to the combination of echoes having regular phase difference is known as Echelon effect. The reflected sound waves from regularly spaced reflecting surfaces such as equally spaced stair cases or a set of railings produce musical note due to the regular succession of echoes of the original sound to the listener. This makes of the original sound confused or unintelligible. This may be avoided by forming the staircases with unequal spacings between them, and covering them with sound absorbing materials like carpet.

**(vi) Resonance:** Some times window panes, loosely fitted wooden portions, wall separators, hollows and crevices start vibrating by absorbing the sound produced in the hall. These may create sound. Certain tones of the original music and the created sound combine to produce an interference such that the original sound gets distorted. This effect can be suppressed by hanging a large number of curtains in the hall.

**(vii) Noise:** Generally there are three types of noise. They are (a) air-borne noise, (b) structure-borne noise and (c) inside noise. These are explained below:

(a) Air-borne noise: The noise that enters the hall from outside through open windows, doors and ventilators is known as air-borne noise. The method of reducing this is given below.

- (1) By using heavy glass doors, windows and ventilators.
- (2) By using double-wall doors and windows with insulating material in between them.
- (3) Forming double wall construction.
- (4) By fixing doors and windows at proper places
- (5) Air conditioning the hall and sealing the openings perfectly.

(b) Structure-borne noise: The noise that reaches through the structures of buildings are known as structural noise. The activity around the building may cause a structural vibration of the building. For example, foot steps, operating machinery, street traffic, etc. The remedy for this is given below.

- (1) By using double walls with air space in between them.
- (2) By using anti-vibration mounts.
- (3) By properly insulating the equipments such as refrigerators, lifts, fans, etc.
- (4) By using carpets on the floor.

(c) Inside noise: The noise produced inside big halls or offices due to equipment such as air conditioners, type writers and fans are called inside noise. This noise may be minimised as follows:

- (1) Placing the machinery on sound absorbent pads.
- (2) Using noise-free air conditioners.
- (3) Covering the floor with carpets.
- (4) Covering the floor, walls and ceiling with sound absorbing materials.

## 13.8 Acoustic quieting

### Introduction

The vibrations of machinery produces sound waves in air, hydro-acoustic waves in liquids and produces mechanical stress in solid matter. The hydro-acoustic waves coming from submarines make them easy to be detected by sonar. One of the major military goal is to prevent the detection of submarines by sonar. For this the subject of acoustic quieting has been developed. Acoustic quieting deals with the suppression of sound coming from machinery by damping the vibrations or by absorbing the vibrational energy coming from them, or by redirecting the waves coming towards observer, so that the observer is free from machinery disturbances. This technology has been extended to many industries and products, such as computers and automobiles.

### Aspects of Acoustic Quietting

There are a number of aspects of acoustic quieting. The aim of each aspect is to minimise the noise received by an observer. Various aspects of acoustic quieting are given below.

- (i) **Noise generation:** This is to minimise the noise at the source, for example, use of plastic gears reduce the noise producing effects of the impact between teeth.
- (ii) **Sympathetic vibrations:** This should decouple the acoustic waves.

- (iii) **Resonations:** Resonations can be suppressed by acoustic damping or by changing the stiffness and size of the resonator. In case of machines, to suppress resonance, the running speed can be changed.
- (iv) **Sound transmissions:** Different methods are used to reduce sound transmission. The selection of these methods depends on the transmission medium such as air, liquid or solid.
- (vi) **Sound reflections:** Reflection of sound can be reduced by using acoustic absorption (deadening) materials, trapping the sound and providing window for the sound to go out. An acoustic scientist can use various methods to quieten the machine. This quieting might be tested by changing materials of source, using damping material, isolating the machine, running the machine in vacuum or running it at low speed.

## 13.9 Methods of quieting

The various methods of quieting are given below

- (i) **Sound isolation:** Here, the transferring of sound (noise) and vibrational energy from one area to another is prevented by using sound control barriers made of deadening materials like fibre glass or synthetic rubber. Machines can be mounted on isolating springs to reduce the transmission of vibration to the floor surfaces and to the building structure. In the construction of homes and offices, sound control barriers (fibre glass) are placed in the walls to arrest the transmission of noise. An enclosure may be successful in reducing noise level, but the noise energy would be bottled up within the enclosure due to high reverberation. This can be reduced by lining the inside walls of the enclosure with sound-absorbing materials.
- (ii) **Noise absorption:** The unwanted sounds or noise that are produced inside a room can be made to be absorbed by suitable materials; instead of being reflected towards the listener. Thus the listener receives only the direct sound but not echo reflections. For example, sound proofing rooms are constructed using acoustic tiles for recording studios.
- (iii) **Acoustic damping:** Damping mounts have been used to suppress the vibrations in many degrees of freedom. The damping materials prevent the vibrations from being transferred to another material. Motors and rotating shafts are fitted with damping mounts. These are used at the points where they are in contact such as with a building or the chassis of a large machine.
- (iv) **Acoustic decoupling:** Some of the machine parts like frame, chassis or external shaft are built in such a way that they keep receiving unwanted vibrations from a moving part due to acoustic decoupling.
- (v) **Preventing stalls:** Whenever a machine enters into an aerodynamic stall, it will suddenly vibrate. The motion of fan blades through the air is the main source of energy in the aerodynamic state.
- (vi) **Preventing cavitation:** There is a large chance for a machine to undergo cavitation when it is in contact with a fluid. The rapid formation and vanishing of bubbles produce noise. The cavitation of screws in ships and in submarines may facilitate their detection through the sonar.
- (vii) **Preventing water hammer:** The abrupt opening and closing of valves present in a water hammer may generate considerable noise in hydraulics and in plumbing.
- (viii) **Shock absorption:** The shock absorbers present in vehicles prevent mechanical shocks from reaching the passengers. They receive quieting shocks also.

**(ix) Reduction of resonance:** Every object vibrates with its natural frequency. Many parts of a machine vibrate and produce waves. These waves resonate and form noise.

**(x) Material selection:** The transmission of sound and vibrations can be minimized by using non-metallic components in place of metal components. This reduces noise. In some cases air can be removed from a machine and hermetically sealed. The vacuum inside the machine will arrest noise transmission.

## 13.10 Quieting for specific observers

- (i) *Under-water acoustics:* All the quieting methods are applicable to submarines. Submarines are operated below the depth of the sound-channel axis, where the speed of sound in water is the lowest. So a submarine can escape being detected by surface ships.
- (ii) *Sound refraction:* Similar to submarines, sound refraction can be used to prevent certain observers from hearing the noise. For example an outdoor observer close to the ground will receive sound waves refracted towards him when the ground is cooler than ambient air, but the sound waves will refract away when the ground is hotter than ambient air.
- (iii) *Sound redirection:* The observer placed out of the path of sound of the highest amplitude will receive much quieter sounds. For example, the sound is loudest in line with a jet's exhaust. Perpendicular to the exhaust, the sound is significantly quieter.
- (iv) *Hearing Protection:* In highly noise-polluted regions such as open air firing region or airport region, an observer wearing ear plugs may receive less sound.
- (v) *Electronic quieting:* Noise can be controlled using electronic methods. A few devices used for electronic quieting are mentioned below.
  - (a) **Electronic vibration control:** Electronics, sensors and computers are now employed to reduce vibration. Using high speed logic, vibration can be damped quickly and effectively by encountering the motion before it exceeds a certain level.
  - (b) **Electronic noise control:** The noise can be reduced by using phase cancellation, employing electronics, sensors and computers. This method is used in active sound generating devices such as loudspeakers.

## 13.11 Muffler (or silencer)

A muffler is a device for reducing the noise emitted by a machine. After internal combustion in engines the exhaust comes out through the muffler. A muffler is a long straight cylindrical barrel that merges perfectly at the end of the exhaust pipe. In internal combustion engines, the muffler (or silencer) is parallel to the fire-arm suppressor. The exhaust system of an internal combustion engine contains an exhaust pipe and muffler to reduce its exhaust noise. The muffler accomplishes with a resonating chamber, which is specifically tuned to cause destructive interference of sound waves. Mufflers reduce back pressure relative to earlier models, such that the engine efficiency, performance and power output are increased. They reduce the wear and tear of engine components and control sound levels.

There are two different type of silencers. They are (i) dissipative (or absorptive) and (ii) reactive silencers.

- (i) In dissipative silencers, acoustic energy is converted into heat by the sound absorbing process. Because of the frequency characteristics of the absorbing materials, it is more effective at medium and high frequencies.
- (ii) Reactive silencers provide an impedance mismatch to the sound waves, causing reflection back towards the source. This causes destructive interference to particular frequencies. It is more effective at low frequencies.

In addition to the above we have mini mufflers. They can be fixed in the place of a normal muffler in a car exhaust system to increase the sound of the exhaust. These are smaller in size.

In cars, a muffler can be fixed length wise in such a way that it blows the exhaust backwards to the rear end, or to the sides before the side wheels. In motor cycles, mufflers are placed beside the engine and the rear wheel, blowing exhaust backwards. In large diesel-powered trucks, the muffler is mounted vertically behind the cab or crosswise under the front of the cab, blowing sideways.

## 13.12 Sound proofing

The process of reducing sound pressure with respect to sound source and the receptor is known as sound proofing. There are different ways of reducing the intensity of sound. They are: increasing the distance between the source and the receiver, keeping a noise barrier to block and absorb the sound energy, using damping structures such as sound baffles or antinoise sound generators, etc. Some of these methods are described below.

(i) *Distance*: The dissipation of sound is proportional to distance. Hence the intensity of sound felt by an observer decreases progressively as the receiver moves away from the source of sound. If any intervening objects are present, they absorb part of the sound energy and vibrate. The dissipation of sound energy also depends on the weather and reflections from the soil.

(ii) *Damping*: During damping the sound energy is converted into heat. Damping can be achieved by adding a layer of material, such as lead or neoprene, which is heavy and soft. This will act as a sound deadening layer. However, since lead and neoprene are costly, a dry wall such as quiet rock is used. Acoustic damping can be obtained by using acoustic foam on the face of the wall or ceiling. Noise damping can be obtained by passing sound waves through different layers of material with different densities. Multiple foam cell air pocket is also used for damping.

(iii) *Noise barriers as exterior sound proofing*: Along major highways, noise barriers are used to protect adjacent residents from road way noise. The noise barriers used may be constructed with wood, masonry, earth or some combination thereof.

(iv) *Noise cancellation*: This is a modern technique. In this, a microphone receives the sound and is analysed by a computer. Then, sound waves with opposite phase (at all frequencies) are produced through a speaker. This produces destructive interference and suppresses a lot of noise.

(v) *Residential sound proofing*: This sound proofing is done mainly reduce or eliminate the effects of exterior noise. Usually, curtains are used to damp sound that enters through doors and windows. Air chambers known as honey combs are also used. To have higher degree of damping, single-, double- and triple honey comb designs are used. Double pane windows give better damping than single pane windows.

(vi) *Room within a room*: In houses, vibrations pass directly through the brick, woodwork and other solid structural elements. The use of acoustic foam and other absorbent materials have no impact on transmitted vibration. Ideal de-coupling eliminates vibrational transfer both in solid material and in air. One method of eliminating the transmittal of sound is to construct a room within a room.

## Formulae

$$(1) \text{ Reverberation time, } T = 0.161 \frac{V}{A} \text{ where } A = \sum_i^n a_i S_i$$

$$(2) \text{ Sound absorption coefficient, } \alpha = \frac{0.161}{S_s} \left[ \frac{1}{T_2} - \frac{1}{T_1} \right]$$

## Solved Problem

1. The volume of a hall is  $2265 \text{ m}^3$  and its absorption is equal to  $92.9 \text{ m}^2$  of open window. If the hall is filled with audience, then the absorption becomes double. Find the reverberation time when the hall is without and with audience.

**Sol.** The Sabines formula for reverberation time is

$$T = \frac{0.161V}{A} \quad \text{where } A = \text{total absorption in the hall}$$

$V$  = volume of hall

$$A = 92.9 \text{ m}^2 \text{ of open window}$$

$$V = 2265 \text{ m}^3$$

$$\therefore \text{Reverberation time of hall without audience, } T_1 = \frac{0.161 \times 2265}{92.9} = 3.9 \text{ seconds}$$

and

$$\text{Reverberation time of hall with audience, } T_2 = \frac{0.161 \times 2265}{92.9 \times 2} = 1.95 \text{ seconds}$$

## Multiple Choice Questions

1. Acoustics deals with \_\_\_\_\_ of sound. ( )  
(a) origin                    (b) propagation                    (c) hearing                    (d) all the above
  2. Architectural acoustics deals with ( )  
(a) design of acoustically good buildings.  
(b) construction of acoustically good buildings.  
(c) Both a and b.  
(d) None of the above.
  3. A reflected sound that reaches the ear within \_\_\_\_\_ after the orginal sound, due to prolonged reflections is called reverberation. ( )  
(a) 60 milliseconds            (b) 600 milliseconds            (c) 1 second                    (d) 2 seconds
  4. The time taken for the intensity of sound to fall to \_\_\_\_\_ of its initial intensity is called reverberation time. ( )  
(a)  $\frac{1}{10^3}$                     (b)  $\frac{1}{10^2}$                     (c)  $\frac{1}{10^4}$                     (d)  $\frac{1}{10^6}$

5. Inside a big hall, the reverberation time is \_\_\_\_\_ of the hall. ( )
- (a) directly proportional to volume
  - (b) inversely proportional to sound absorption
  - (c) Both a and b
  - (d) None of the above.
6. If the total volume of hall is  $V$  and its total absorption is  $A$ , then the expression for reverberation time is ( )
- (a)  $0.161 \frac{V}{A}$
  - (b)  $0.161 \frac{A}{V}$
  - (c)  $0.161AV$
  - (d)  $\frac{0.161}{AV}$
7. While deriving an expression for reverberation time, Sabine assumed that ( )
- (a) the enclosure should be big.
  - (b) standing wave formation is negligible.
  - (c) sound absorption by air is negligible.
  - (d) All the above.
8. The unit of coefficient of sound absorption is ( )
- (a) Sabine
  - (b) open window unit
  - (c) a or b
  - (d) None of the above
9. The sound absorption coefficient of human body is ( )
- (a) 0.75
  - (b) 0.50
  - (c) 0.25
  - (d) 1.00
10. The basic requirement for an acoustically good hall is: ( )
- (a) Echoes, interference, resonance and echelon effects should not occur in the hall.
  - (b) The reverberation time for speech should be 0.5 to 1 second and for music it should be 1 to 2 seconds.
  - (c) There should not be concentration of sounds at any part of the hall.
  - (d) All the above.
11. For optimum architectural acoustics, the following factors should be considered: ( )
- (a) The time of reverberation for a hall should neither be too large nor too small.
  - (b) Sufficient loudness at every portion of the hall
  - (c) Reduction of air-borne, structure-borne and inside noise
  - (d) All the above.
12. Noise that enters into a hall from the outside through \_\_\_\_\_ is known as air-borne noise ( )
- (a) open windows
  - (b) open doors
  - (c) open ventilators
  - (d) All the above.
13. Air-borne noise can be reduced by ( )
- (a) forming a double wall construction.
  - (b) by using heavy glass doors, windows and ventilators.
  - (c) by using double wall doors and windows.
  - (d) All the above.
14. Structure-borne noise can be reduced ( )
- (a) by using anti-vibrating mounts.
  - (b) by using double walls with air space in between them.
  - (c) by properly insulating refrigerators, lifts, fans, etc.
  - (d) All the above
15. Noise produced due to air conditioners, typewriters, fans etc. present inside a hall is called ( )
- (a) structure-borne noise
  - (b) inside noise
  - (c) air-borne noise
  - (d) All the above.

## 13-16 | Applied Physics

16. Acoustic quieting deals with the suppression of sound coming from machinery by ( )  
(a) damping the vibrations. (b) absorbing the vibrational energy.  
(c) redirecting the waves coming towards observer. (d) All the above.
17. The aspect of acoustic quieting is \_\_\_\_\_ of noise received by an observer. ( )  
(a) minimisation (b) maximisation (c) optimisation (d) All the above.
18. Acoustic quieting can be obtained ( )  
(a) by minimising the noise at the source.  
(b) by generating sympathetic vibrations.  
(c) by reducing sound transmission and sound reflection using acoustic absorption materials.  
(d) All the above.
19. Acoustic quieting can be achieved ( )  
(a) by sound isolation. (b) by using acoustic tiles.  
(c) by using damping mounts. (d) All the above.
20. Hearing protection is used ( )  
(a) in a highly noise polluted region. (b) an airport region.  
(c) an open air firing region. (d) All the above.
21. A muffler ( )  
(a) is a device for reducing the noise emitted by a machine.  
(b) accomplishes with a resonating chamber, which is tuned to cause destructive interference of sound waves.  
(c) Both a and b.  
(d) None of the above.
22. The process of reducing the sound pressure with respect to sound source and the receptor is known as ( )  
(a) acoustic quieting (b) sound proofing (c) reverberation (d) None of the above.
23. Sound proofing can be achieved ( )  
(a) by moving the receiver away from the source of sound.  
(b) by damping the sound using acoustic foam, lead or neoprene on the face of the wall or ceiling.  
(c) by using noise cancellation.  
(d) All the above.

### Answers

1. d      2. c      3. a      4. d      5. c      6. a      7. d      8. c      9. b      10. d      11. d      12. d  
13. d      14. d      15. b      16. d      17. a      18. d      19. d      20. d      21. c      22. b      23. d

### Review Questions

- (1) Write an essay about the acoustics of buildings.
- (2) Derive Sabine's mathematical relation for reverberation time.
- (3) Explain reverberation and reverberation time.
- (4) Define and explain the sound absorption coefficient of materials.

- (5) What are the basic requirements of an acoustically good hall?
- (6) Explain the various factors that affect architectural acoustics. What are their remedies?
- (7) What is acoustic quieting ? What are the different aspects of acoustic quieting?
- (8) Explain the various methods of acoustic quieting.
- (9) Write notes on quieting for specific observers.
- (10) What is sound proofing? Explains the different methods of sound proofing.

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## CHAPTER

# 14

## Nanotechnology

### 14.1 Basic principle of nanoscience and nanotechnology

Nanotechnology is the extension of existing science into the nanoscale. It pushed towards microminiaturization. The word ‘nano’ means ‘one-billionth’, ( $10^{-9}$ ). Feynman, a noble laureate in physics, brought this nanotechnology into daylight by delivering lectures in 1959. Nanoscience is the study of the fundamental principles of molecules and structures having sizes in between 1 and 100 nm. These are known as nanostructures. The 20th century scientists called this as top-down science. The physical, chemical, biological properties associated with the nanostructures constituted from atoms and molecules is known as bottom-up process. The top-down process refers to machining and etching techniques and the bottom-up process refers to building organic and inorganic structures atom-by-atom or molecule-by-molecule.

Nanotechnology deals with the design, manufacturing and applications of nanostructures in useful nanoscale devices such as electronic circuits and mechanical devices at the molecular level. These are the smallest solid things possible to make. In nanotechnology, the fundamental properties of materials and machines depend on their size. For example, a nanoscale wire or circuit component does not necessarily obey Ohm’s law.

The principle of the nanoscale science and engineering refers to the fundamental understanding and technological advances from the exploitation of new physical, chemical, electrical and biological properties of systems having size in between molecules [or atoms] and bulk materials. Nanotechnology refers to the field of applied science and technology that deals with the fabrication of devices or materials which lie in the sizes of 1 to 100 nm.

Through nanotechnology, we can understand many new things. For example, if we properly arrange carbon atoms in coal then it may become diamond. By rearranging atoms in sand, silicon chip can be made. Single atom manipulation has been known in late 1980s using the scanning tunneling microscope (STM). The probe of the STM is as sharp as an atom at the tip. The distance between the tip and the flat surface of the specimen is nearly 1 nm and kept constant by monitoring the tunneling current. By applying a voltage pulse in this condition, a single atom can be extracted from the surface of the specimen and then placed at a desired position. The STM is also useful for manipulating single molecules, observing molecular shapes, microfabrication technology for

semiconductor devices and bio-chemical technology. Nanotechnology produces materials that are built up atom-by-atom. With carbon atoms tubular molecules are made and they are called carbon nanotubes. Spherical molecules with 60 carbon atoms having a diameter slightly less than 1 nm can also be made and these are called bucky balls or fullerenes. The factors that differentiate nanomaterials from bulk materials is the increase in surface area to volume ratio and quantum confinement effects. These are explained below.

**(a) Surface area to volume ratio:** This value is very large for nanomaterials. To understand this concept, consider a spherical material of radius 'r' then:

$$\frac{\text{Surface area of the sphere}}{\text{Volume of the sphere}} = \frac{4\pi r^2}{\left(\frac{4}{3}\right)\pi r^3} = \frac{3}{r}$$

As the size of the sphere decreases, the above ratio increases. Alternatively, if the material is cubic, as it is divided into small cubes, then also the surface area to volume ratio increases. Hence, the nanomaterials possess large value of surface area to volume ratio as compared to the bulk material.

**(b) Quantum confinement effects:** According to band theory, solid materials have energy bands and isolated atoms possess discrete energy levels. Nanomaterials are intermediate to the above two cases. For nanomaterials, if the dimensions of potential wells or potential boxes are of the order of the de Broglie wavelength of electrons or mean free path of electrons, then the energy levels of electrons change, and the electron will remain confined to a small region of the material. This is called quantum confinement.

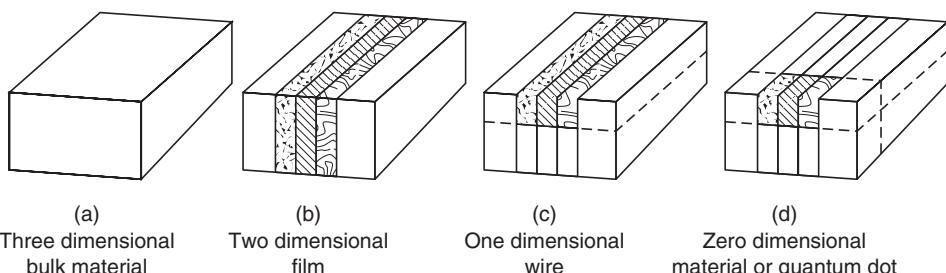
Nanomaterials are very strong, hard, wear resistant, corrosion resistant, erosion resistant and chemically active.

The electrons in bulk solid material possess alternatively discrete allowed and forbidden bands of energies. As the material changes from bulk to nanoparticle size, the energies of electrons change. A graph plotted between the density of electron states versus the energies of electrons for a bulk material is a parabola, whereas this is not the case for nanoparticle materials. The quantum effects are dominant in nanoparticle materials. So, we come across quantum dots, quantum wires and quantum wells (or quantum films) in nano-science. They are zero, one and two dimensional nanoparticles. The concept of the above materials and their electron density states are illustrated below.

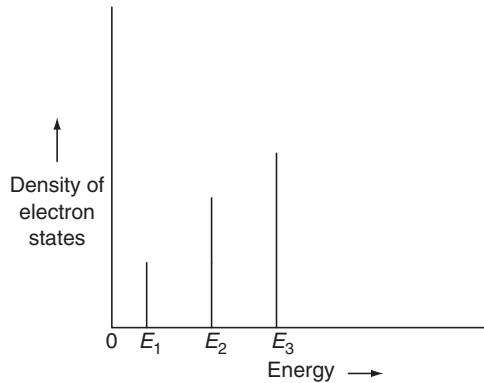
When a bulk nanoparticle material is reduced in one, two and three dimensions to nanometers then it results in the formation of quantum film, quantum wire and quantum dot as shown in Fig. 14.1.

Figure 14.1

Representation of quantum film, quantum wire and quantum dot in a bulk nanoparticle material



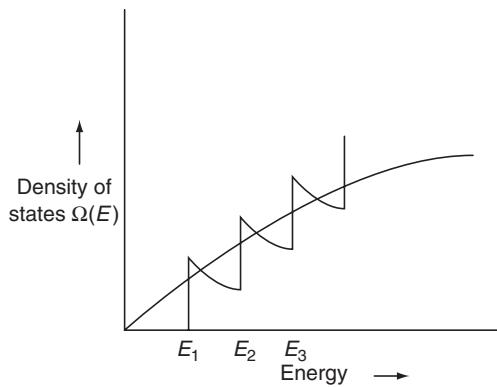
The energies of electrons in quantum dots appear as clusters. The density of electron states vary from cluster to cluster as shown in Fig. 14.2a.

**Figure 14. 2a** Density of electron states versus energy of electrons for quantum dots

In the case of quantum wires, the density peaks are high at energy values  $E_1$ ,  $E_2$ ,  $E_3$  ... and decrease rapidly for ranges in between as shown in Fig. 14.2b. The density of states

$$\Omega(E) dE = \frac{\sqrt{2m}}{\pi\hbar} \sum \left[ \frac{n_i H(E - E_i)}{\sqrt{E - E_i}} \right] dE$$

Where  $n_i$  is degeneracy factor and  $H(E - E_i)$  is the Heaviside function. The density of states is of the order of  $10^9/\text{m eV}$ .

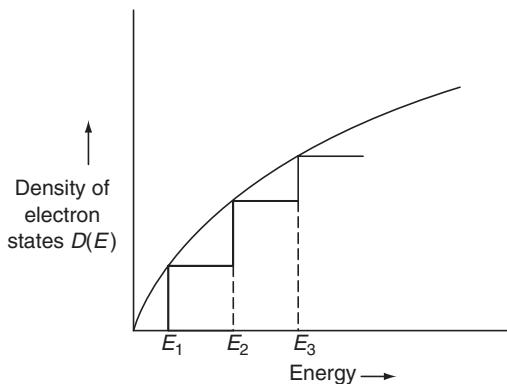
**Figure 14. 2b** Density of states versus energy of electrons for quantum wire

In quantum wells, the graph between density of electron states and energy is a step function as shown in Fig. 14.2c. The density of states

$$D(E) dE = \frac{m^*}{\pi\hbar^2} \sum H(E - E_i) dE$$

Where  $m^*$  = effective mass of electron and  $H(E - E_i)$  is a step function called the Heaviside function. This value is zero for  $E < E_i$  and 1 for  $E \geq E_i$ . The density of states is of the order of  $10^{18}/\text{m}^2 \text{ eV}$ . The locus of all corners of the step function is a parabola.

**Figure 14. 2c Density of electron states versus energy of electrons for quantum film**



## 14.2 Physical properties

At the macro scale, the physical and chemical properties are not dependent on the size of the material, but at the nanoscale every thing will change including colour, melting point and chemical properties. This is due to the difference in the nature of interactions between atoms in nanostructures and in bulk materials. Materials reduced to the nanoscale can suddenly show very different properties compared to what they exhibit on a macroscale. The various physical properties have been explained below:

### (i) Geometric structure

Large nanoparticles have the same crystal structure as that of the bulk material but different lattice parameters. In cluster nanoparticles, the structure is deviated. In nanomaterials, the surface to volume ratio increases. Similarly, the interatomic distance decreases by reducing the size of nanoparticles.

### (ii) Optical properties

Different-sized nanoparticles scatter different wavelengths of light incident on it and hence they appear with different colours. For example, nanogold doesn't act like bulk gold. The nanoscale gold particles can be orange, purple, red or greenish in colour depending on their grain size. The bulk copper is opaque whereas nanoparticle copper is transparent. Porous silicon exhibits red photoluminescence, but bulk silicon will not show this effect. In nanoparticle semiconductor elements (such as Ge, Si), a shift in optical absorption spectra (towards blue) have been observed. The electroabsorption effects are observed in CdTe quantum dots.

### (iii) Thermal properties

There is a change in thermal properties of some materials as they go from bulk to nanoparticles. A few of them are given below. The melting point of nanogold decreases from 1200 K to 800 K as the size of particles

decreases from  $300\text{\AA}$  to  $200\text{\AA}$ . The Debye temperature and ferroelectric phase transition temperature are lower for nanomaterials. The diffusion coefficient and solid state phase transition pressure are high for nanomaterials. At higher temperatures, there is breakdown in symmetry of nanoparticles due to high thermal vibrations of surface atoms in nanostructures. Superplasticity of nanomaterial occurs at lower temperatures by reducing the grain size. Stable aluminium becomes combustible in nanophase. Solid gold changes into liquid as it goes from bulk to nanomaterial at room temperature.

#### (iv) Magnetic properties

The magnetic properties of nanomaterials are different from that of bulk materials. In small ferromagnetic particles, the magnetic properties are different from that of bulk material. They are saturated magnets. In nanomaterials, we use single domains unlike large number of domains in bulk materials. The coercivity of single domain is very large. Small clusters [containing less than 80 atoms] of non-magnetic substances show spontaneous magnetic moment whereas in case of magnetic nanoparticles, the magnetic moment is reduced. For example, Fe, Co, Ni and Gd are ferromagnetic in bulk but they exhibit super paramagnetism in the nanophase. Na, K and Rh are paramagnetic in bulk but in nanophase, they are ferromagnetic. Cr is anti-ferromagnetic in bulk, in nanophase it shows frustrated paramagnetic property. At higher temperatures, clusters show less magnetic moment called super paramagnetism because thermal vibrations change the alignment of magnetic moment. Clusters of non-magnetic element supported on metal substrates also show magnetism. This shows that small particles possess more magnetism than the bulk material.

#### (v) Electronic properties

The electrical conductivity and energy bandwidth of some materials change when they pass from bulk phase to nanoparticle phase. For example, bulk silicon is an insulator; it becomes a conductor in the nanophase. Nanomaterial semiconductors such as Ge and Si do not show semiconducting property. In nanoceramics and in nanomagnetic composites, electrical conductivity increases with reducing particle size. In metals, electrical conductivity decreases with reducing particle size. By reducing the size of metal particles from bulk to nano, the energy bands become narrower and hence the ionization potential energy increases.

#### (vi) Mechanical properties

The mechanical behaviour of nanostructures is dominated by the nature of interfaces in them. Mechanical properties such as hardness, toughness, elastic modulus, scratch resistance, fatigue strength, crack initiation and propagation are significantly different for nanostructures than bulk materials. In metals and alloys, the hardness and toughness are increased by reducing the size of nanoparticles. In ceramics, ductility and superplasticity are increased on reducing particle size. Nanostructured composites offer an increased density of inhibitors to slip crack migration so that the strength of the material increases. Hardness increases 4 to 6 times as one goes from coarse grain Cu to nanocrystalline Cu and it is 7 to 8 for Ni.

It is observed that the materials with smaller grain size are stronger, because crack propagation can be delayed or reduced in nanostructures than bulk materials. Fe and Ni continue to harden with decreasing grain size. By decreasing the size of nanocrystalline metals from  $1\text{ }\mu\text{m}$  to  $10\text{ nm}$ , the hardness increases 2 to 7 times. As the grain size is reduced below  $10\text{ nm}$ , the hardness reduces in some nanomaterials.

The transition from bulk to nanophase reduces elastic strength and increases plastic behaviour. Brittle materials [ceramics, intermetallics] can become ductile by reducing their grain size. At higher temperatures, nanozirconia material possesses superplastic property. When the material is superplastic, it can undergo large tensile deformation without necking and fracture. Creep involves atomic transport along grain boundaries, and materials having large number of grains have large creep rates. This leads to superplasticity. The creep rates can be increased by 6 to 8 times by reducing the grain size from microns to nanometers. The reduction of the size of nanoparticles in steel leads a reduction in ductile-to-brittle transition temperature.

## 14.3 Chemical properties

Nanocrystalline materials are strong, hard, wear resistant, erosion and corrosion resistant. They are chemically active and have the following chemical properties.

(a) The nanostructures in chemistry are colloids and these are formed in a condensed phase having sizes in the range from 1 to 100 nm. Nanoscale catalysts have a high degree of dispersion, and this maximizes the contact area of a catalyst with the reactant.

(b) **The effect of nanoscale materials on chemical reactivity:** Changes in chemical reactivity of nanoscale materials have been expected. Chemical reactions are governed by electrons, electron affinities [or ionizational potential] and electron orbital densities. Coupling exists between chemical reactivity and the electronic character of the reactants and any catalyst. It was known that the ionizational potential increases as the cluster size drops below the bulk limit and it has limited applicability.

The electronic properties of a catalyst is host-dependent and possibly even reaction-dependent. Clusters of platinum, iridium or osmium reduced to a size of 1 nm and supported on alumina or silica exhibited electronic properties similar to those found for large crystallites of the metal. The electronic structure of metal nanocrystallites depends on supported non-conducting oxides. The reactivity of a cluster depends on the cluster size. This is useful in the preparation of catalytic agents. Some chemically inert bulk materials become good chemical catalysts in the nanophase, for example: platinum and gold.

(c) **Electrochemical reactivity:** Nanostructure size effects have been observed in catalysis. In the case of metal nanocrystallites supported on conductors, we see that in nanocrystallites of platinum supported on titanium or glassy carbon, the photocurrent increases whereas the photoemission current for palladium nanocrystallites supported on glassy carbon decreases relative to that of the bulk metal. So, we say that photoemission currents vary as a function of the crystallite size i.e., as compared to the bulk metal, increased reactivity for supported platinum nanocrystallites and decreased reactivity for glassy carbon supported palladium nanocrystallites was observed.

(d) **Effect of nanostructures on mass transport:** In chemical or electrochemical reactions, the rate of increase in mass transport increases as the particle size decreases.

(e) **The effect of chemistry on nanostructures:** The equilibrium vapour pressure, chemical potentials and solubilities of nanoparticles are greater than that for the same bulk material. Exposure to high temperatures or to certain chemicals can increase the size of a nanostructure. The high surface area of atoms or molecules of nanocrystallites supports heterogeneous catalysis.

(f) **Hydrogen storage in metals:** Most of the metals do not adsorb hydrogen, those adsorb have a metal to hydrogen atom ratio of 1. The small positively charged clusters of Ni, Pd and Pt containing atoms in between

2 to 60 can adsorb hydrogen atoms up to 8 per metal atom. This hydrogen adsorption decreases with an increase of cluster size. So, small metallic clusters are used as hydrogen storage devices.

## 14.4 Fabrication

Fabrication applies to the building of machines, structures or process equipment by cutting, shaping and assembling components made from raw materials. In nanotechnology, the scanning instruments help to a large extent in the development of nanoscience. In these instruments, the tip of the probe slides along a surface. The tip has nanoscale dimensions, usually of single-atom size. During sliding, the instrument measures different properties. To determine these properties, there are different types of scanning probe measurements. They are described in brief below.

**(i) Atomic force microscopy (AFM):** In this, electrons are used to measure the force applied on the probe tip as it moves on the object surface.

**(ii) Scanning tunneling microscopy (STM):** In this, the amount of electrical current flowing between the scanning tip and the object surface is used to measure local electrical conduction and geometry of the object at that place.

**(iii) Magnetic force microscopy [MFM]:** In this, the tip scans the magnetic surface. This locally detects the magnetic structure of the substance.

All other scanning microscopes also work on the principle of STM. The scanning is used to find nanoscale structure by measuring force, current, magnetic drag, chemical identity, etc.

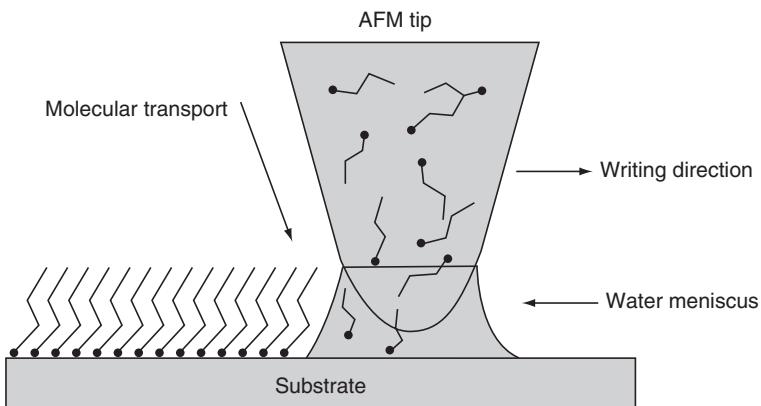
The scanning probe instrument uses the dragging finger analogy. This helps us to see structures and modifies a surface with the help of the tip of the scanning probe. The individual atoms or molecules can be moved on the surface by pushing on the surface or by picking them off the surface, moving and putting them back down. In this process, the scanning tip acts as a sort of earth mover at the nanoscale. Some scanning instruments have hundreds or even thousands of probe tips. The various nanostructure fabrication processes are described below.

**(i) Nanolithography:** Optical or X-ray lithography is used to make the present computer chips. In this, a master mask is made using chemical methods. A lithograph is an image that is produced by carving a pattern on the stone. Lithography is used for making objects from stones. In addition, there is microimprint lithography. This method works in the same way as the rubber stamp.

**(ii) Dip pen nanolithography (DPN):** The DPN is a direct writing technique that is used to create nanostructures on a substrate by delivering molecules through a capillary present at the tip of an atomic force microscope (AFM), as shown in Fig. 14.3. AFM tips are the ideal nanopens to construct arbitrary nanostructures on surfaces. The principle of DPN is similar to that of using the fountain pen. In this method, a reservoir of ink (atoms or molecules) is present at the top of the probe tip and are arranged across the surface.

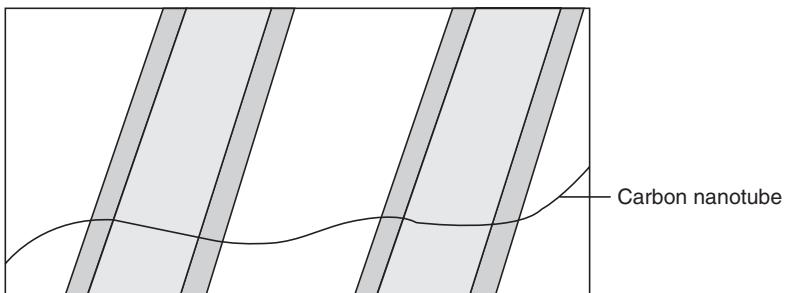
The ink is alkylthiol molecules; these molecules possess a head group of a thiol and 1–4 nm length hydrocarbon tail group. These molecules are taken as delivery molecules and a gold substrate is used to collect the molecules. The thiol molecules form a single layer on the substance with the thiol group forming a strong bond with gold and the tail group aligning perpendicular to the surface. The DPN device is used to image and write a pattern. Using software, the DPN plotter can write complicated patterns also.

**Figure 14.3 Representaion of dip pen lithography**



**(iii) Electron beam lithography:** The use of light of small wavelengths generate some problems, so instead of light beam electron beam is to be used in lithography. The structures at nanoscale can be manufactured using e-beam lithography. Figure 14.4 shows the formation of two electrodes using electron beam lithography. The structure lying across is a single molecule carbon nanotube.

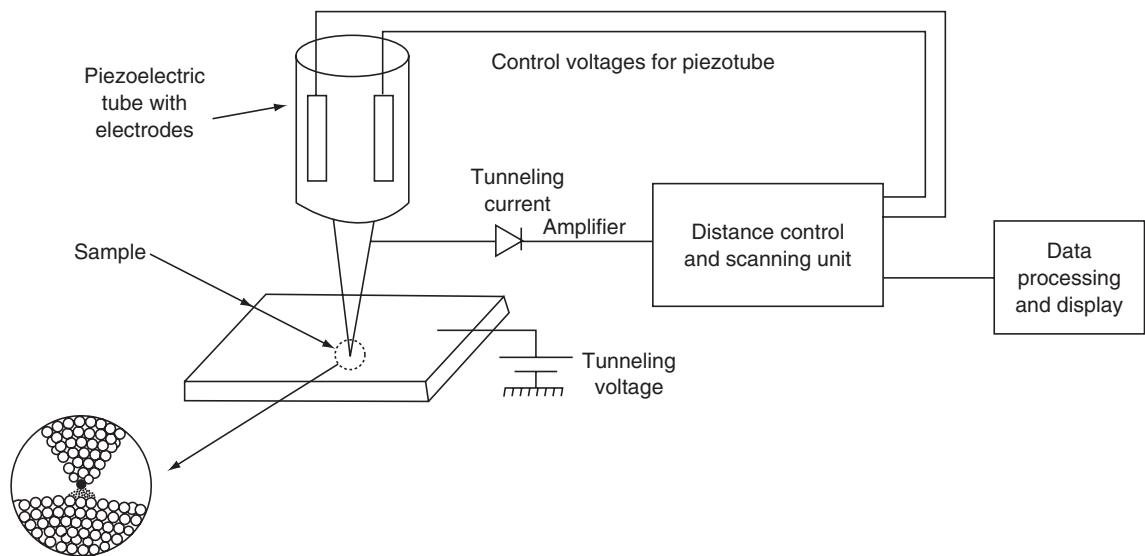
**Figure 14.4 Two electrodes made using electron beam lithography. The horizontal structure one is the carbon nanotube**



In this method, the resolution depends on the granularity of the resist used, the contrast of the resist developer, spatial distribution of deposited energy and the statistical distribution of photons at each pixel. During lithographic process, the whole system is kept under vacuum and a single beam of electrons is focused at the surface of the resist-coated semiconductor wafer. Using pattern generator, the electron beam is moved across the surface under computer control.

**(iv) Atomic lithography:** The scanning tunneling microscope [STM] used in this method is capable of imaging individual atoms i.e., directly observe the atoms on the surface of a material. The resolution is of the order of a fraction of atomic diameter. The STM works [Fig. 14.5] by using a very sharp tip that is positioned over the electrically conducting sample.

**Figure 14.5 A schematic diagram of the operation of a STM**



The magnitude of tunneling current monitors the separation between the tip and the sample surface. As the tip moves, the tunneling current changes, and this shows the distance between the tip and surface. The change in tunneling current is fed back to an electrical circuit, which controls the up and down motion of the tip. The decrease in tunneling current is an indication of larger separation, then the feedback circuit lowers the tip. A voltage difference applied between tip and surface causes a small number of electrons to tunnel from the tip to the sample surface. By applying a few volts between the tip and surface, an electric field is produced, this field can break local chemical bonds or initiate a chemical reaction, resulting in atom displacement, removal and deposition of individual atoms or knocking off of individual atoms.

## 14.5 Production of nanoparticle

Nanoparticles can be produced by a number of ways. They are described below:

### (i) Plasma arcing

Plasma is an ionized gas. Plasma can be produced by the discharge of gas between two electrodes, so that the gas dissociates into electrons and positive ions. Using plasma arcing, very thin films of the order of atomic dimensions can be deposited on the surface of an electrode. This deposition is carried in vacuum or in an inert gas. An arc passes from one electrode to the other. The first electrode [anode] vapourizes, so positively charged ions are produced. These ions deposit on the cathode. By using carbon electrodes, carbon nanotubes can be formed on the surface of the cathode. A mixture of conducting and non-conducting materials is also used in electrodes to form thin layers of the materials on the cathode.

## (ii) Sol–gel method

In solutions, nano-sized molecules are dispersed randomly. Whereas in colloids, the molecules [or particles] have diameters in the range of 20  $\mu\text{m}$  to 100  $\mu\text{m}$  and are suspended in the solvent. So, the colloid appears cloudy. A colloid that is suspended in a liquid is called a sol. The gelation of the sol in the liquid to form a network is called gel. The formation of sol–gel involves hydrolysis, condensation, growth of particles and the formation of networks. Using the sol–gel method, silica gels, zirconia and yttrium gels and aluminosilicate gels are formed. Nanostructured surfaces are formed using the sol–gel method.

## (iii) Chemical vapour deposition

In this method the material is heated to gaseous phase and allowed to condense on a solid surface in vacuum. Nanomaterials of metallic oxides or metallic carbides can be formed by heating metal and carbon or metal and oxygen in a vacuum chamber to gaseous phase and allowed to deposit on the surface of a solid. Metal nanoparticles are formed by exposing the metal to tuned metal-exciting microwaves so that the metal is melted, evaporated and formed into plasma at 1500°C. By cooling this plasma with water in a reaction column, nanoparticles are produced. The grain size of nanoparticles depends on the concentration of metal vapour, its rate of flow in the reaction column and temperature.

## (iv) Ball milling

In this method, small balls of the material are made to rotate inside a drum and drop under the influence of gravity on to a solid present in the drum. The balls are broken into nanocrystallites. This is also known as mechanical crushing. This method is used for a large number of elements and metal oxides. For example, iron nanoparticles of sizes 13 to 30 nm can be formed.

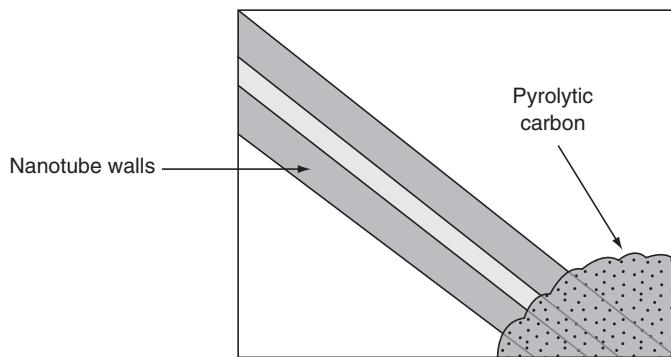
## (v) Electrodeposition

As current is passed between the electrodes immersed in an electrolyte, some substances will be deposited on the surface of one electrode. By controlling the current, a single layer of atoms can be deposited. Nanostructured films of Au, Cu, Pt, Ni, polymers, oxides and semiconductors can be deposited. These films are robust, flat, uniform and shiny. The deposited plates are used in batteries, solar cells, fuel cells, sensors, photonic devices and field emitters.

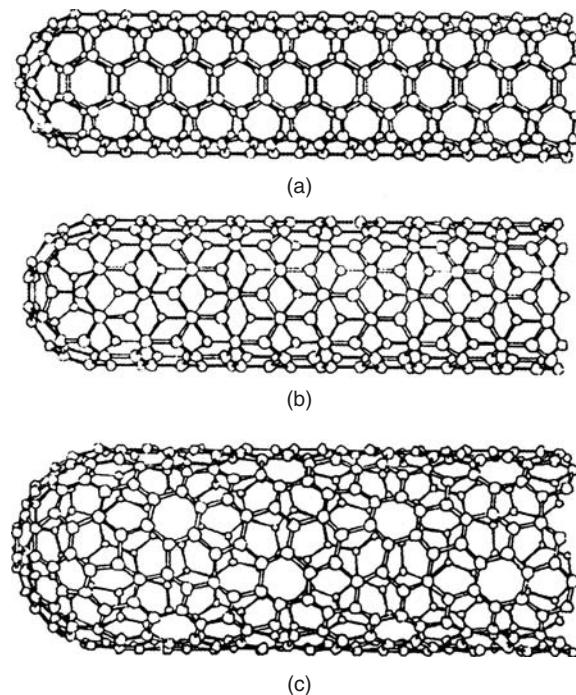
# 14.6 Carbon nanotubes

## (a) Introduction

Carbon nanotubes are hollow cylindrical tubes. The length of carbon nanotubes may vary from several micrometers to millimeters and the diameter will vary from 1 to 20 nm. The ends are closed with caps containing pentagonal rings. A tube may contain one cylindrical wall of graphite or a number of concentric cylindrical walls. Under the transmission electron microscope, these cylindrical walls appear as planes. Single wall nanotubes appear with two planes whereas the multiwall nanotubes appear with more than two planes and are seen as a series of parallel lines as shown in Fig. 14.6.

**Figure 14.6 Carbon nanotubes**

The single-walled carbon nanotubes are of three different types. They are: (i) arm chair, (ii) zig-zag and (iii) chiral type structures. These are shown in Fig. 14.7. In these, a single hexagonal wall is seen.

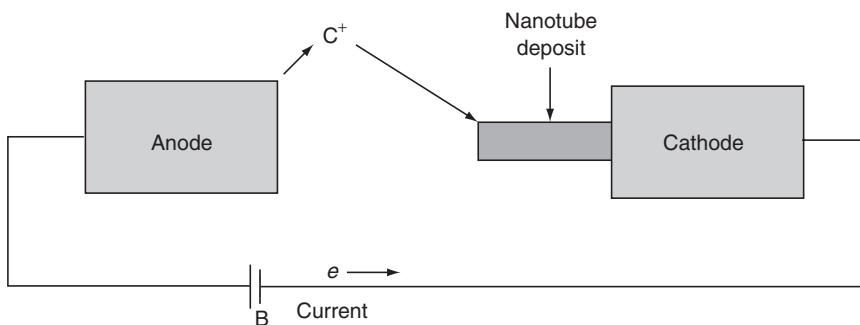
**Figure 14.7 Single-walled carbon nanotubes: (a) Arm chair, (b) Zig-zag, and (c) Chiral type**

### (b) Formation of nanotubes

There are a number of methods of making nanotubes.

**(i) Plasma arcing method:** Carbon nanotubes are prepared by putting an electric current across two carbonaceous electrodes [graphite] as in a helium or argon atmosphere as shown in Fig.14.8. This method is called the plasma arcing method. In this method, evaporation of one electrode [anode] takes place as cations, and the particles are deposited at the other electrode. The deposition on the cathode are nanotubes. Normally, multi-walled nanotubes are formed from plasma arcing. Single-walled nanotubes are formed if the electrodes are bored out and cobalt or other metals are included.

**Figure 14.8 Carbon nanotube formation**



**(ii) Laser method:** Large quantities of single-walled nanotubes can be prepared by dual-pulsed laser vapourization method. In this method, the samples can be prepared by laser vapourization of graphite rods with equal amounts of cobalt and nickel powder at 1200°C in flowing argon. After this, heat treatment is carried out at 1000°C in vacuum to remove  $C_{60}$  and other fullerenes. The first laser vapourization pulse is followed by a second pulse for more uniform vapourization. The product appears as a mat of ropes having a diameter of 10–20 nm and a length of 100  $\mu\text{m}$  or more. The diameter of tubes can be controlled by varying the parameters such as growing temperature and catalyst composition.

The other methods include arcing in the presence of cobalt, chemical vapour deposition method, ball milling, diffusion flame synthesis, electrolysis, solar energy pyrolysis at low temperature, heat treatment of a polymer, etc.

### (c) Properties of nanotubes

- (i) The tubes are mechanically robust.
- (ii) Nanotubes are about 6 times lighter, 10 times stiffer and 20 times stronger than steel.
- (iii) The tube behaves as a metal and as a semiconductor. As a metal, its electrical conductivity is 1000 times more than that of copper.
- (iv) The electrical conductivity of nanotubes is a function of diameter, conductivity in multiwalled nanotubes is quite complex.

### (d) Applications of nanotubes

**(i) Electronics:** The single-walled nanotube can act as a transistor. Pairs of nanotubes or crossed nanotubes show as logic structures. If a line of hexagons form a helix, then the tube acts as a semiconductor. A single

nanotube with a natural junction acts as a rectifying diode. Transistor nanotube circuits are built by drawing a single nanotube over three parallel gold electrodes, adding a polymer between the electrodes and sprinkling potassium atoms on the top. The potassium atoms add electrons to the nanotube. In flat panel displays, a nanotube works due to its field emission property. Nanotubes are used in batteries.

- (ii) **Hydrogen storage:** Nanotubes can store hydrogen and also helium, oxides and metals like copper.
- (iii) **Mechanical machines:** Nanotubes can act as axles in nanomachines. Building gear teeth on nanotube is favoured to translate different rotational motions.
- (iv) **Space elevators:** Long filaments of nanotubes are used in fibre-reinforced plastics, these have less weight. So they are used in aeroplanes, space ships and land vehicles. Carbon nanotubes, like graphite, withstand high temperatures, so they are used for thermal protection of spacecraft during re-entry into the atmosphere. Carbon nanotubes have high Young's modules, so they withstand aeronautical strains.
- (v) **Hospitals:** Carbon nanotubes are thin, so they can penetrate the skin without pain. Blood can be drawn from diabetic patients through nanostraws to know glucose levels and to inject insulin whenever required.

## 14.7 Applications of nanotechnology

Nanomaterials are found in both biological systems and man-made structures. Nature has been using nanomaterials for millions of years. The large surface area to volume ratio increases the chemical activity. Nanomaterials have the following applications.

- (i) **In microelectronics:** In microelectronics, the reduction in size of electronic components leads to faster switching times. Nanotechnology includes fabrication of nanowires used in semiconductors. Porous silicon emits visible light, so it finds application in optoelectronics. Quantum dot lasers are nanoscaled objects, they emit good-quality laser beam compared to semiconductor laser diodes. They are cheaper and the emitted wavelength depends on the diameter of the dot.
- (ii) **Machine tools:** Some nanocrystalline materials such as tungsten carbide, tantalum carbide and titanium carbide are harder than conventional materials; they are more wear-resistant and erosion-resistant, so they are used in cutting tools and drill bits. Nanocrystalline silicon nitride and silicon carbide are used in the manufacturing of high-strength springs, ball bearings and valve lifters because of their excellent physical, chemical and mechanical properties. Nanocrystalline ceramics such as zirconia ( $ZrO_2$ ) are softer than conventional materials, so they can be easily pressed and sintered into various shapes at significantly lower temperatures.
- (iii) **High-power magnets:** The magnetic strength of a material is directly proportional to the surface area per unit volume. The magnetic nanocrystalline yttrium – samarium – cobalt possess very high magnetic properties due to large surface area. The typical applications of high-power rare earth magnets are in submarines, generators, electric motors, automobile alternators, magnetic resonance imaging (MRI) instruments and in ultrasensitive analytical instruments.
- (iv) **In television or in a monitor:** In television or in a monitor, the resolution depends on the size of the pixel made of phosphors. The phosphor glows when a beam of electrons strike them. The resolution of images in these instruments increases as the size of pixels reduces. Materials like nanocrystalline selenide, zinc sulphide, lead telluride and cadmium sulphide synthesized by the sol-gel method improve the resolution. The use of nano-phosphors may reduce the making cost of high resolution television. In new generation batteries, the separator

plates are made up of nanocrystalline materials prepared by the sol-gel method, and they hold more energy. For example, batteries made of nanocrystalline nickel and metal hydrides are long lasting and requires minimal recharging.

**(v) Motor vehicles and air craft:** The thermal energy generated in engines is wasted to a large extent. This can be reduced by coating the cylinders with nanocrystalline ceramics such as zirconia and alumina. By retaining more heat energy, combustion of the fuel takes place completely. In air crafts, by decreasing the grain size of the materials the fatigue strength increases. By using nanomaterials, the fatigue life increases as much as 300%. The components made of nanomaterials are stronger and operate at higher temperatures. So air crafts can fly faster using the same amount of aviation fuel.

**(vi) Aerogels:** Aerogels are nanocrystalline materials. They are porous and hence air is trapped at the interstices. Using these materials for insulation at offices and homes leads to drastic reduction in cooling and heating bills by saving power. These materials are also used as materials for smart windows, so that the materials become darkened when the sun is too bright and lightened when the sun is not shining brightly.

**(vii) Energy efficiency:** For illumination, energy consumption can be greatly reduced by using quantum caged atoms or light emitting diodes (LEDs) instead of ordinary filament bulbs. Nanostructures with a continuum of energy band gaps have an increased solar energy conversion efficiency as compared to ordinary semiconductor solar cells.

In hydrogen fuel cells, nanostructured catalyst material is used on carbon-supported noble metal particles with diameters between 1 and 5 nm. For hydrogen storage, materials with nanosized pores like nanotubes, zeolites, etc. are under investigation.

**(viii) Medical field:** Nanomaterials are used in biology for the development of diagnostic devices, drug delivery vehicles, analytical tools and in physical therapy applications. The genetic sequence of a sample can be detected by tagging gold nanoparticles with short segments of DNA. Magnetic nanoparticles are used to label molecules, structures or micro-organisms of an antibody. Iron nanoparticles are used in cancer treatment. Nanotechnology is used to reproduce or to repair damaged tissue.

**(ix) Textiles:** Clothes made of nanofibres are water and stain repellent and wrinkle-free. They can be washed less frequently at low temperatures.

**(x) Computer:** Quantum computers use fast quantum algorithms and have quantum bit memory space (qubit), so it involves in several computations at the same time.

**(xi) Cosmetics:** Sun screens based on mineral nanoparticles such as titanium dioxide offer several advantages. They have high UV protection compared to the bulk material.

**(xii)** In addition to the above, we have quantum dots, suntan lotion, nanotubes, protective coatings. Fullerenes [ $C_{60}$ ] are used as lubricants [molecular ball bearings], diamond seeding, diamond production, xerographic materials, photochromic goggles, etc.

**(xiii)** There is a scientific evidence that some nanomaterials are toxic to humans or to the environment. Nanomaterials are able to cross biological membranes and access cells, tissues and organs. Normally, this cannot be done by larger sized particles. Some materials penetrate the skin. Nanomaterials have the potential to cause DNA mutation and induce major structural damage to mitochondria, even resulting in cell death.

## Multiple Choice Questions

1. Nanotechnology was brought into day light by delivering lectures by: ( )  
(a) Feymann                    (b) Einstein                    (c) Newton                    (d) Max Planck
2. Nanostructures have sizes in between: ( )  
(a) 1 and 100 Å                    (b) 1 and 100 nm  
(c) 100 and 1000 nm                    (d) None of the above
3. Nanotechnology deals with \_\_\_\_\_ of nanostructures into useful nanoscale devices such as electronic circuits and mechanical devices at the molecular level. ( )  
(a) the design                    (b) manufacturing                    (c) applications                    (d) All the above
4. Choose the correct statement: ( )  
(a) If we properly arrange carbon atoms in coal then it may become diamond  
(b) By rearranging atoms in sand, silicon chip can be made  
(c) Both a and b  
(d) None of the above
5. The probe of scanning tunneling microscope is as sharp as ( )  
(a) an atom at the tip                    (b) many atoms at the tip  
(c) a needle                                (d) None of the above
6. Choose the correct statement ( )  
(a) Scanning tunneling microscope probe can extract single atom from the surface of the specimen and place it at the desired position.  
(b) Scanning tunneling microscope is useful for manipulating single molecules and observing molecular shapes.  
(c) Spherical molecules with 60 carbon atoms can be made and it is called bucky ball or fullerenes.  
(d) All the above
7. The surface area to volume ratio is \_\_\_\_\_ for nanomaterials. ( )  
(a) very large                            (b) very less  
(c) moderate                              (d) None of the above
8. The bulk materials, when reduced to nanoparticles will show \_\_\_\_\_ physical and chemical properties. ( )  
(a) same                                    (b) different                            (c) Both a and b                            (d) None of the above
9. The interatomic distance \_\_\_\_\_ by reducing the size of nanoparticles. ( )  
(a) decreases                              (b) increases  
(c) remain same                            (d) None of the above
10. The different sized nanoparties scatter different wave lengths of light incident on it and they appear with: ( )  
(a) same colour                            (b) different colours  
(c) colourless                              (d) None of the above
11. Choose the correct statement: ( )  
(a) Porous silicon exhibits red photoluminescence.  
(b) Nanogold particles can be orange, purple, red or greenish in colour depending on their grain size.  
(c) Nanoparticle copper is transparent  
(d) All the above

## 14-16 | Applied Physics

12. When a bulk material is changed into nanoparticles material then their \_\_\_\_\_ properties changes. ( )  
(a) optical                    (b) thermal                    (c) magnetic                    (d) All the above
13. Choose the correct statement: ( )  
(a) The melting point of nanogold decreases from 1200k to 800k as the size of particles decreases form 300Å to 200Å  
(b) The Debye temperature and ferroelectric phase transition temperature are lower for nanomaterials.  
(c) Stable aluminium turns to combustible in nanophasse.  
(d) All the above
14. Fe, Co, Ni and Gd are ferromagnetic in bulk but they show \_\_\_\_\_ magnetic in nanophasse. ( )  
(a) super para                (b) para                    (c) ferri                    (d) dia
15. Na, K and Rh show paramagnetic properties in bulk whereas in nanophasse they show \_\_\_\_\_ properties. ( )  
(a) diamagnetic                (b) ferrimagnetic  
(c) ferromagnetic              (d) antiferromagnetic
16. By reducing the size of metal particles from bulk to nano, the energy bands are:  
(a) narrower                    (b) remains same            (c) wider                    (d) None of the above
17. Choose the correct statement: ( )  
(a) In metals and alloys, the hardness and toughness are increased by reducing the size of nanoparticles and in ceramics, ductility and super plasticity are increased.  
(b) The hardness increases by 4 to 6 times for nanocrystalline copper than coarse grain copper and it is 7 to 8 for nickel.  
(c) By reducing the size of nanocrystalline metals from  $1\mu\text{m}$  to 10 nm, the hardness increases by 2 to 7 times.  
(d) All the above
18. The nanomaterials with smaller grain size are stronger, because crack propagation can be \_\_\_\_\_ than in bulk materials. ( )  
(a) reduced                    (b) increased  
(c) a or b                      (d) None of the above
19. The creep rates can be increased by \_\_\_\_\_ times by reducing the grain size from microns to nanometres. ( )  
(a) 4 to 6                    (b) 6 to 8                    (c) 8 to 10                    (d) 2 to 4
20. Choose the correct statement: ( )  
(a) Some chemically inert bulk materials like Pt and Au can become good chemical catalysts in nanophasse.  
(b) Nanocrystalline materials are strong, hard, wear resistant, erosion resistant, corrosion resistant and are chemically active.  
(c) The equilibrium vapour pressure, chemical potentials and solubilities of nanoparticles are greater for nanomaterials than bulk materials.  
(d) All the above
21. Choose the correct statement: ( )  
(a) Single walled carbon nanotube can act as a transistor.  
(b) Single walled carbon nanotube with a natural junction can act as a rectifying diode.  
(c) Carbon nanotubes can act as axles in nanomachines.  
(d) All the above

22. Nanostructures are made using \_\_\_\_\_ methods. ( )
- (a) optical or X-ray lithography
  - (b) dip pen nanolithography
  - (c) electron beam lithography and atomic lithography
  - (d) All the above
23. Nanoparticles are produced using ( )
- (a) sol-gel method
  - (b) plasma arcing and ball milling methods
  - (c) chemical vapour deposition and electro deposition methods
  - (d) All the above
24. The length of a carbon nanotube will vary from: ( )
- (a) several micrometres to millimetres
  - (b) millimetres to centimetres
  - (c) centimetres to metres
  - (d) None of the above
25. The diameter of a carbon nanotube will vary from ( )
- (a) 1 to 20 nm
  - (b) 20 to 50 nm
  - (c) 50 to 100 nm
  - (d) 100 to 200 nm
26. Carbon nanotube ends are closed with caps containing \_\_\_\_\_ rings. ( )
- (a) tetragonal
  - (b) pentagonal
  - (c) hexagonal
  - (d) None of the above
27. The different types of single wall carbon nanotubes are: ( )
- (a) arm chair
  - (b) zig-zag
  - (c) chiral type
  - (d) All the above
28. Carbon nanotubes are prepared using: ( )
- (a) laser method and electrolysis method
  - (b) plasma arcing method and chemical vapour deposition method
  - (c) ball milling method and diffusion flame synthesis method
  - (d) All the above
29. Carbon nanotubes are: ( )
- (a) 6 times lighter, 10 times stiffer and 20 times stronger than steel
  - (b) robust
  - (c) having electrical conductivity 1000 times more than that of copper
  - (d) All the above
30. Choose the correct statement: ( )
- (a) In atomic force microscopy, electrons are used to measure the force applied on the probe tip as it moves on the object surface.
  - (b) In scanning tunneling microscopy, the electrical current flowing between the scanning tip and the object surface to measure local electrical conduction and geometry of the object at that place.
  - (c) In magnetic force microscopy, the tip scans the magnetic surface and locally detects the magnetic structure of the substance.
  - (d) All the above
31. The nanocrystalline tungsten carbide, tantalum carbide and titanium carbide are: ( )
- (a) harder than their conventional materials
  - (b) more wear-resistant and erosion-resistant
  - (c) used in cutting tools and drill bits
  - (d) All the above

## 14-18 | Applied Physics

32. Nanocrystalline silicon nitride and silicon carbide are used in the manufacturing of : ( )  
(a) high strength springs  
(b) ball bearings and valve lifters  
(c) both a and b  
(d) None of the above
33. The nanophosphors may \_\_\_\_\_ the making cost of high resolution television. ( )  
(a) reduce (b) increase  
(c) have no change in (d) None of the above
34. In new generation batteries, the separator plates are made up of with nanocrystalline nickel and metal hydrides because they: ( )  
(a) hold more energy (b) are long lasting  
(c) require rare recharging (d) All the above
35. In air crafts, by decreasing the grain size of nanomaterials the fatigue strength increases and the fatigue life increases as much as: ( )  
(a) 50% (b) 200% (c) 300% (d) 100%
36. The thermal energy generated in engine cylinders is wasted to a large extent, this wastage can be reduced by coating the cylinders with nanocrystalline ceramics such as: ( )  
(a) zirconia (b) alumina  
(c) Both a and b (d) None of the above
37. Aerogels are used: ( )  
(a) for insulation in offices and homes  
(b) for smart windows  
(c) both a and b  
(d) None of the above
38. Nanomaterials are used in ( )  
(a) micro electronics, machine tools and high power magnets  
(b) monitors, television, engine cylinders and aerogels  
(c) textiles, computers and in medical fields  
(d) All the above
39. In the medical field nanotechnology is used: ( )  
(a) to reproduce or to repair damaged tissue  
(b) iron nanoparticles are used in cancer treatment  
(c) for the development of diagnostic devices, drug delivery vehicles and analytical tools  
(d) All the above
40. Clothes made up of nanofibres are: ( )  
(a) water and stain repellent (b) wrinkle free  
(c) less frequently washed (d) All the above
41. Choose the correct statement: ( )  
(a) Quantum computers have quantum bit memory space so it involves in several computations at the same time  
(b) Sun Screens based on mineral nanoparticles have high UV Protection compared to the bulk material  
(c) Both a and b  
(d) Nanomaterials are not toxic to humans or to the environment

**Answers**

1. a	2. b	3. d	4. c	5. a	6. d	7. a	8. b	9. a	10. b	11. d
12. d	13. d	14. a	15. c	16. a	17. d	18. a	19. b	20. d	21. d	22. d
23. d	24. a	25. a	26. b	27. d	28. d	29. d	30. d	31. d	32. c	33. a
34. d	35. c	36. c	37. c	38. d	39. d	40. d	41. c			

**Review Questions**

1. Write a detailed note on nanoscience and nanotechnology. (Set-1, Set-3–May 2008), (Set-2–Sept. 2008)
2. Write a detailed note on nanoscience. (Set-1–Sept. 2008), (Set-4–May 2008)
3. How the physical and chemical properties of nanomaterials vary with their size? (Set-4–Sept. 2008) (Set-2–May 2008)
4. Write the important applications of nanomaterials. (Set-4–Sept. 2008), (Set-2–May 2008)
5. Write the important applications of nanomaterials in medicine. (Set-2–Sept. 2008), (Set-1, Set-3–May 2008)
6. Why nanomaterials exhibit different properties? Explain. (Set-1–Sept. 2008), (Set-4–May 2008)
7. What are nanomaterials? Explain. (Set-3–Sept. 2008)
8. Nanomaterials exhibit different properties. Explain the reason. (Set-3–Sept. 2008)

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## A P P E N D I X

A

### Hexagonal Close Pack (HCP) Structure

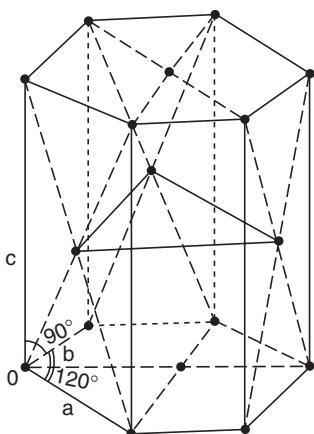
Hexagonal close packed (HCP) crystal structure has two layers of atoms. One layer of atoms is present at the bottom face of the unit cell, and it is referred to as the 'A' layer of atoms. Above the bottom layer, we have a second layer of atoms. This is the middle layer in the unit cell and is referred to as the 'B' layer of atoms. The atoms in the 'B' layer are seated in the voids between any three atoms of the bottom layer. Above the second layer, we have a third layer of atoms. This is the top layer of atoms in the unit cell and it is a repetition of the bottom layer. Hence, the stacking of a hexagonal close packed crystal structure consists of a series of *ABABAB...* layers.

The unit cell structure of HCP is shown in Fig. A.1. The unit cell parameters  $a$ ,  $b$ ,  $c$  are shown in the diagram.

$$a = b \neq c;$$

$$\alpha = \beta = 90^\circ \quad \text{and} \quad \gamma = 120^\circ$$

**Figure A.1** Unit-cell structure of HCP



In the unit cell, the atoms are present at the six corners of a hexagon and at the centre of the hexagon at the bottom and top faces. Three more atoms are present at the centres of alternate side faces. The bottom face atoms are on one plane and the central atoms of the side faces are in another plane. So, it has two layers of atoms and these layers repeat themselves in the crystal.

Each corner atom of the unit cell is shared by six unit-cells. Hence, the total number of atoms at the twelve corners of a unit cell is  $12 \times \frac{1}{6} = 2$ .

The central atom at the base is shared by two unit cells. Hence, the number of atoms shared from the centres of the bottom and top faces of the unit cell  $= 2 \times \frac{1}{2} = 1$ .

The second layer inside the unit cell has 3 atoms.

$\therefore$  The number of atoms per unit cell of HCP = 6

Along the edge of any of the bottom or top face, the surfaces of two atoms are in contact, hence the bottom face edge length,  $a = 2r$  or  $r = \frac{a}{2}$ .

To get the coordination number, imagine the central atom at the base. This is surrounded by six atoms on the basal plane, three atoms on its top layer and three atoms on the bottom layer. Hence, the coordination number is 12.

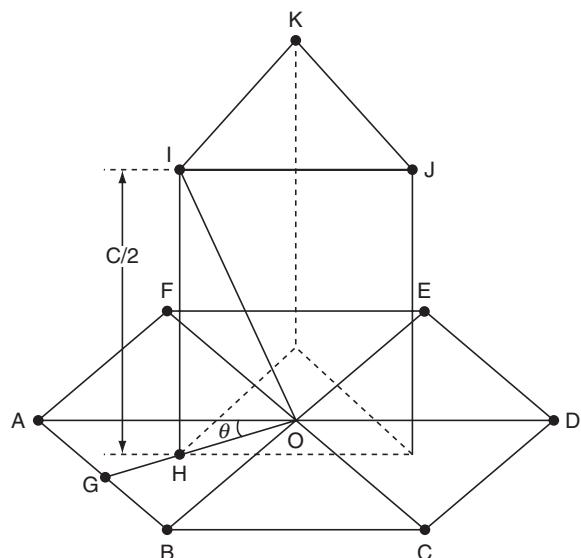
To find the relation between the height of the unit cell  $c$  and the length of the bottom face edge  $a$ , consider the bottom and middle planes of the atoms are shown in Fig. A.2. The separation between these two planes is  $c/2$ .

From Fig. A.2, the triangle OHI is a right angle triangle, the angle at H is  $90^\circ$ .

$$\begin{aligned}\therefore OI^2 &= a^2 = HI^2 + OH^2 \\ &= \left(\frac{c}{2}\right)^2 + OH^2 \quad \text{_____ (A.1)}\end{aligned}$$

Since the surfaces of atoms present at 'O' and at 'I' are in contact so  $IO = 2r = a$ .

**Figure A.2** The bottom and middle layer of atoms in a HCP unit cell



To find OH, consider the triangle ABO in which  $\cos\theta = \frac{GO}{AO}$   
or  $GO = AO \cos\theta = a \cos\theta = a \cos 30^\circ \quad (\therefore \theta = 30^\circ)$

$$\therefore GO = \frac{\sqrt{3}a}{2}$$

As H is the centre point of the triangle ABO,

$$OH = \frac{2}{3}GO = \frac{2}{3} \times \frac{\sqrt{3}}{2}a = \frac{a}{\sqrt{3}} \quad \text{(A. 2)}$$

Substituting equation (A. 2) in equation (A. 1)

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

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

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

$$\text{or} \quad 4 \times \frac{2}{3} = \left( \frac{c}{a} \right)^2$$

$$\frac{c^2}{a^2} = \frac{8}{3} \quad \text{(A. 3)}$$

$$\Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}} = 1.6329$$

This is the axial ratio for hcp crystal structure. Lastly, the packing factor can be estimated in the following way.

$$\text{Packing factor (PF)} = \frac{\text{Volume of all atoms in the unitcell}}{\text{Volume of unit cell}} = \frac{v}{V} \quad \text{(A. 4)}$$

$$\text{Volume of all atoms in the unit cell, } v = \left\{ \begin{array}{l} \text{number of atoms} \\ \text{per unit cell} \end{array} \right\} \times \left\{ \begin{array}{l} \text{Volume of} \\ \text{an atom} \end{array} \right\}$$

$$v = 6 \times \frac{4}{3} \pi r^3 = \frac{24}{3} \pi \left( \frac{a}{2} \right)^3 = \pi a^3 \quad \text{(A. 5)}$$

$$\text{Volume of unit cell, } V = \left\{ \begin{array}{l} \text{bottom face area of} \\ \text{the unit cell} \end{array} \right\} \times \text{height of the unit cell}$$

$$V = [6 \times \text{area of triangle ABO}] \times \text{height of the unit cell}$$

## A-4 Appendix

$$= 6 \times \left[ \frac{\text{base}}{2} \times \text{height of the triangle} \right] \times \text{height of the unit cell}$$
$$\therefore V = 6 \times \left[ \frac{a}{2} \times a \sin 60^\circ \right] \times c = 3a^2 \frac{\sqrt{3}}{2} c = \frac{3\sqrt{3}a^2 c}{2} \quad \text{(A. 6)}$$

Substituting equation (A. 5) and equation (A. 6) in equation (A. 4)  
we get

$$PF = \frac{v}{V} = \frac{\pi a^3 \times 2}{3\sqrt{3}a^2 c} = \frac{2\pi}{3\sqrt{3}} \frac{a}{c} = \frac{2\pi}{3\sqrt{3}} \sqrt{\frac{3}{8}} = \frac{\pi}{3\sqrt{2}} = 0.74$$

or 74 % using equation (A. 3)

The above value of packing factor is equal to the packing factor of FCC.



## A P P E N D I X

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# B

## Surface Defects

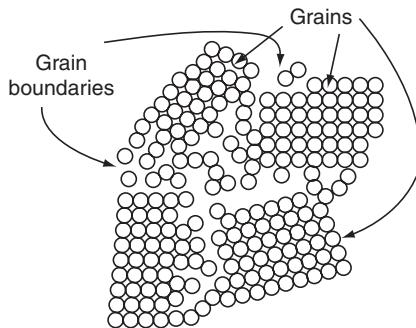
Two-dimensional crystal imperfections are known as surface defects or plane defects. In surface defects, the imperfections should lie about a surface having few atomic dimensions thick. Surface defects are of two types (a) external surface defects and (b) internal surface defects.

**(a) External surface imperfections:** Every atom present inside the crystal has a large number of surrounding atoms, whereas the atoms present on the surface of the crystal has no neighbouring atoms on one side of the surface. Hence atomic bonds do not extend beyond the surface of the crystal. Because of this, the surface atoms possess larger energy than the interior atoms. This larger energy at the surface causes imperfection at the external surface itself.

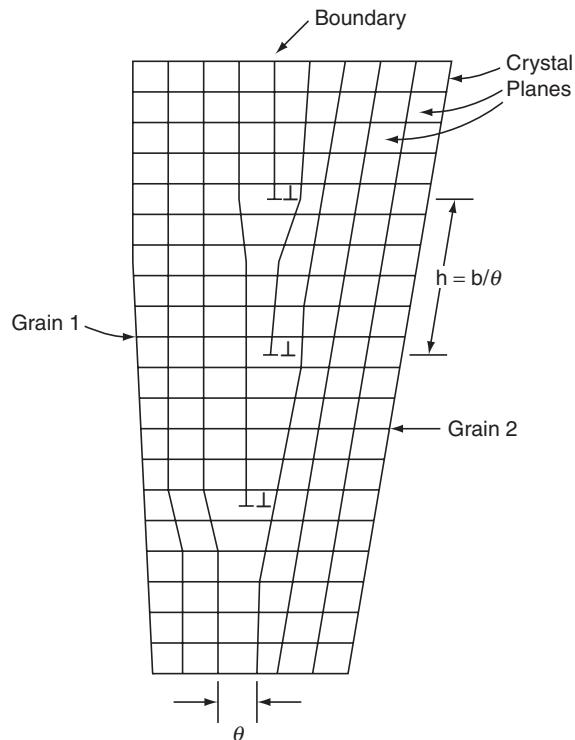
**(b) Internal surface imperfections:** The change in stacking of atomic planes across a boundary in the crystal is known as internal surface imperfection. Some of the internal surface imperfections are explained below:

**(i) Grain boundaries:** The non-periodicity of atoms between the crystallites (grains) of a polycrystalline material causes grain boundary surface defect. During recrystallization or during solidification of a polycrystalline material, the atoms from adjacent regions of two crystallites eventually impinge on each other, while the atoms between the crystallites are pulled to take up a compromised position between the two crystallites.

The thickness of this non-periodic region is of the order of 2 to 10 atomic distances or more. This boundary region is called a crystal boundary or a grain boundary and is shown in Fig. B.1. The orientation of the crystallites changes sharply at the grain boundary. If the misorientation angle between the crystallites is greater than  $10$  to  $15^\circ$ , then it is called a high-angle grain boundary. On the other hand, if the misorientation angle between the adjacent crystals is of the order of a few degrees or less than  $10^\circ$ , then it is called a low-angle grain boundary.

**Figure B.1** High-angle grain boundaries

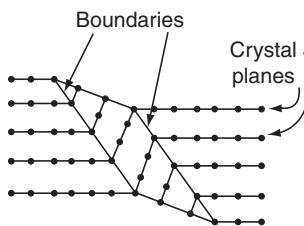
**(ii) Tilt and Twist boundaries:** Tilt boundary has an array of edge dislocations as indicated by ( $\perp$ ) in Fig. B.2. In the figure, ' $h$ ' is the vertical spacing between two consecutive edge dislocations and ' $b$ ' is the length of Burger's vector. Here  $\tan \theta \approx \theta = \frac{*b}{h}$ , is the angle of tilt or misorientation. This is a low-angle boundary. Twist results from a set of screw dislocations, it is also a low-angle boundary.

**Figure B.2** Tilt boundary

**(iii) Twin boundaries** This is a surface imperfection that separates two mirror orientations of a crystal.

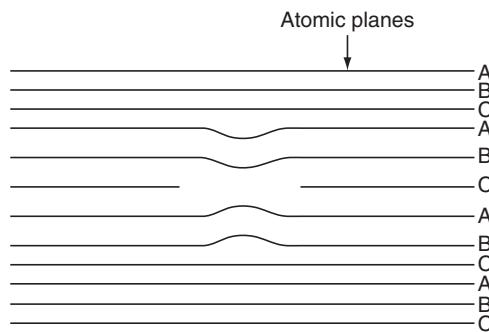
As shown in Fig. B.3, the atomic arrangement on one side of a twin boundary is a mirror reflection of the atomic arrangement on the other side of the twin boundary. The region between the two boundaries is called the twinned region. The twin boundaries can be seen under an optical microscope.

**Figure B.3** Twin boundaries



**(iv) Stacking fault:** Stacking fault is a surface imperfection in which there is a discrepancy in the stacking sequence of atomic planes. As shown in Fig. B.4, the stacking sequence in close packed FCC structure is ABCABCABC...

**Figure B.4** Stacking fault



Suppose that in a small region in atomic layer 'C', the atoms are not positioned properly. Then at this region, the stacking sequence is different and here the stacking sequence becomes ... *ABAB* ... . This is the stacking sequence of *HCP* structure. Thus the missing atoms in a small area of atomic layer 'C' gives rise to a stacking fault in close packed *FCC* crystal. The crystal will be sound on both sides of the fault.

**(v) Ferro-magnetic domain walls:** A ferro-magnetic material contains a large number of ferro-magnetic domains. Each domain is magnetised to saturation in a particular direction inside the material. The intensity of magnetic field and hence the magnetic field energy is almost uniform inside the domains. However, the intensity of magnetic field and the magnetic field energy is more at the surface of the domains. This large magnetic field energy on the surface of the domains gives rise to a surface imperfection known as magnetic domain-wall imperfection.

**(2) volume defects:** The cracks that are formed due to small electrostatic dissimilarity between the stacking layers, or due to sudden thermal waves or by using the material for some application cause volume defects.

The presence of large vacancies or voids due to missing clusters of atoms, non-crystallized regions, and inclusion of foreign particles with a dimension of at least 10 to 30Å are considered as volume defects.



## Dictionary of Selected Terms

### Chapter - I

**Appreciable:** Large enough to be noticed.

**Approach:** To come near to in distance or time.

**Available:** That you can get, buy or find.

**Bond:** A representation or a valency link by which one atom is attached to another in a chemical compound.

**Bound:** Held together firmly, to tie

**Cleave:** To split or cut

**Cohesion:** The attraction existing between molecules of the same kind. The force of reaction between similar molecules or molecules of the same substance.

**Consequence:** As a result of

**Considerable:** Great in amount, size, importance etc.

**Consists:** To have, possess

**Crystal:** A natural solid bounded by planes, a substance in which the constituents are arranged in a definite geometrical form

**Crystal structure:** The arrangement of atoms, ions or molecules in a crystal is called crystal structure

**Dielectric:** A non conductor of electric charge in which an applied electric field causes a displacement of charge but not a flow of charge.

**Dipole:** Two equal and opposite charges that are separated by a distance

**Directional:** Producing or receiving signals, sound, etc, better in one particular direction.

**Dispersion:** The process by which people or things are spread over a wide area

**Dominate:** To control or have a lot of influence on an unpleasant way.

**Electricity:** Any effect resulting from the existence of stationary or moving electric charges.

**Electrostatic field:** Electric field produced by stationary charges or charges at rest.

**Equilibrium:** A body is said to be equilibrium if (i) sum of the force acting on it is zero and (ii) there is no net torque acting on the body.

**Evolve:** To develop gradually, especially from a simple to a more complicated form.

**Exist:** to be real; to be present in a place or situation.

**Extent:** How large, important, serious etc.

**Fluctuate:** To change frequently in size, amount, quality etc.,

**Fracture:** A break in a material

**Incapable:** Not able to do

**Indicate:** To show, to mention, to represent information without using words.

**Infinite:** Very great; Impossible to measure without limits, with out end.

**Influence:** The effect on the way that behaves or thinks

**Instantaneous:** Happening immediately

**Insulator:** A substance that is poor conductor of heat and electricity

**Inter:** Between, from one to another

**Inter atomic forces:** Forces between atoms

**Intermolecular forces:** Forces between molecules and atoms, such forces are attractive in nature

**Ion:** An electrically charged atom formed by the loss (positive ion) or gain (negative ion) of one or more electrons. Positive ions are called cations and negative ions are called anions.

**Isolate:** To separate physically from other things.

**Migrate :**To move from one place to another

**Moment:** The product of force and the perpendicular of its line of action from the point on which it acts.

**Occur:** To happen

**Opaque:** Not allow light through

**Overlap:** Part of one thing covers part of the other.

**Polar:** Connected with the poles.

**Potential energy:** Energy possessed by a body by virtue of its position

**Primary:** Basic, main, most important

**Proximity:** The state of being near in terms of distance or time.

**Represent:** To show, to present, to describe

**Rigid:** Very strict and difficult to change

**Rigidity:** Stiffness, resistance to change of form

**Secondary:** Less important

**Share:** To have or use at the same time, to divide between two or more

**Solvent:** A substance, especially a liquid that can dissolve another substance.

**Stable:** Firmly fixed, not likely to move

**Stress:** The force per unit area on a body that tends to cause it to deform

## Chapter - II

**Base:** The first or main part of a substance to which other things are added.

**Constitute:** To be the parts that together form

**Crystal structure:** The atoms, ions or molecules forming the crystal have a regular arrangement.

**Crystalline:** Made of or similar to crystals.

**Crystallography:** The study of crystal form and structure

**Distribution:** The act of giving or delivering to a number of people

**Efficient:** Doing well and thoroughly with no wast of time money or energy.

**Exist:** To be real, to be present in a place or situation

**Geometric:** Having regular shapes or lines

**Identical:** Similar in every detail.

**Interpenetrate:** To spread one thing to another in each direction.

**Intersection:** A place where two or more roads, lines etc. meet or crosses each other.

**Isotropic:** Having the same properties in all direction.

**Lattice:** Regular arrangement of atoms, ions or molecules in a crystalline solid.

**Occupy:** To fill or use a space, an area or an amount of time.

**Parameter:** Some thing that decides or limits a way in which it can be done

**Periodical:** Happening fairly often and regularly

**Poly:** Many

**Primitives:** Very simple and old fashioned

**Projection:** The act of putting an image on to a surface

**Represent:** To show

**Sequence:** A set of events, actions, numbers, etc. which have a particular order and which lead to a particular order.

**Stack:** A pile, usually neatly arranged, to arrange object neatly in a pile.

**Symmetries:** Symmetry operations which transform the body into itself i.e., original position or shape.

**Unit cell:** The group of particles (atoms, ions or molecules) in a crystal that is repeated in three dimension in the crystal.

## Chapter - III

**Accommodate:** To provide with a room or place

**Anion:** Negative ion

**Arbitrary:** Determined by chance, not limited by law.

**Cation:** Positive ion

**Complicated:** Made of many different things or parts that are connected, difficult to understand.

**Concentric:** Having the same centre for circles.

**Consecutive:** following one after another in a series, without interruption.

**Constructive:** Having a useful and helpful effect rather than being negative.

**Defect:** Discontinuity in a crystal lattice.

**Deformation:** The process of changing and spoiling the normal shape

**Destructive:** Causing damage.

**Diffraction:** The bending of waves as they pass through an aperture or round the edge of a barrier

**Dislocate:** Out of its normal position

**Disorder:** lack of order

**Entropy:** a measure of the degree of disorder of a system.

**Equidistant:** Equally far from two or more places.

**Extrinsic:** Not belonging naturally, coming from or existing out side

**Fluctuate:** To change frequently in size, amount, quantity, etc.

**Glides:** To move smoothly and quietly.

**Hammering:** The act of hitting with a hammer

**Indicate:** To show, to be a sign of, to mention, to make notice.

**Intercept:** To stop.

**Interference:** The effect produced by the superposition of waves

**Interior:** connected with the inside part of

**Interplanar:** Between planes

**Interpretation:** the particular way in which a thing is understood or explained.

**Intersect:** To meet or cross each other lines

**Interstitials:** A small space

**Monochromatic radiation:** electromagnetic radiation having only one wavelength or frequency.

**Neutral:** having neither a positive charge nor a negative electrical charge

**Orientation:** The act of directing your aims towards a particular thing.

**Pattern:** A regular arrangement of lines, shapes, colours, etc. and a design on a material, carpets etc.

**Reciprocal:** Counterpart, complement

**Represent:** To show

**Scattering:** The spreading out or diffusion of a beam of radiation when it is incident on matter.

**Semiconductor:** A substance whose conductivity lies between that of an insulator and a conductor.

**Shear:** to break under pressure.

**Spiral:** A shape or design, consisting of a continuous curved line that winds around a central point.

**Substitute:** Instead of

**Succeed:** to achieve that you have been trying to do

**Successive:** Following immediately one after the other

**Vacancy:** Empty

**Vibration:** A continuous shaking moment or feeling

## Chapter - IV

**Associate:** joined or connected with a profession or an organization

**Associated:** the two things are connected because they happen together or one thing causes the other.

**Collision:** Hitting of bodies

**Complex:** Made of many different things or parts that are connected.

**Compton effect:** When an X-ray or  $\gamma$ -ray photon collides with an electron. Some of the photon's energy is transferred to the electron and consequently the wavelength of the radiation is increased. This is known as Compton effect.

**Concentric:** circles having the same centre.

**Conjugate:** to have different forms, showing number, person, tense, etc.

**Counter:** Any device for detecting and counting objects or events, often incident charged particles or photons.

**Damping:** a decrease in the amplitude of an oscillation as a result of energy being drained from the oscillating system to overcome from frictional or other resistive forces.

**Degeneracy:** The number of different arrangements of a system having the same energy.

**Derive:** to get from

**Distribution:** Arrangement or classification of particles in a system.

**Diffract:** to break up a beam of light into a series of dark and light bands

**Diffraction grating:** a glass plate with a very large number of closely spaced parallel lines (about 6000 per cm) is used to produce a spectrum of a given light.

**Discrete:** independent of other things of the same type.

**Dual:** having two parts or aspects

**Eigen function:** An allowed wave function of a system in quantum mechanics. The associated energies are eigen values.

**Evacuate:** Remove air

**Existence:** The state or fact of being real or living.

**Fluorescent:** producing bright light by using some forms of radiation

**Foil:** Metal made into very thin sheets that is used for covering or wrapping things

**Hypothesis:** An assumption as basis for investigation or reasoning. An idea or explanation based on a few known facts, which has not yet been proved to be true or correct.

**Incident:** Falling or striking on something.

**Indicate:** To show, to make notice.

**Individual:** considered separately rather than as a part of a group.

**Infinite:** Very great, impossible to measure, without limits, without end.

**Intensity:** The strength, degree or extent of any given quality.

**Instant:** happening immediately

**Macro:** large

**Momentum:** A quantity expressing the motion of a body or system. It is equal to the product of the mass of a body and its velocity. For a system, it is equal to the vector sum of the products of mass and velocity of each particle in the system.

**Observe:** to see, to notice or to watch

**Oriented:** to direct for a particular purpose

**Photo electric effect:** When photon of sufficient energy incident on alkali metals, electrons are emitted is known as photoelectric effect.

**Photon:** A quantum or 'packet' of electromagnetic radiation, usually considered as an elementary particle.

**Position:** Location, refers to the place occupied by a body or system

**Potential barrier:** A region containing a maximum of potential that prevents a particle on one side of it from passing to the other side.

**Probability:** How likely a thing is to happen

**Process:** A series of things that are done in order to achieve a particular result.

**Quantize:** To restrict a variable to discrete values, each of which is an integral multiple of the same value.

**Quantum Mechanics:** A theory based on the idea that most physical quantities like energy, angular momentum, etc. can take up only certain values and can not vary continuously

**Radiation:** The process by which energy given off by one body is transmitted through a medium or through space and absorbed by another body.

**Receive:** to get or accept or given to you

**Relativism:** in relation to other things

**Relativity:** According to this theory the mass of a body increases with velocity, length and time also changes with velocity

**Respectively:** In the same order as the people or things already mentioned

**Scatter:** to throw or drop things in different directions so that they cover an area of ground.

**Scattering:** The spreading out or diffusion of a beam of radiation when it is incident on matter

**Spur:** A sharp pointed object

**Substitute:** Instead of the one you normally use or have

**Suggest:** To put forward an idea or a plan for other people to think about.

**Target:** An object that people practice shooting at

**Validity:** The state of being logical and true.

## Chapter - V

**Absolute:** Not dependent on or relative to anything else.

**Acceptable:** Agree or approve of most people in the society.

**Acquire:** To gain by your own efforts, ability or behaviour

**Allowed:** be done, happen

**Assumption:** a belief or feeling that is true or that will happen. Although there is no proof.

**Coefficient:** a number which is placed before another quantity and which multiplies it.

**Collision:** Hitting of bodies

**Conductive:** Able to conduct electricity, heat, etc.

**Consequence:** as a result of.

**Core:** The central region of a star, planet, atom, etc.

**Distribution:** the way that some thing is shared, the act of giving or delivering to a number of people.

**Drift:** the movement of current carriers in a semiconductor under the influence of an applied voltage.

**Drop:** to fall or allow to fall.

**Equipartition:** the total energy of a molecule is equally distributed among the various degrees of freedom of the molecule

**Existence:** The state or fact of being real or living

**Forbidden:** Not allowed

**Inflection:** A change in the form.

**Insulator:** A substance that is a poor conductor of heat and electricity

**Isolate:** to separate physically or socially from other people or things

**Occupy:** To fill or use a space, an area or an amount of time

**Propagate:** To spread an idea, a belief or a piece of information among many people.

**Quantum mechanics:** The branch of mechanics that deals with moment and force in pieces of matter smaller than atoms.

**Random:** done, chosen, etc. without thinking or deciding in advance what is going to happen.

**Scatter:** To throw or drop things in different directions so that they cover an area of ground.

**Specific heat:** Heat supplied to a unit mass of a body to rise its temperature through one degree centigrade.

**Specimen:** a small amount of

**Successive:** Following immediately one after the other

**Superimpose:** To put one image on top of another so that two can be seen combined.

## Chapter - VI

**Ability:** the state of being able to do, a level of skill or intelligence.

**Alignment:** Arrangement in a straight line

**Anomalous Dispersion:** A sudden discontinuity in the graph of refractive index versus wave length of light due to the high absorbivity of the medium at wave lengths in the region of absorption band.

**Approach:** To come near to in distance or time.

**Continuum:** a series of similar items

**Contribute:** the act of giving,

**Contribution:** the act of giving, especially money, to help a person or an organization.

**Damping:** A decrease in the amplitude of an oscillation or motion with time.

**Dielectric:** A non conductor of electric charge in which an applied electric field causes a displacement of charge but not a flow of charge.

**Dipole:** Two equal and opposite charges that are separated by a distance.

**Dissipate:** To gradually become or make become weaker until it disappears.

**Distribute:** to give things to a large number of people.

**Distribution:** the way that something is shared, the act of giving or delivering to a number of people.

**Equipment:** the things that are needed for a particular purpose or activity.

**Extinguish:** to make a fire stop burning or light stop shining, to destroy

**Ignite:** to start to burn, to make start to burn

**Induce:** to influence, to cause

**Insulator:** A substance that is a poor conductor of heat and electricity

**Intercept:** to stop going from one place to another from arriving.

**Isotropic:** Exhibiting identical properties in all directions.

**Laminated:** made by sticking several thin layers together

**Microscopic:** Extremely small and difficult or impossible to see without a microscope.

**Moderate:** That is neither very good, large, hot, etc. nor very bad, small, cold, etc.,

**Optic axis:** A direction in a double refracting crystal along which the ordinary and extra- ordinary rays travel at the same speed.

**Orientation:** the direction in which an object faces.

**Permittivity:** the ratio of the electric displacement in a medium to the intensity of the electric field producing it.

**Polar:** connected with or near the north or south pole.

**Polarization:** When an insulator is placed in an electric field, the charges in its molecules separate so that one face has a net positive charge and the other a net negative charge. This effect is called electric polarization.

**Prevent:** to stop from doing

**Random:** different directions or ways

**Remance (retentivity):** The magnetic flux density remaining in a ferromagnetic substance when the saturation field is reduced to zero.

**Resonance:** An oscillation of a system at its natural frequency of vibration as determined by the physical parameters of the system.

**Restore:** to bring back a situation or feeling that existed before, to bring back to a former condition.

**Saturation:** The state or process that happens when no more of it can be accepted or added because there is already too much of it or too many of them.

**Specimen:** A small amount of that shows what the rest of it is like

**Spontaneous:** done naturally without being forced.

**Stability:** The quality or state of being steady and not changing or being disturbed in any way.

**Suggest:** to put forward an idea or plan for other people to think about.

**Susceptibility:** The state of being very likely to be influenced or affected.

**Transducer:** Device for converting a non electrical signal, such as sound, light, heat, etc. into an electrical signal or vice versa.

## Chapter - VII

**Acquire:** To gain by your own efforts, ability or behaviour.

**Agitation:** The act of stirring or shaking a liquid.

**Alloy:** A material that is formed by mixing a metal with other metal or other elements.

**Analogous:** Similar in some way to another thing or situation.

**Anisotropic:** denoting a medium in which certain physical properties are different in different directions.

**Bulk:** The main part of

**Configuration:** an arrangement of the parts or a group of things

**Confirm:** To state or how that is definitely true or correct, especially by providing evidence.

**Crystallography:** the study of crystal form and structure

**Disruption:** Difficult to continue in the normal way

**Domain:** Region inside a ferromagnetic material in which the atomic magnetic moments all point in the same directions.

**Existence:** the state or fact of being real or living.

**Feebly:** Very weak

**Gyromagnetic ratio:** the ratio of the angular momentum of an atomic system to its magnetic moment.

**Illuminate:** To shine, light on

**Intimate:** having a close and friendly relationship, very close

**Lateral:** connected with the side of or with movement to the side.

**Magnetic Induction:** The number of magnetic lines passing per unit area perpendicular to lines.

**Magnetization:** The act of acquiring or communicating magnetism.

**Magnetostriction:** Change in length of a ferromagnetic material when it is magnetized.

**Orient:** To direct towards

**Oven:** the part of a cooker like a box in which food is cooked or heated.

**Permeability:** The ratio of the magnetic flux density in a substance to the external field strength.

**Predominant:** Having more power or influence than others

**Propagate:** To spread

**Propose:** to suggest a plan, an idea, etc., for people to think about and decide on, to intended to do.

**Saturate:** to make completely

**Shrink:** to become smaller

**Specimen:** A small amount of that shows what the rest of it is like

**Suspension:** A liquid with very small pieces of solid matter floating in it.

**Unfavourable:** not good likely to cause problems or make more difficult.

**Vacuum:** A space from which the air or any matter has been exhausted.

## Chapter - VIII

**Accumulate:** To gradually get more and more of, over a period of time, gradually increase in number or quality over a period of time.

**Acquire:** to gain by yours own efforts, ability or behaviour

**Coefficient:** A number which is placed before another quantity and which multiplies it.

**Diffusion:** the process by which different substances mix as a result of the random motions of their component atoms, molecules and ions

**Drift velocity:** Average velocity at which electrons or ions progress through a medium.

**Excess:** More than is necessary, larger than

**Exert:** To make a big effort, to use power or influence to affect.

**Extrinsic semiconductor:** a semiconductor in which the current carrier density is mainly due to the presence of impurities

**Generation:** a stage in the development of a product, generation of electricity, heat etc.

**Identify:** to recognize and be able to say who or what they are

**Infinite:** very great, impossible to measure, without limits.

**Inject:** To add a particular quantity to a body.

**Insulator:** A substance that is a poor conductor of heat and electricity.

**Intrinsic semiconductor:** It is a pure semiconductor

**Minority:** The smaller part of a group, less than half of the people or things in a large group.

**Mobility:** The ability to move easily from one place to another.

**Occupy:** To fill or use a space, an area or an amount of time.

**Participate:** To take part in or become involved in an activity.

**Representation:** The act of presenting

**Rupture:** To burst or break apart inside the body.

**Semiconductor:** A substance whose conductivity lies between that of an insulator and a conductor.

**Vacancy:** A place that is available

## Chapter - IX

**Accurate:** Correct and true in every detail.

**Afloat:** Floating on water

**Approach:** To come near in distance or time.

**Attenuate:** To make weaker or less effective.

**Concept:** An idea or a principle that is connected with

**Confirm:** To state or show that is definitely true or correct by providing evidence.

**Convert:** To change or make change from one form, purpose, system, etc to another.

**Correlate:** To show that there is a close connection between two or more facts, figures, etc.

**Critical:** Serious, uncertain and possibly dangerous

**Cryotron:** A switch that relies on superconductivity.

**Diagnose:** To say exactly what an illness or the cause of a problem.

**Drop:** To fall or make fall deliberately, fall down.

**Enclosure:** Something that is placed, in an envelope

**Epilepsy:** Disorder of the nervous system that causes a person to become unconscious suddenly, often with violent movements of the body.

**Exceed:** To be greater than a particular number or amount.

**Exclusion:** The act of excluding.

**Exist:** To be real, to be present in a place or situation.

**Forbidden:** Not allowed.

**Gradually:** slowly, over a long period of time.

**Imply:** To suggest

**Interact:** To communicate with

**Invent:** To produce or design that has not existed before

**Levitate:** To rise and float in the air with no physical support

**Magnetic Induction:** The number of magnetic lines passing per unit area perpendicular to magnetic lines.

**Magnetization:** The act of acquiring or communicating magnetism.

**Magnetometer:** An instrument used for comparing magnetic moments or fields

**Mal:** Word prefix meaning bad or badly, not correct

**Participate:** To take part in or become involved in an activity.

**Penetration:** process of making a way into or through

**Persistent:** Continuing for a long period of time without interruption.

**Phonon:** A quantum of sound wave energy

**Resolution:** Giving a clear image

**Resonator:** A device for making sound louder and stronger

**Sandwich:** To fit into a very small space between two other things.

**Scatter:** To throw or drop things in different directions so that they cover an area of ground

**Segment:** A part that is separate from the other parts

**Significantly:** in a way that has a special or secret meaning

**Super:** More or better than normal, extremely

**Superconductivity:** The absence of measurable electrical resistance in certain substances at a temperature close to 0K.

**Susceptibility:** The state of being very likely to be influenced or affected

**Transition:** The process of changing from one state or condition to another

**Tunnel effect:** An effect in which there is a finite probability that electrons are able to tunnel through a narrow potential barrier.

**Variation:** Change

**Virtual:** Almost or very nearly the things described, made to appear to exist.

## Chapter - X

**Affected:** influenced in a harmful way

**Anaesthesia:** A reversible loss of sensation in all or part of the body, usually induced by drugs which may be inhaled or injected.

**Attenuation:** A loss of intensity suffered by sound, radiation, etc. as it pass through a medium.

**Automobile:** A motor car.

**Brewster's angle:** When unpolarized light incident on a medium of refractive index  $n$  at a particular angle  $x$ , called Brewster's angle, such that  $n = \tan x$

**Bury:** To place in a grave, to hide some thing in the ground.

**Caries:** decay in teeth or bones

**Choroid:** A layer, which lies between the retina and the sclerotic

**Collisions:** Hitting of bodies.

**Container:** An object designed for holding or storing, such as a box, tin, carton, etc.

**Conventional:** Traditional, normal, customary

**Converge:** To move towards a place from different directions and meet to form a large crowd

**Destroy:** To damage so badly that it no longer exist, works, etc.

**Distortion:** The extent to which a system fails to reproduce the characteristics of its input in its output.

**Etching:** To cut lines onto a piece of glass, metal, etc. in order to make words or picture.

**Excited:** Having energy higher than that of the ground state

**Flash:** A sudden brief blaze of light, a sudden and temporary increase in brightness

**Hetero:** Different,

**Homo:** Same

**Incoherent light:** Electromagnetic radiation energy not all of the same phase, also consisting of various wavelengths.

**Interaction:** Action or influence of people or things on each other

**Isotope:** An element having same atomic number but different mass number

**Metastable state:** A state of system in which it is apparently in a stable equilibrium, however, if slightly disturbed the system changes to a new state of lower energy.

**Nuclear fusion:** A type of nuclear reaction in which atomic nuclei of low atomic number fuse to form a heavier nucleus with the release of large amount of energy.

**Plasma:** A gas that has been heated to very high temperature so that most of its atoms or molecules are broken down into free electrons and positive ions

**Pollution:** The adverse effect on the natural environment including human, animal or plant life of a harmful substance that does not occur naturally

**Population inversion:** To form a situation in which the number of atoms in higher energy level is larger than that in lower energy level is called population inversion.

**Predominant:** more numerous, powerful

**Pulse:** A signal of light or electric current of very short duration.

**Recombination process:** The process in which a neutral atom or molecule is formed by the combination of a positive ion and a negative ion.

**Resonance:** Vibration that occurs when an object or system is made to oscillate at its natural frequency.

**Resonant cavity:** A closed space within a conductor in which an electromagnetic field can be made to oscillate at a frequency above those at which a resonant circuit will operate.

**Satellite:** A relatively small natural body that orbits a planet

**Spontaneous:** Occurring naturally not influenced from outside, voluntary

**Stimulated:** Increase activity, to excite

**Strip:** A long narrow flat piece of material

**Temper:** The degree of hardness and toughness of metal or glass

**Threshold:** A starting point, the minimum value of a quantity or variable that must be reached before it has a specified effect.

**Transition:** A change or passage from one condition, state, subject, place, etc. to another.

**Trimming:** The parts cut

**Unstable:** A body move away from its original position on being slightly disturbed.

**Vicinity:** The area around a particular place.

**Vital:** Necessary or essential in order

**Weapon:** An object such as a knife, gun, bomb, etc. that is used for fighting or attacking

## Chapter - XI

**Acceptance:** The act of accepting a gift, an invitation, an offer etc.,

**Aperture:** An opening that allows light to reach

**Attenuation:** A loss of intensity, suffered by sound, radiation etc. as it pass through a medium.

**Cladding:** A protective covering of a hard material

**Communication:** The activity or process of expressing ideas and feelings or of giving people information. Method of sending information especially telephones, radio, computers, etc.

**Conventional:** Traditional method or style, considered acceptable by society in general

**Core:** The central part of an object

**Coupling:** A link for joining things together.

**Critical angle:** The angle of incidence in denser medium for which the angle of refraction in rarer medium is 90 degree

**Delay:** To slow some one or something down or make them late

**Deliver:** To give.

**Dipstick:** A stick used to measure the level of a liquid in a container

**Distortion:** The extent to which a system fails to reproduce characteristics of its input.

**Encode:** To express something in or converted into code

**Extensive:** Covering a large area, great in amount, dealing with a wide range of information

**Flexible:** Bending easily, readily adaptable to suit circumstances

**Fringes:** alternate dark and bright regions produced by interference or diffraction of light

**Interferometer:** An optical instrument, which divides the incident beam and then combines to produce interference.

**Launch:** To send into

**Modulate:** To alter the tone or volume of

**Profile:** The edge or outline of that you see against a back ground.

**Pulse:** A signal of light or electric current of very short duration.

**Receive:** To get, be given, accept, welcome

**Reflection:** The action or process of sending back light, heat, sound, etc. from a surface

**Refract:** The bending of light when it goes from one medium to another

**Regenerate:** To produce again, to renew, to be brought back

**Reliable:** to depend on, to be certain of

**Repeater:** Someone or something that repeats

**Sensor:** any of various devices that detect or measure a change in a physical quantity, usually by converting it into an electrical signal

**Span:** the interval, length, distance etc. between two points in space or time.

**Split:** to divide or break into, to divide or separate

**Spreading:** Increasing in size, extent

**Submarine:** A ship that can travel under water

**Successive:** Following immediately one after the other

**Superimpose:** on top of another

**Tolerance:** the ability to resist or endure pain or hardship

**Total internal reflection:** The total reflection of a beam of light in the denser medium at the interface of denser medium and rarer medium (of lower refractive index) when the angle of incidence in the denser medium exceeds critical angle.

**Transmission:** The act or process of passing from one person, place or thing to another, the act or process of sending out an electronic signal.

**Transmitter:** The equipment that transmits the signals

## Chapter - XII

**Coding:** A set of rules and characters for converting one form of data to another.

**Coherent:** Having a constant phase relationship.

**Construct:** Make by fitting parts together, build, form.

**Conventional:** Custom, usual or general agreement.

**Destructive:** Make useless.

**Diffraction:** The process of spreading waves of light or other things by passing through a narrow aperture or across sharp edge of an object.

**Exposing:** Lay open or leave uncovered.

**Flaws:** An imperfection, a crack or similar fault.

**Foetus:** An unborn mammalian offspring.

**Hologram:** A photograph of the interference pattern, which when suitably illuminated produces a three dimensional image.

**Illuminate:** Light up, make bright, spread luster on.

**Information:** Something told, the act of telling news.

**Interference:** Combine of light (or other) waves to produce a pattern.

**Monochromatic:** Containing only one colour or light of single wave length.

**Non-destructive:** Does not involve destruction or damage.

**Pregnant:** A woman having a child developing in the uterus.

**Reconstruction:** Build or form again.

**Virtual:** Relating to the points at which rays would meet if produced backwards.

## Chapter - XIII

**Absorption:** To take in or receive; the removal of energy by the medium through which it passes.

**Acoustics:** The branch of physics that deals with sound and sound waves.

**Architecture:** The design and construction of buildings with focus on stability and sense of beauty.

**Cavitation:** The formation and collapse of vapour pockets in a flowing liquid in regions of low pressure.

**Damping:** To cause a decrease in the energy of something.

**Decoupling:** To cause to become separated or disconnected.

**Empirical:** Derived from or guided by experience or observation, without using scientific methods.

**Quieting:** To make something quiet, or to prevent it from making sound.

**Remedy:** Something that corrects or restores to the correct or proper condition.

**Resonance:** A large vibration produced in a system when it is subjected to an external stimulus whose frequency is the same or nearly the same as the natural frequency of the system.

**Reverberation:** Reflection or replication of sound.

**Stall:** The condition of an engine being stopped because of poor supply or overload of fuel mixture.

**Standing wave:** A wave that remains in a constant position.

**Sympathetic vibration:** The vibration of a body at its natural frequency in response to the vibration of a neighbouring body at that frequency.

## Chapter - XIV

**Alignment:** Put in a straight line or bring into line.

**Alternator:** A dynamo that generates an alternating current.

**Amenable:** Responsive, tractable.

**Analytical:** Using analytic methods.

**Aviation:** The skill or practice of operating air craft.

**Bulk:** The greater part of number, a large bodily volume or a large mass.

**Catalyst:** A substance, that without itself undergoing any permanent chemical change, increases the rate of a reaction.

**Cluster:** A close group or bunch of similar things growing or occurring.

**Coercive:** restrain or persuade.

**Colloids:** A substance consisting of ultra microscopic particles dispersed in a second substance, as in gels, soils and emulsions.

**Confine:** Hold captive or restrict.

**Corrosion:** The process of wear away by chemical action or destroy gradually.

**Cosmetic:** intended to adorn or beautify the body.

**Design:** A preliminary plan or sketch for making something.

**Desire:** A longing or craving

**Deviate:** Turn aside or diverge.

**Diabetes:** Any disorder of the metabolism with excessive thirst and the production of a large amount of urine.

**Disperse:** Distribute or derive in different directions.

**Drag:** Draw on, pull along with effort.

**Ductility:** Capable of being drawn into wire or easily moulded.

**Erosion:** Wear away, destroy or destroyed gradually.

**Exist:** Be alive, occur, be found, have being under specified Conditions.

**Exploitation:** A daring feat, take advantage of

**Extension:** A part enlarging or added onto a main structure or an instance of extending the process.

**Extract:** Remove, takeout, select or reproduce for quotation.

**Fabricate:** Construct from prepared components.

**Fatigue:** Weakness in materials caused by repeated variation of stress.

**Gelatin:** A virtually colourless, tasteless transparent water-soluble protein derived from collagen and used in food, photography, etc.

**Granular:** Like grains or granules.

**Host:** A person who receives or entertains another as a guest.

**Illumination:** The act or process of illuminating.

**Inhibit:** Prevent or restrain.

**Interface:** A surface forming a Common boundary between two regions.

**Isolation:** The sate of being isolated.

**Lithography:** A process of printing from a plate so that ink adheres only to the design to be printed.

**Manipulate:** Manage to one's own advantage, alter.

**Manufacture:** The making of articles.

**Monitor:** Any of various persons or devices for checking or warning about a situation, operation, etc.

**Mutation:** The process or an instance of change or alteration.

**Nanotechnology:** The branch of technology that deals with dimensions and tolerances of less than 100 nanometres.

**Opaque:** Not transmitting light, impenetrable to sight.

**Pattern:** A model or design from which copies can be made.

**Pixels:** A grid of display elements made up of dots of phosphor that glows when stimulated by electrons.

**Photolithography:** Lithography using plates made photo graphically.

**Porous:** Full of pores, pore is a minute opening in surface through which gas, liquid or fine solids may pass.

**Probe:** A penetrating investigation, a small device for measuring, testing, etc.

**Random:** Made, done, etc. without method or conscious choice, with equal chances for each item.

**Resist:** Offer opposition, a protective coating of a resistance substance, withstand the action, prevent from reaching, penetrating.

**Robust:** Strong and sturdy in physique or construction.

**Specimen:** An individual or part taken as an example of a class.

**Stain:** Spoil, damage, discolour or be discoloured by the action of liquid sinking in.

**Tag:** A label tied to an object to show its address or an electronic device that can be attached to a person or thing for monitoring purposes.

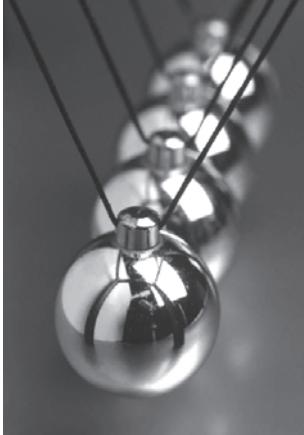
**Therapy:** The treatment of physical or mental disorders, other than by surgery.

**Tough:** Hard to break, cut, tear or chew, durable.

**Wafer:** Very thin; a very thin slice of a semiconductor crystal.

**Wrinkle:** Slight crease in the skin such as is produced by age.

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## Question Papers

### Set - 1

I - B.Tech. Supplementary Examinations, Aug/Sep – 2008  
(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)

Time: 3 hours

Max. Marks: 80

Note: Answer any FIVE questions  
All questions carry equal marks

- 1a. Define coordination number and packing factor of a crystal.  
b. Describe BCC crystal structure, with a suitable example.  
c. Obtain an expression for the packing factor of FCC structure. (4 + 6 + 6)
- 2a. Derive 3-dimensional, time independent Schrodinger wave equation for an electron.  
b. What is the physical significance of wave function?  
c. Deduce the expression for energy of an electron confined to a potential box of width 'x'. (6 + 4 + 6)
- 3a. Discuss with suitable mathematical expressions, the Kronig-Penney model for the energies of an electron in a metal.  
b. Explain the classification of metals, semiconductors and insulators based on band theory. (10 + 6)
- 4a. Explain the following:
  - i. Electric Polarization and
  - ii. Polarizability.  
b. Derive Clausius-Mosotti relation in dielectrics subjected to static fields.  
c. Argon gas contains  $2.70 \times 10^{25}$  atoms/m<sup>3</sup> at 0°C and at 1 atm. Pressure. Calculate the dielectric constant, if the diameter of argon atom is 0.384 nm. (4 + 8 + 4)

Q-2 | **Question Papers**

- 5a. Distinguish between intrinsic and extrinsic semiconductors with suitable examples.
- b. Derive an expression for the density of holes in valence band of an intrinsic semiconductor. (8 + 8)
- 6a. What is population inversion relating to laser action? Explain.
- b. Show that the ratio of Einstein's coefficient of spontaneous emission to Einstein's coefficient of absorption, is proportional to the cube of the frequency of the incident photon. (6 + 10)
- 7a. Describe the structure of an optical fiber.
- b. Explain, in detail, the basic principle of an optical fiber.
- c. Write the applications of fiber optics in medicine and industry. (6 + 6 + 4)
- 8a. Write a detailed note on nanoscience.
- b. Why nanomaterials exhibit different properties? Explain. (6 + 10)

**Set - 2**

**I - B.Tech. Supplementary Examinations, Aug/Sep – 2008  
(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel & E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the formation of an ionic crystal, with a suitable example.
- 1b. Derive an expression for the cohesive energy of an ionic crystal. (6 + 10)
- 2a. Show that the energies of a particle in a 3-dimensional potential box, are quantized.
- 2b. Discuss, in detail, the physical significance of wave function.
- 2c. A neutron beam of kinetic energy 0.04 eV is diffracted at the plane (1 0 0) of a simple cubic crystal for which  $d_{110}$  is 0.314 nm. Calculate the glancing angle at which first order Bragg diffraction will be observed. (6 + 4 + 6)
- 3a. Discuss with suitable mathematical expressions, the Kronig-Penney model for the energies of an electron in a metal.
- 3b. Explain the classification of metals, semiconductors and insulators based on band theory. (10 + 6)
- 4a. What are the sources of permanent dipole moment in magnetic materials?
- 4b. Explain the hysteresis loop observed in Ferro-magnetic materials.
- 4c. Write notes on Ferro-electricity. (6 + 6 + 4)
- 5a. Write notes on direct band gap and indirect band gap semiconductors.
- 5b. Show that for a p-type semiconductor the Hall coefficient,  $R_H = (1/ne)$ . (8 + 8)
- 6a. Explain the characteristics of a LASER.
- 6b. Describe the construction and working of a semiconductor laser.
- 6c. Write any four applications of laser. (4 + 8 + 4)
- 7a. What is the basic principle of holography? Explain.
- 7b. How to construct and reconstruct a hologram? (6 + 10)
- 8a. Write a detailed note on nanoscience and nanotechnology.
- 8b. Write the important applications of nanomaterials in medicine. (10 + 6)

**Set - 3**

**I - B.Tech. Supplementary Examinations, Aug/Sep – 2008  
(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)**

**Time: 3 hours**

**Max. Marks: 80**

**Note: Answer any FIVE questions**

**All questions carry equal marks**

- 1a. Explain the terms
  - i. basis
  - ii. space lattice
  - iii. lattice parameters and
  - iv. unit cell.b. Deduce the expression for the inter-planar separation in terms of Miller indices for a cubic structure. (6 + 10)
- 2a. Derive one-dimensional, time independent Schrodinger wave equation for an electron.  
b. What is the physical significance of wave function?  
c. An electron is confined to a box of length  $10^{-8}$ m. Calculate the minimum uncertainty in velocity. (8 + 4 + 4)
- 3a. Explain the terms (i) mean free path, (ii) relaxation time and (iii) drift velocity of an electron in a metal.  
b. Discuss the origin of electrical resistance in metals.  
c. Calculate the mobility of the electrons in copper obeying classical laws. Given that the density of copper =  $8.92 \times 10^3$  kg/m<sup>3</sup>, Resistivity of copper =  $1.73 \times 10^{-8}$  ohm-m, atomic weight of copper = 63.5 and Avogadro's number =  $6.02 \times 10^{26}$  per k-mol. (6 + 6 + 4)
- 4a. Explain the terms:
  - i. Magnetic flux density
  - ii. Magnetic field strength
  - iii. Magnetization and
  - iv. Magnetic susceptibility. How they are related to each other?b. What are hard and soft magnetic materials? Write their characteristic properties and applications. (8 + 8)
- 5a. Write a note on intrinsic semiconductors.  
b. Derive an expression for the number of electrons per unit volume in the conduction band of an intrinsic semiconductor. (6 + 10)
- 6a. Describe the various methods to achieve population inversion relating to lasers.  
b. With the help of a suitable diagram, explain the principle, construction and working of a helium-neon laser. (6 + 10)
- 7a. Explain the principle of an optical fiber.  
b. Explain how the optical fibers are classified.  
c. Calculate the angle of acceptance of a given optical fibre, if the refractive indices of the core and the cladding are 1.563 and 1.498 respectively. (6 + 6 + 4)
- 8a. What are nanomaterials Explain.  
b. Nanomaterials exhibit different properties. Explain the reasons. (6 + 10)

**Set - 4**

**I - B.Tech. Supplementary Examinations, Aug/Sep – 2008  
(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Describe, in detail, the seven crystal systems with diagrams.
- 1b. Sketch the planes  $(1\ 2\ 0)$ ,  $(2\ 1\ 3)$  and directions  $[1\ 0\ 0]$  and  $[2\ 1\ 1]$  (10 + 6)
- 2a. Discuss the de Broglie hypothesis of duality of matter particles.
- 2b. Describe, in detail, with a neat diagram, Davisson and Germer experiment to show that particles behave like waves. (6 + 10)
- 3a. Distinguish between Drude-Lorentz theory and Sommerfeld's theory of metals.
- 3b. Explain the Fermi-Dirac distribution function of electrons.
- 3c. For a metal having  $6.5 \times 10^{28}$  conduction electrons per  $\text{m}^3$ , calculate relaxation time of electrons, if the metal has the resistivity  $1.43 \times 10^{-8}$  ohm-m. [Mass of electron =  $9.1 \times 10^{-31}$  Kg] (6 + 6 + 4)
- 4a. Explain the following:
  - i. Polarization vector and
  - ii. Electric displacement.
- 4b. Deduce an expression for Lorentz field relating to a dielectric material.
- 4c. The radius of the helium atom is  $0.55 \text{ \AA}$ . Calculate the polarizability of He and its relative permittivity. The number of He atoms in a volume of one metre cube is  $2.70 \times 10^{25}$  atoms. [permittivity of free space =  $8.85 \times 10^{-12} \text{ F/m}$ ] (4 + 8 + 4)
- 5a. Distinguish between intrinsic and extrinsic semiconductors with suitable examples.
- 5b. Derive an expression for the density of electrons in conduction band of an intrinsic semiconductor. (8 + 8)
- 6a. What is population inversion relating to laser action? Explain.
- 6b. Distinguish between homo-junction semiconductor laser and hetero-junction semiconductor laser.
- 6c. A semiconductor diode laser has a peak emission wavelength of  $1.55 \mu\text{m}$ . Find its band gap in eV. (4 + 8 + 4)
- 7a. Derive the expressions for
  - i. acceptance angle and
  - ii. numerical aperture, of an optical fiber.
- 7b. Describe different types of fibers by giving the refractive index profiles and propagation details. (8 + 8)
- 8a. How the physical and chemical properties of nano-particles vary with their size?
- 8b. Write the important applications of nanomaterials. (10 + 6)

**Set - 1****I - B.Tech. Regular Examinations, May/June – 2008****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the forces between the two interacting atoms when they are brought nearer to form a molecule.  
b. Derive the expression for the equilibrium spacing of two atoms for which the potential energy is minimum. (6 + 10)
- 2a. Explain de-Broglie hypothesis.  
b. Describe G.P.Thomson's experiment in support of this hypothesis.  
c. Find the wavelength associated with an electron rose to a potential 1600 V. (4 + 8 + 4)
- 3a. Distinguish between Drude-Lorentz theory and Sommerfeld's theory of metals.  
b. Define Fermi level of electron.  
c. Find the drift velocity of free electrons in a copper wire of cross-sectional area  $10 \text{ mm}^2$ , when the wire carries a current of  $100 \text{ A}$ . Assume that each copper atom contributes one electron to the electron gas. [Density of copper =  $8.92 \times 10^3 \text{ kg/m}^3$ , Atomic weight of copper = 63.5 and Avagadro's number =  $6.02 \times 10^{26}$  per k-mol] (10 + 2 + 4)
- 4a. Explain the following:
  - i. Dielectric constant
  - ii. Electric susceptibility
  - iii. Electric polarization and
  - iv. Polarizability.(6 + 10)  
b. Write notes on:
  - i. Ferro-electricity and
  - ii. Piezo-electricity.(6 + 10)
- 5a. Explain the critical parameters and their significance in superconductors.  
b. Write notes on:
  - i. isotope effect and
  - ii. energy gap, in superconductors.  
c. A Josephson junction having a voltage of  $8.50 \mu\text{V}$  across its terminals, then calculate the frequency of the alternating current. [Planck's constant =  $6.626 \times 10^{-34} \text{ J - sec}$ ] (4 + 8 + 4)
- 6a. Explain the characteristics of a LASER.  
b. Describe the construction and working of ruby laser.  
c. Write any four applications of laser. (4 + 8 + 4)
- 7a. Derive an expression for the 'numerical aperture' of an optical fiber.  
b. Explain the advantages of optical communication system.

- c. The numerical aperture of an optical fiber is 0.39. If the difference in the refractive indices of the material of its core and the cladding is 0.55, calculate the refractive index of material of the core, when the light is launched into it in air. (8 + 4 + 4)
- 8a. Write a detailed note on nanoscience and nanotechnology.
- b. Write the important applications of nanomaterials in medicine. (10 + 6)

**Set - 2****I - B.Tech. Regular Examinations, May/June – 2008****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. What is Bragg's law? Explain.  
 b. Describe Laue's method for the determination of crystal structure.  
 c. The Bragg's angle in the first order for (2 2 0) reflection from nickel (FCC) is  $38.2^\circ$  when X-rays of wavelength  $1.54 \text{ \AA}$  are employed in a diffraction experiment. Determine the lattice parameter of nickel.  $(4 + 8 + 4)$
- 2a. Explain, in detail, the properties of matter waves.  
 b. Describe Davisson and Germer experiment to verify the wave nature of matter  $(6 + 10)$
- 3a. Distinguish between classical free electron theory and quantum free electron theory of metals.  
 b. Explain the Fermi-Dirac distribution function of electrons. Explain the effect of temperature on the distribution.  $(8 + 8)$
- 4a. Explain the following:  
 i. Dielectric constant  
 ii. Electric susceptibility,  
 iii. Electric polarization and  
 iv. Polarizability.  
 b. Write notes on:  
 i. Ferro-electricity and  
 ii. Piezo-electricity.  $(6 + 10)$
- 5a. What is Meissner effect? Explain.  
 b. Describe the difference between Type-I and Type-II superconductors.  
 c. The critical field for niobium is  $1 \times 10^5 \text{ amp/m}$  at  $8 \text{ K}$  and  $2 \times 10^5 \text{ amp/m}$  at absolute zero. Find the transition temperature of the element.  $(4 + 8 + 4)$
- 6a. Distinguish between spontaneous emission and stimulated emission.  
 b. Distinguish between homo-junction semiconductor laser and hetero-junction semiconductor laser.  
 c. A semiconductor diode laser has a peak emission wavelength of  $1.55 \mu\text{m}$ . Find its band gap in eV.  $(4 + 8 + 4)$
- 7a. Derive the expressions for  
 i. acceptance angle and  
 ii. numerical aperture of an optical fiber.  
 b. Describe different types of fibers by giving the refractive index profiles and propagation details.  $(8 + 8)$
- 8a. How the physical and chemical properties of nano-particles vary with their size?  
 b. Write the important applications of nanomaterials.  $(10 + 6)$

**Set - 3**

**I - B.Tech. Regular Examinations, May/June – 2008**  
**(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Plot and explain the variation of (i) attractive potential energy (ii) repulsive potential energy and (iii) resultant potential energy with inter-atomic distance, when two atoms are brought nearer.
- b. The Madelung constant of KCl is 1.75. Its neighbour separation is 0.314 nm. Find the cohesive, energy per atom. [Given that the Repulsive exponent value = 5.77; Ionization energy of potassium = 4.1 eV; Electron affinity of chlorine = 3.6 eV] (10 + 6)
- 2a. Discuss the de Broglie hypothesis of duality of matter particles.
- b. Describe GP Thomson's experiment to verify the wave nature of matter. (6 + 10)
- 3a. Explain the terms (i) mean free path, (ii) relaxation time and (iii) drift velocity of an electron in a metal.
- b. Discuss the origin of electrical resistance in metals.
- c. Calculate the mobility of the electrons in copper obeying classical laws. Given that the density of copper =  $8.92 \times 10^3$  kg/m<sup>3</sup>, Resistivity of copper =  $1.73 \times 10^{-8}$  Ohm-m, atomic weight of copper = 63.5 and Avogadro's number =  $6.02 \times 10^{26}$  per k-mol. (6 + 6 + 4)
- 4a. Describe the phenomenon of electronic polarization and obtain an expression for electronic polarizability.
- b. Write notes on:
  - i. Ferro-electricity and
  - ii. Piezo-electricity.(8 + 8)
- 5a. write a note on intrinsic semiconductors.
- b. Derive an expression for the carrier concentration in n-type extrinsic semiconductors. (6 + 10)
- 6a. Distinguish between spontaneous emission and stimulated emission.
- b. Distinguish between homo-junction semiconductor laser and hetero-junction semiconductor laser.
- c. Calculate the wavelength of emitted radiation from GaAs which has a band gap of 1.44 eV. (4 + 8 + 4)
- 7a. What are important features of optical fibers.
- b. Describe the communication process using optical fibers.
- c. Write the uses of fiber optics in different fields. (4 + 6 + 6)
- 8a. Write a detailed note on nanoscience and nanotechnology.
- b. Write the important applications of nanomaterials in medicine. (10 + 6)

**Set - 4****I - B.Tech. Regular Examinations, May/June – 2008****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the various types of bonding in solids with suitable examples.
- 1b. The Madelung constant of KCl is 1.75. Its neighbour separation is 0.314 nm. Find the cohesive energy per atom. [Given that the Repulsive exponent value = 5.77; Ionization energy of potassium = 4.1 eV; Electron affinity of chlorine = 3.6eV] (10 + 6)
- 2a. Distinguish between a matter wave and an electromagnetic wave.
- 2b. Describe GP Thomson's experiment to study electron diffraction.
- 2c. Find the wavelength associated with an electron rose to a potential 1600 V. (4 + 8 + 4)
- 3a. Explain the following:
  - i. Electrical resistivity and
  - ii. Fermi energy.
- 3b. Explain briefly the quantum free electron theory of metals.
- 3c. On the basis of band theory how the crystalline solids are classified into metals, semiconductors and insulators? (4 + 6 + 6)
- 4a. Explain the hysteresis loop observed in ferro-magnetic materials.
- 4b. Explain clearly difference between hard and soft magnetic materials. (8 + 8)
- 5a. How are 'superconductors' classified? Explain their properties.
- 5b. What is Meissner effect? Explain
- 5c. Write notes on the applications of superconduction materials. (6 + 4 + 6)
- 6a. Describe the various methods to achieve population inversion relating to lasers.
- 6b. With the help of a suitable diagram, explain the principle, construction and working of a semiconductor laser. (6 + 10)
- 7a. Distinguish between light propagation in
  - i. step index optical fiber and
  - ii. graded index optical fiber.
- 7b. Write a note on fiber optic medical endoscopy. (10 + 6)
- 8a. Write a detailed note on nanoscience.
- 8b. Why nanomaterials exhibit different properties? Explain. (6 + 10)

**Set - 1**

**I - B.Tech. Regular Examinations, April/May – 2007**  
**(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel& & E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Show that FCC is the most closely packed of the three cubic structures by working out the packing factors. (10)  
b. Describe the structure of NaCl. (6)
- 2a. Draw the (112) and (120) planes and the (112) and (120) directions of a simple cubic crystal. (4)  
b. Derive an expression for the inter-planar spacing in the case of a cubic structure. (8)  
c. Calculate the glancing angle at (110) plane of a cubic crystal having an axial length of 0.26 mm corresponding to the second order diffraction maximum for the X-rays of wavelength of 0.065 mm. (4)
- 3a. What is Frenkel defect? Explain. (6)  
b. Derive an expression for the concentration of Frenkel defects present in a crystal at any temperature. (10)
- 4a. Explain the origin of energy bands in solids. (6)  
b. Assuming the electron-lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons. (6)  
c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy. (4)
- 5a. Explain the polarization mechanism in dielectric materials. (8)  
b. What are the important requirement of good insulating materials? (4)  
c. A parallel plate capacitor of area  $650 \text{ mm}^2$  and a plate separation of 4 mm has a charge of  $2 \times 10^{-10} \text{ C}$  on it. When a material of dielectric constant 3.5 is introduced between the plates, what is the resultant voltage across the capacitor? (4)
- 6a. Distinguish between metals, semiconductors and insulators. (6)  
b. Explain the effect of temperature on resistivity of a semiconductor. (4)  
c. Derive an expression for the number of electrons per unit volume in the conduction band of an intrinsic semiconductor. (6)
- 7a. What do you understand by population inversion? How it is achieved? (6)  
b. Derive the relation between the probabilities of spontaneous emission and stimulated emission in terms of Einsteins coefficients. (10)
- 8a. Define the relative refractive index difference of an optical fibre. Show how it is related to numerical aperture. (6)  
b. Draw the block diagram of an optical fibre communication system and explain the function of each block. (10)

**Set - 2****I - B.Tech. Regular Examinations, April/May – 2007****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Define crystal lattice, unite cell, lattice parameter and coordination number. (8)  
 b. Consider a body centered cubic lattice of identical atoms having radius R. Compute  
     i. the number of atoms per unit cell  
     ii. the coordination number and  
     iii. the packing fraction (8)
- 2a. What are Miller indices? Draw (111) and (110) planes in a cubic lattice. (6)  
 b. Explain Bragg's law of X-ray diffraction. (6)  
 c. The Bragg's angle for reflection from the (111) plane in a FCC crystal is  $19.2^\circ$  for an X-ray wavelength of 1.54 A.U. Compute the cube edge of the unit cell. (4)
- 3a. Explain Schottky and Frenkel defects with the help of suitabl figures. (10)  
 b. Explain the significance of Burgers vector. (6)
- 4a. How does the electrical resistance of a metal change with temperature? (4)  
 b. Discuss the motion of an electron in a periodic lattice. (8)  
 c. Find the relaxation time of conduction electrons in a metal having resistivity  $1.54 \times 10^{-8} \Omega\text{-m}$ , if the metal has  $5.8 \times 10^{28}$  conduction electrons per cubic meter. (4)
- 5a. Obtain a relation between electronic polaratization and electric susceptibility of the dielectric medium. (6)  
 b. What is dielectric breakdown? Explain briefly the various factors contributing to breakdown in dielectrics. (6)  
 c. A parallel plate capacitor having a plate separation of  $2 \times 10^{-3}$  m across which a potential of 10 V is applied. Calculate the dielectric displacement, when a material of dielectric constant 6.0 is introduced between the plates. (4)
- 6a. Explain Meissner effect. (6)  
 b. What is meant by isotopic effect? Explain with suitable example. (6)  
 c. A superconducting material has a critical temperature of 3.7 K, and a magnetic field of 0.0306 Tesla at 0 K. Find the critical field at 2 K. (4)
- 7a. Explain the terms:  
     i. Absorption  
     ii. Spontaneous emission  
     iii. Stimulated emission  
     iv. Pumping mechanism  
     v. Population inversion  
     vi. Optical cavity. (12)  
 b. Mention the medical applications of lasers. (4)

- 8a. Explain the principle behind the functioning of an optical fibre. (4)
- b. Derive an expression for acceptance angle for an optical fibre. How it is related to numerical aperture? (8)
- c. An optical fibre has a numerical aperture of 0.20 and a cladding refractive index of 1.59. Find the acceptance angle for the fibre in water which has a refractive index of 1.33. (4)

**Set - 3****I - B.Tech. Regular Examinations, April/May – 2007****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Show that FCC is the most closely packed of the three cubic structures by working out the packing factors. (10)  
b. Describe the structure of NaCl. (6)
- 2a. Explain Bragg's law of X-ray diffraction. (6)  
b. Describe Laue's method for determination of crystal structure. (6)  
c. A beam of X-ray is incident on a NaCl crystal with lattice spacing 0.282 nm. Calculate the wavelength of X-rays if the first order Bragg reflection takes place at a glancing angle of  $8^\circ 35'$ . Also calculate the maximum order of diffraction possible. (4)
- 3a. What is Frenkel defect? Explain. (6)  
b. Derive an expression for the concentration of Frenkel defects present in a crystal at any temperature. (10)
- 4a. Explain the origin of energy bands in solids. (6)  
b. Assuming the electron-lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons. (6)  
c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy. (4)
- 5a. What is ferromagnetic? What are the distinguishing features of ferromagnetism? (8)  
b. What are ferrites? Explain the magnetic properties of ferrites and mention their industrial applications. (8)
- 6a. Derive the continuity equation for electrons. (8)  
b. What physical law is manifested in the continuity equation? (4)  
c. Find the diffusion coefficient of electrons in silicon at 300 K if  $\mu$  is  $0.19 \text{ m}^2/\text{V-S}$ . (4)
- 7a. What do you understand by population inversion? How is it achieved? (6)  
b. Derive the relation between the probabilities of spontaneous emission and stimulated emission in terms of Einstein's coefficients. (10)
- 8a. Define the relative refractive index difference of an optical fibre. Show how it is related to numerical aperture. (6)  
b. Draw the block diagram of an optical fibre communication system and explain the function of each block. (10)

**Set - 4****I - B.Tech. Regular Examinations, April/May – 2007****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the “Unit Cell” and “Lattice” parameters. What is a primitive cell and how does it differ from unit cell? (6)
- b. Describe the crystal structure of CsCl. (4)
- c. Chromium has BCC structure. Its atomic radius is 0.1249 nm. Calculate the free volume / unit cell. (6)
- 2a. What are Miller indices? Draw (111) and (110) planes in a cubic lattice. (6)
- b. Explain Bragg's law of X-ray diffraction. (6)
- c. The Bragg's angle for reflection from the (111) plane in a FCC crystal is  $19.2^\circ$  for an X-ray wavelength of 1.54 Å.U. Compute the cube edge of the unit cell. (4)
- 3a. Show that the wavelength of an electron accelerated by a potential difference 'V' volts, is  $\lambda = 1.227 \times 10^{-10} \sqrt{V} \text{ m}$  for non-relativistic case. (6)
- b. Describe an experiment to establish the wave nature of electrons. (6)
- c. Explain the difference between a matter wave and an electromagnetic wave. (4)
- 4a. Explain the origin of energy bands in solids. (6)
- b. Assuming the electron-lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons. (6)
- c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy. (4)
- 5a. What is intrinsic break down in dielectric materials? (4)
- b. Explain electronic polarization in atoms and obtain an expression for electronic polarisability in terms of the radius of the atom. (8)
- c. A parallel plate capacitor has an area of  $100 \text{ cm}^2$ , with a separation of 1 cm and is charged to a potential of 100 V. Calculate the capacitance of the capacitor and the charge on the plates. (4)
6. Explain the following: (6 + 5 + 5)
  - a. Critical magnetic field of a superconductor as a function of temperature.
  - b. Meissner effect.
  - c. Cryotrons.
- 7a. Explain with a neat diagram.
  - i. absorption
  - ii. spontaneous emission and
  - iii. stimulated emission of radiation. (8)
- b. What is population inversion? How it is achieved by optical pumping? (8)

Q-16 | **Question Papers**

- 8a. Describe the construction of a typical optical fibre and give the dimensions of the various parts. (4)
- b. Define the acceptance angle and numerical aperture. Obtain an expression for the numerical aperture of an optical fibre. (8)
- c. Calculate the numerical aperture and acceptance angle for an optical fibre with core and cladding refractive indices being 1.48 and 1.45 respectively. (4)

**Set - 1**

**I - B.Tech. Regular Examinations, May/June – 2006**  
**(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Define coordination number and packing factor of a crystal. (4)  
b. Describe the FCC crystal structure. (6)  
c. Obtain an expression for the packing factor of FCC structure. (6)
- 2a. What are Miller indices? How are they obtained? (8)  
b. Explain Bragg's Law of X-ray diffraction. (8)
- 3a. Explain the concept of matter waves (6)  
b. Describe Davison and Germer's experiment and explain how it enabled the verification of wave nature of matter. (6)  
c. Calculate the velocity and kinetic energy of an electron of wavelength  $1.66 \times 10^{-10}$  m. (4)
- 4a. How does the electrical resistance of a metal change with temperature? (4)  
b. Discuss the motion of electrons in a periodic lattice. (4)  
c. Find the relaxation time of conduction electron in a metal having resistivity  $1.54 \times 10^{-8} \Omega\text{-m}$ , if the metal has  $5.8 \times 10^{28}$  conduction electrons per cubic meter. (4)
- 5a. Define the terms magnetic susceptibility, magnetic induction and permeability. How is magnetic susceptibility of a material measured? (10)  
b. Explain the salient features of anti-ferromagnetic materials. (6)
- 6a. Describe the drift and diffusion currents in a semiconductor. (6)  
b. Derive their expressions. (6)  
c. Deduce Einstein relation (4)
- 7a. Explain the following:
  - i. Life time of an energy level
  - ii. Optical pumping processes.
  - iii. Metastable states. (6)
- b. Distinguish between spontaneous and stimulated emission processes of light. (4)  
c. Discuss briefly the different methods of producing laser light (6)
- 8a. Describe the construction of a typical optical fibre and give the dimension of the various parts. (4)  
b. Define the acceptance angle and numerical aperture. Obtain an expression for the numerical aperture of an optical fibre. (8)  
c. Calculate the numerical aperture and acceptance angle for an optical fibre with core and cladding refractive indices being 1.48 and 1.45 respectively. (4)

**Set - 2****I - B.Tech. Regular Examinations, May/June – 2006****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the forces between the two interacting atoms when they are brought nearer to form a molecule. (6)
- b. Derive the expression for the equilibrium spacing of two atoms for which the potential energy is minimum and hence obtain the dissociation energy. (10)
- 2a. State and explain Bragg's law. (6)
- b. Describe with suitable diagram, the powder method for determination of crystal structure. (6)
- c. A beam of X-ray of wavelength 0.071 nm is diffracted by (110) plane of rock salt with lattice constant of 0.28 nm. Find the glancing angle for the second order diffraction. (4)
- 3a. Distinguish between Frenkel and Schottky defects. (8)
- b. Derive an expression for the energy change due to creation of vacancies in side a solid. (8)
- 4a. Explain the origin of energy bands in solids. (6)
- b. Assuming the electron – lattice interaction to be responsible for scattering of conduction electrons in a metal. Obtain an expression for conductivity in terms of relaxation time and explain any three draw backs of classical theory of free electrons. (6)
- c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy. (4)
- 5a. What is meant by ferror-magnetic materials? Give example. (4)
- b. Explain the hysteresis properties of ferromagnetic materials. (6)
- c. Mention the various properties of para-magnetic materials. (6)
- 6a. How are the superconductors classified? Explain their properties. (6)
- b. What is Meissner effect? (6)
- c. Write notes on the applications of superconducting materials. (6)
- 7a. With necessary theory and energy level diagram, explain the working of a Helium-Neon gas laser.(10)
- b. Mention some important applications of lasers. (6)
- 8a. Distinguish between light propagation in
  - i. step index and
  - ii. graded index optical fibres.
- b. Discuss the various advantages of communication with optical fibres over the conventional coaxial cables. (6)
- c. Calculate the refractive indices of core and cladding of an optical fibre with a numerical aperture 0.33 and their fractional difference of refractive indices being 0.02. (4)

**Set - 3****I - B.Tech. Regular Examinations, May/June – 2006****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Define coordination number and packing factor of a crystal. (4)  
b. Describe the FCC crystal structure. (6)  
c. Obtain an expression for the packing factor of FCC structure. (6)
- 2a. Explain how the X-ray diffraction can be employed to determine the crystal structure (10)  
b. The distance between (110) planes in a body-centered cubic structure is 0.203 nm. What is the size of the unit cell? What is the radius of the atom? (6)
- 3a. Explain the concept of matter waves. (6)  
b. Describe Davison and Germer's experiment and explain how it enabled the verification of wave nature of matter. (6)  
c. Calculate the velocity and kinetic energy of an electron of wavelength  $1.66 \times 10^{-10}$ m (4)
- 4a. Explain the origin of energy bands in solids. (6)  
b. Assuming the electron – lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons. (6)  
c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy. (4)
- 5a. Explain the electrochemical breakdown in dielectric materials. (4)  
b. Explain the concept of internal field in solids and hence obtain an expression for the static dielectric constant of elemental solid dielectric. (8)  
c. A parallel plate capacitor having an area  $6.45 \times 10^{-4}$ m<sup>2</sup> and a plate separation of  $2 \times 10^{-3}$ m, across which a potential of 12 V is applied. If a material having a dielectric constant 5.0 is positioned within the region between the plates, compute the polarization. (4)
- 6a. Define the terms of superconductivity;
  - i. Critical temperature
  - ii. Critical magnetic field and
  - iii. Critical current(6)  
b. What are Cooper pairs? Explain. (4)  
c. Write notes on any four applications of superconductors. (6)
- 7a. Explain the following typical characteristics of laser:
  - i. coherence
  - ii. divergence and
  - iii. monochromaticity(6)  
b. Explain the principle and working of a ruby laser. (10)

Q-20 | **Question Papers**

- 8a. Explain the principle behind the functioning of an optical fibre. (4)
- b. Derive an expression for a acceptance angle for an optical fibre. How it is related to numerical aperture? (8)
- c. An optical fibre has a numerical aperture of 0.20 and a cladding refractive index of 1.59. Find the acceptance angle for the fibre in water which has a refractive index of 1.33 (4)

**Set - 4****I - B.Tech. Regular Examinations, May/June – 2006****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the terms (6)  
 i. basis  
 ii. space lattice and  
 iii. unit cell.
- b. Describe the seven crystal systems with diagrams. (10)
- 2a. Describe Bragg's law of X-ray diffraction. (6)
- b. Describe Bragg's X-ray spectrometer and explain how Bragg's law can be verified. (6)
- c. Monochromatic X-ray of  $\lambda = 1.5 \text{ \AA}$  are incident on a crystal face having an interplanar spacing of  $1.6 \text{ \AA}$ . Find the highest order for which Bragg's reflection maximum can be seen. (4)
- 3a. Describe edge and screw dislocations. Draw Burgers circuit and slip planes for them. (10)
- b. Explain the significance of Burgers vector. (6)
- 4a. What is Fermi level? (2)
- b. Explain Fermi-Dirac distribution for electrons in a metal. Discuss its variation with temperature. (8)
- c. Calculate the free electron concentration, mobility and drift velocity of electrons in aluminum wire of length of 5 m and resistance  $0.06 \Omega$  carrying a current of 15 A, assuming that each aluminum atom contributes 3 free electrons for conduction.  
 Given: Resistivity for aluminum =  $2.7 \times 10^{-8} \Omega\text{-m}$ .  
 Atomic weight = 26.98  
 Density =  $2.7 \times 10^3 \text{ kg/m}^3$   
 Avagadro number =  $6.025 \times 10^{23}$  (6)
- 5a. Explain the electrochemical breakdown in dielectric materials. (4)
- b. Explain the concept of internal field in solids and hence obtain an expression for the static dielectric constant of elemental solid dielectric. (8)
- c. A parallel plate capacitor having an area  $6.45 \times 10^{-4} \text{ m}^2$  and a plate separation of  $2 \times 10^{-3} \text{ m}$ , across which a potential of 12 V is applied. If a material having a dielectric constant 5.0 is positioned within the region between the plates, compute the polarization. (4)
- 6a. Explain n-type and p-type semiconductors. Indicate on an energy level diagram the conduction and valence bands, donor and acceptor levels for an intrinsic and extrinsic semiconductors. (10)
- b. Explain the detailed mechanism of current conduction in n and p type semiconductors. (6)
- 7a. Describe the principle, construction and working of a semiconductor laser. (10)
- b. Write the applications of laser. (6)
- 8a. Explain the terms 'numerical aperture' and 'acceptance angle'. (6)
- b. With the help of a suitable diagram explain the principle, construction and working of an optical fibre as a wave guide. (6)
- c. An optical fibre has a core material of refractive index of 1.55 and cladding material of refractive index 1.50. The light is launched into it in air. Calculate its numerical aperture. (4)

**Set - 1****I - B.Tech. Regular Examinations, June – 2005****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the terms  
i. basis ii. space lattice and iii. unit cell.
- b. Describe the seven crystal systems with diagrams.
- 2a. What are Miller indices? How are they obtained?  
b. Explain Schottky and Frankel defects with the help of suitable figures.
- 3a. Show that the wavelength of an electron accelerated by a potential difference 'V' volts, is  $\lambda = 1.227 \times 10^{-10} / \sqrt{V}$  m for non-relativistic case.  
b. Describe an experiment to establish the wave nature of electrons.  
c. Explain the difference between a matter wave and an electromagnetic wave.
- 4a. Explain the origin of energy bands in solids.  
b. Assuming the electron - lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three drawbacks of classical theory of free electrons.  
c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy.
- 5a. Explain Clausius - Mosotti relation in dielectrics subjected to static fields.  
b. What is orientational polarization. Derive an expression for the mean dipole moment when a polar material is subjected to an external field.  
c. The relative dielectric constant of sulphur is 3.75 when measured at 27° C. Assuming the internal field constant  $\gamma = 1/3$  calculate the electronic polarizability of sulphur if its density at this temperature is 2050 kg/m<sup>3</sup>. The atomic weight of sulphur being 32.
- 6a. Draw the B-H curve for a ferro-magnetic material and identify the retentivity and the coercive field on the curve.  
b. What are paramagnetic and diamagnetic materials.  
c. An atom contains 10 electrons revolving in a circular path of radius  $10^{-11}$  m. Assuming homogeneous charge distribution, calculate the orbital dipole moment of the molecule in Bohr magneton.
- 7a. When donor impurities are added to a semiconductor, the concentration of holes decreases. Explain with reasons.  
b. Show that the Fermi level is nearer to the conduction band in a n-type semiconductor. Discuss the variation of conductivity with temperature of an n-type semiconductor.
- 8a. Explain the terms 'numerical aperture' and 'acceptance angle'.  
b. With the help of a suitable diagram explain the principle, construction and working of an optical fiber as a waveguide.  
c. An optical fiber has a core material of refractive index of 1.55 and cladding material of refractive index 1.50. The light is launched into it in air. Calculate its numerical aperture.

**Set - 2**

**I - B.Tech. Regular Examinations, June – 2005**  
**(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)**

**Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Show that FCC is the most closely packed of the three cubic structures by working out the packing factors.  
b. Describe the structure of NaCl.
- 2a. What are Miller indices? How are they obtained?  
b. Explain Schottky and Frankel defects with the help of suitable figures.
- 3a. Explain the concept of matter waves.  
b. Describe Davison and Germer's experiment and explain how it enabled the verification of wave nature of matter.  
c. Calculate the velocity and kinetic energy of an electron of wavelength  $1.66 \times 10^{-10}$  m.
- 4a. What is Fermi level?  
b. Explain Fermi-Dirac distribution for the electrons in a metal. Discuss its variation with temperature.  
c. Calculate the free electron concentration, mobility and drift velocity of electrons in aluminum wire of length of 5 m and resistance  $0.06 \Omega$ , carrying a current of 15 A, assuming that each aluminum atom contributes 3 free electrons for conduction.  
Given: Resistivity for aluminum =  $2.7 \times 10^{-8} \Omega\text{-m}$   
Atomic weight = 26.98  
Density =  $2.7 \times 10^3 \text{ kg/m}^3$   
Avagadro number =  $6.025 \times 10^{23}$
- 5a. Explain briefly the classification of ferro-electric materials.  
b. What is meant by a local field in a solid dielectric. Derive an expression for the local field for structures possessing cubic symmetry.  
c. There are  $1.6 \times 10^{20}$  NaCl molecules/m<sup>3</sup> in a vapour. Determine the orientational polarization at room temperature if the vapour is subjected to an electric field 5000 V/cm. Assume that the NaCl molecule consists of sodium and chlorine ions separated by 0.25 nm
- 6a. Explain clearly the difference between hard and soft magnetic materials. What are mixed ferrites? Mention their uses.  
b. How ferrites are superior to ferromagnetic materials?
- 7a. Distinguish between metals, semiconductors and insulators.  
b. Explain the effect of temperature on resistivity of a semiconductor.  
c. Derive an expression for the number of electrons per unit volume in the conduction band of an intrinsic semiconductor.
- 8a. Explain the characteristics of a laser beam.  
b. Mention any two applications of laser, each in the field of scientific research, engineering and medicine.  
c. Describe the construction and working of a ruby laser.

**Set - 3****I - B.Tech. Regular Examinations, June – 2005****(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel&E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the terms
  - i. basis
  - ii. space lattice and unit cell.
- b. Describe the seven crystal systems with diagrams.
- 2a. What are Miller indices? How are they obtained?  
b. Explain Schottky and Frankel defects with the help of suitable figures.
- 3a. Explain the concept of matter waves.  
b. Describe Davison and Germer's experiment and explain how it enabled the verification of wave nature of matter.  
c. Calculate the velocity and kinetic energy of an electron of wavelength  $1066 \times 10^{-10}$  m.
- 4a. What is Fermi level?  
b. Explain Fermi-Dirac distribution for electrons in a metal. Discuss its variation with temperature.  
c. Calculate the free electron concentration, mobility and drift velocity of electrons in aluminum wire of length of 5 m and resistance  $0.06 \Omega$ , carrying a current of 15 A, assuming that each aluminum atom contributes 3 free electrons for conduction.  
Given: Resistivity for aluminum =  $2.7 \times 10^{-8} \Omega\text{-m}$   
Atomic weight = 26.98  
Density =  $2.7 \times 10^3 \text{ kg/m}^3$   
Avagadro number =  $6.025 \times 10^{23}$
- 5a. Discuss the variation of spontaneous polarization of Roschelle salt with temperature.  
b. Obtain an expression for the static dielectric constant of a monoatomic gas.  
c. Explain the phenomenon of anomalous dielectric dispersion.
- 6a. What are the characteristics of soft magnetic materials?  
b. What is ferro-magnetic curie temperature? Discuss the behaviour of a ferro-magnetic material below the curie temperature.  
c. The magnetic field in the interior of a certain solenoid has the value of  $6.5 \times 10^{-4}$  T when the solenoid is empty. When it is filled with iron, the field becomes 1.4 T. Find the relative permeability of iron.
- 7a. Explain d.c. Josephson effect.  
b. Describe the BCS theory of superconductivity.  
c. Write applications of superconductivity.
- 8a. Describe the principle, construction and working of a semiconductor laser.  
b. Write the applications of laser.

**Set - 4****I - B.Tech. Regular Examinations, June – 2005  
(E.E.E, E.C.E, C.S.C, C.S.I.T, E.I.E, B.M.E, E.Con.E, C.S.S.E, E.Tel& E.Com.E)****Time: 3 hours****Max. Marks: 80****Note: Answer any FIVE questions****All questions carry equal marks**

- 1a. Explain the formation of an ionic crystal.  
b. Derive an expression for the cohesive energy of an ionic crystal.  
c. Calculate the cohesive energy of NaCl from the following data:  
Equilibrium separation between the ion pair = 0.281 nm.  
Ionization energy of Na = 5.14 eV.  
Electrton affinity of Cl = 3.61 eV.  
Born repulsive exponent = 9  
Madelung constant = 1.748.
- 2a. What are Miller indices? How are they obtained?  
b. Explain Schottky and Frankel defects with the help of suitable figures.
- 3a. Derive time independent Schrödinger's wave equation for a free particle.  
b. Explain the physical significance of wave function.  
c. An electron is bound in a one-dimensional infinite well of width  $1 \times 10^{-10}$  m.  
Find the energy values in the ground state and first two excited states.
- 4a. Explain the origin of energy bands in solids.  
b. Assuming the electron - lattice interaction to be responsible for scattering of conduction electrons in a metal, obtain an expression for conductivity in terms of relaxation time and explain any three draw backs of classical theory of free electrons.  
c. Find the temperature at which there is 1% probability of a state with an energy 0.5 eV above Fermi energy.
- 5a. What are the important characteristics of ferro-electric materials?  
b. Describe-thepossible mechanism of polarization in a dielectric material.  
c. The dielectric constant of Helium gas at NTP is 1.0000684. Calculate the electronic polarizability of He atoms if the gas constains  $2.7 \times 10^{25}$  atoms/m<sup>3</sup>.
- 6a. Draw the B-H curve for a ferro-magnetic material and identify the retentivity and the coercive field on the curve.  
b. What are paramagnetic and diamagnetic materials.  
c. An atom contains 10 electrons revolving in a circular path of radius  $10^{-11}$  m. Assuming homogeneous charge distribution, calculate the orbital dipole moment of the molecule in Bohr magneton.
- 7a. Derive the continuity equation for electrons.  
b. What physical law is manifested in the continuity equation.  
c. Find the diffusion coefficient of electrons in silicon at 300 K if  $\mu$ , is 0.19 m<sup>2</sup>/V-S.
- 8a. Describe the construction of a typical optical fiber and give the dimensions of the various parts.  
b. Define the acceptance angle and numerical aperture. Obtain an expression for the numerical aperture of an optical fiber.  
c. Calculate the numerical aperture and acceptance angle for an optical fiber with core and cladding refractive indices being 1.48 and 1.45 respectively.

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# Index

## A

absorption 10.3  
absorption coefficient of sound 13.7  
acceptance angle 11.2  
acoustic quieting 13.10  
  aspects of 13.10  
  electronic quieting 13.12  
  methods of 13.11  
acoustics 13.1  
  echo 13.1  
  pitch 13.1  
  timbre 13.1  
  tone 13.1  
acoustics attenuation 9.6  
activators 10.10  
a.c. resistivity 9.4  
aerogels 14.14  
amorphous solid 2.1  
anisotropy energy 7.14  
anti-ferromagnetic 7.5–7.6, 7.17–7.19, 9.3, 14.3  
applications of lasers 10.17–10.19  
  communication 10.17  
  computer 10.17  
  industrial 10.17  
  medical 10.18  
  military 10.19  
  thermonuclear fusion 10.19  
application of superconductivity 9.18–9.21  
application:

carbon nanotubes 14.10–14.13  
holography 12.3  
nanotechnology 14.1  
  aerogels 14.14  
  computer 14.14  
  cosmetics 14.14  
  energy efficiency 14.14  
  magnets 14.14  
  medical 14.14  
  microelectronics 14.13  
  motor vehicles 14.13  
  television 14.13  
  textiles 14.14  
architectural acoustics 13.8  
  factors affecting 13.8  
arm chair 14.11  
attractive forces 1.5  
attractive potential energy 1.6  
atomic lithography 14.8  
atomic force microscopy 14.7  
attenuation in optical fibres 11.9

## B

ball milling 14.10  
band  
  conduction 8.1–8.22  
  valence 8.1–8.22  
band theory 5.12  
barium titanate 6.17–6.19

battery 4.23, 8.10, 9.13  
 BCS ground state 9.17  
 BCS theory 9.15  
 beam splitter 11.15, 12.2  
 Becker 7.12  
 black body radiation 4.10–4.12  
   Planck's law 4.12  
   Planck's quantum theory 4.17–4.18  
   Rayleigh–Jeans law 4.11  
   Wein's law 4.10  
 Bloch 5.12  
 Bloch theorem 5.19  
 Bloch wall 7.14  
 Bohr magneton 7.2  
 Boltzmann's constant 5.3  
 bonds  
   covalent 1.2  
   dipole 1.4  
   dispersion 1.3  
   hydrogen 1.4  
   inter molecular 1.3  
   ionic 1.1  
   metallic 1.3  
   primary 1.1  
   secondary 1.1  
 Bose–Einstein distribution 4.5–4.7  
 Bragg's law 3.14  
 Bragg's plane 4.24  
 Bravais lattice 2.2, 2.4  
 Brewster  
   angle 10.8  
   windows 10.8  
 bucky ball 14.2  
 Burger's vector 3.10  
 buried heterostructure laser 10.14

**C**

caesium chloride structure 2.13  
 carbon dioxide laser 10.15  
 carbon nanotubes 14.10–14.13  
   applications 14.12–14.13  
   formation 14.12  
 carrier concentration  
   electron 8.4  
   extrinsic 8.17  
   hole 8.6  
   intrinsic 8.9  
   intrinsic semiconductors 8.1  
 chemical properties of nanomaterials 14.6–14.7  
 chemical vapour deposition 14.10

chiral 14.11  
 cladding 11.1–11.8  
 classical free electron theory 5.2–5.5  
 classification of magnetic materials 7.5–7.6  
 classification of metals, semiconductors  
   and insulators 5.24  
 Clausius–Mosotti relation 6.4  
 cluster nanoparticles 14.4  
 coherent length 9.17  
 coherent 10.1  
 cohesive energy  
   calculation 1.6–1.9  
   of NaCl molecule 1.8  
 communication  
   fibre optics 11.11–11.13  
   lasers 10.1  
 Compton effect 4.12  
 condition for ray propagation in a fibre 11.5  
 conduction band 8.1  
 continuity equation 8.25–8.29  
 conventional light 10.1  
 Cooper pair 9.16  
 coordination number 2.8  
 core 11.1–11.10  
 cosmetics 14.14  
 critical currents 9.4  
 cryotron switch 9.19  
 crystal defects 3.7–3.10  
   compositional 3.8  
   edge 3.8  
   electronic 3.8  
   Frenkel 3.8  
   line 3.8  
   point 3.7  
   Schottky 3.7  
   screw 3.10  
 crystal directions 3.1  
 crystal planes 3.1  
 crystal structures  
   caesium chloride 2.13  
   diamond 2.11  
   sodium chloride 2.12  
   zinc sulphide 2.14  
 crystal systems 2.3  
   cubic 2.5  
   hexagonal 2.7  
   monoclinic 2.6  
   orthorhombic 2.6  
   rhombohedral 2.7  
   tetragonal 2.6  
   triclinic 2.7

trigonal 2.7  
crystalline solid 2.1  
cubic structures  
  body centred 2.9  
  diamond 2.11  
  face centred 2.10  
  simple 2.8  
Curie constant 7.11

## D

damping 13.13  
Davisson and Germer experiment 4.22  
de Broglie hypothesis 4.12  
Debye-Scherrer 3.16  
degree of freedom 5.23  
density of electron states 4.8 – 4.10  
diamagnetic materials 7.5  
diamond structure 2.11  
dielectric constant 6.1  
dielectric properties 6.1  
dielectrics 6.1  
diffraction 4.20  
diffusion current 8.23–8.24  
dipolar polarization 6.7  
dipole bond 1.4  
dipole moment 6.1, 6.4, 6.7, 6.9–6.15, 6.19  
dip pen nanolithography 14.7  
direct band gap semiconductors 8.31  
discrete values of energy 4.31, 4.33  
dispersion bond 1.3  
displacement sensor 11.13  
domain theory of ferromagnetism 7.12  
double heterostructure laser 10.13  
drift current 8.23–8.25  
drift velocity 5.3  
  expression 5.6  
Drude 5.2

## E

Echelon effect 13.9  
edge dislocation 3.8  
effective mass of electron 5.22–5.24  
Eigen function 4.15  
Eigen values 4.33  
Einstein 4.12  
Einstein relation 8.24  
Einstein's coefficient 10.4–10.6  
E-K diagram 5.18

electrical conductivity 5.2, 8.11  
electron gas 4.7  
electron scattering 5.11  
electron spin 7.2  
electronic polarization 6.11  
electrochemical reactivity 14.6  
electrodeposition 14.10  
electron beam lithography 14.8  
electronic properties of nanomaterials 14.5  
encoder 11.11  
energy efficiency 14.14  
energy gap 8.14  
energy of formation of vacancy 3.10–3.11  
entropy 9.5  
epilepsy 9.21  
exchange energy 7.14  
excited state 10.3  
extrinsic semiconductor 8.14

## F

face-centred cubic structure 2.10  
fabrication of nanomaterials 14.7  
fatigue 14.14  
Fermi-Dirac distribution 4.3 – 4.5, 5.7  
Fermi energy 4.8, 5.7  
ferrimagnetic materials 7.6, 7.19  
ferroelectricity 6.18  
ferromagnetic domains  
  experimental evidence 7.13  
  origin 7.13  
ferromagnetic materials 7.6  
fibre optics 11.1–11.16  
  acceptance angle 11.2–11.3  
  advantages 11.12  
  communication 11.11–11.12  
  condition for ray propagation 11.4  
  graded index 11.5  
  numerical aperture 11.3  
  principle 11.1  
  ray propagation 11.5–11.6  
  sensing application 11.13–11.15  
  step index 11.5  
fluorescent screen 4.9  
flux exclusion 9.6  
flux quantization 9.10  
forces  
  attractive 1.5  
  repulsive 1.5  
formation of carbon nanotubes 14.12

free electron theory  
 classical 5.2–5.5  
 failures 5.4  
 quantum 5.9–5.11  
 Frenkel defect 3.8  
 frequency dependence of dielectric constant 6.20  
 fullerenes 14.2

**G**

galvanometer 4.23  
 general features of superconductivity 9.3–9.7  
 germanium 8.1  
 glassy carbon 14.6  
 gold foil 4.19  
 G.P Thomson experiment 4.19–4.22  
 graded index fibre 11.7  
 ground state 10.3

**H**

Hall effect 8.29–8.31  
 hard magnetic material 7.20  
 heat capacity 9.5  
 Heisenberg uncertainty principle 4.28  
 helium-neon gas laser 10.8–10.10  
 hetero structure laser 10.12  
 hexagonal close pack structure A-1-A-4  
   axial ratio of A-3  
   packing factor of A-3-A-4  
 hexagonal crystal system 2.7  
 high power magnets 14.13  
 hole 8.6  
 holography  
   application 12.3  
   introduction 12.1  
   principle 12.1  
   reconstruction of image 12.2  
   recording of image 12.1  
 homo structure laser 10.12  
 hydrogen bond 1.4  
 hysteresis curve 7.6

**I**

indirect band gap semiconductors 8.31  
 inter molecular bond 1.3  
 interference 4.12  
 internal field 6.2–6.4  
 intrinsic carrier concentration 8.9

intrinsic semiconductors 8.1  
 ionic bond 1.1  
 ionic polarization 6.7, 6.10  
 isotopic effect 9.3

**J**

Josephson effect 9.13–9.15  
 Josephson junction 9.14  
 Josephson junction devices 9.20

**K**

Kamerling Onnes 9.1  
 Kronig–Penney model 5.13–5.19  
 krypton flash lamp 10.10

**L**

lasers 10.1–10.17  
   carbon dioxide 10.15  
   He-Ne 10.8–10.10  
   ruby 10.10–10.11  
   semiconductor 10.11–10.14  
 laser method to form nanotubes 14.12  
 lattice  
   Bravais 2.4  
   parameters 2.3  
   space 2.2  
 Laue method 3.17–3.18  
 line defect 3.8  
 lithography  
   atomic 14.8  
   dip pen nano 14.7  
   electron beam 14.8  
   nano 14.7  
 light emitting diode (LED) 8.46–8.49, 11.11  
 liquid crystal display (LCD) 8.49–8.50  
 local field 6.2  
 Lorentz 6.2  
 loss-less power transmission 9.19

**M**

Madelung constant 1.9  
 Maglev vehicle 9.20  
 magnetic bearings 9.18  
 magnetic force microscopy 14.7  
 magnetic field energy 7.14  
 magnetic flux density 7.1

## magnetic materials

- anti-ferro 7.6, 7.17
- dia 7.5
- ferri 7.6
- ferro 7.6
- hard 7.20
- para 7.6
- soft 7.20

## magnetic momentum

- electron spin 7.4
- nuclear spin 7.5
- orbital motion 7.3

## magnetic permeability 7.1

## magnetic properties 7.1

## magnetic properties of nanomaterials 14.5

## magnetization 7.2

## matter waves 4.12, 4.13

- experimental study of 4.19 – 4.25

## Maxwell–Boltzmann distribution 4.1 – 4.3

## mean collision time 5.6

## mean free path 5.6

## mechanical effects 9.6

## medical applications of nanomaterials 14.14

## Meissner effect 9.6

## memory cell 9.20

## metallic bond 1.3

## metastable state 10.8

## microscopy

- atomic force 14.7
- magnetic force 14.7
- scanning tunneling 14.1, 14.7, 14.8

## Miller indices 3.1

## minority carrier life time 8.19–8.22

## momentum 4.12

## monochromatic 3.15, 10.1

## monoclinic crystal system 2.6

## motor vehicles application of nanomaterials 14.14

## muffler 13.12 – 13.13

## N

## nanotechnology 14.1

- applications of 14.13 – 14.14

- fabrication 14.7 – 14.9

- principle 14.1

## nanoparticles 14.4

- properties of 14.4 – 14.7

- production of 14.9 – 14.10

- quantum effects in 14.2 – 14.4

## Neel temperature 7.17

## nickel 4.23

## non-centrosymmetric 6.17

## non-polar materials 6.1

## normalization 4.34

## noise 13.10

## nuclear magnetic moment 7.5

## numerical aperture 11.3 – 11.5

## O

## optical fibres in communication 11.11–11.12

## optical properties of nanomaterials 14.4

## orbital angular momentum 7.3

## orbital magnetic moment 7.3

## oriental polarization 6.7

## origin of ferromagnetic domains 7.13

## origin of magnetic moment 7.2

## orthorhombic crystal system 2.5

## P

## packing factor 2.8

## paramagnetic material 7.5

## particle in a box 4.31

## one-dimensional box 4.31 – 4.35

## three-dimensional box 4.35 – 4.39

## Pauli's exclusion principle 5.7

## penetration depth 9.9

## permittivity 6.5

## persistent current 9.3

## phase space 4.1

## phonons 9.15

## photoelectric effect 4.12

## photoemission 14.5

## photographic plate 4.19

## photoluminescence 14.4

## photon gas 4.7

## photons 4.5

## photodiodes 8.51

## avalanche 8.52

## p-i-n 8.52

## physical properties of nanomaterials 14.4

## piezoelectricity 6.17

## Planck's equation 4.13

## plasma arcing 14.9

## plasma arcing method 14.9

## p-n diode 8.36

## band diagram of 8.36

## Fermi level 8.36

## Shockley's equation 8.37

V–I characteristics of 8.39  
 p-n junction 8.33  
     alloying method 8.33  
     biasing of 8.37–8.38  
     diffusion method 8.33  
     formation of 8.33  
     grown junction method 8.33  
 point defect 3.7  
 polar material 6.1  
 polarization 4.12  
     dipolar 6.7, 6.8  
     electronic 6.7, 6.12  
     ionic 6.7, 6.10  
     orientational 6.7, 6.18  
 population inversion 10.6  
 potential energy 1.6  
 potential well 4.31  
 powder method 3.16  
 pressure sensor 11.14  
 primary bonds 1.1  
 principle of optical fibre 11.1  
 principle of  
     holography 12.1  
     nanotechnology 14.1  
 probability density 4.30, 4.31, 4.34  
 production of nanomaterials 14.9  
 properties  
     chemical 14.6  
     electronic 14.5  
     magnetic 14.5  
     mechanical 14.5  
     optical 14.4  
     physical 14.4  
     thermal 14.4

**Q**

quantized 4.13  
 quantum confinement effects 14.4  
 quantum free election theory 5.8–5.11  
 quantum tunneling 9.11–9.13  
 quartz crystal 6.17

**R**

ray propagation 11.5, 11.6  
 reconstruction of image from hologram 12.2  
 recording of image on a holographic plate 12.1  
 rectifier 8.41–8.46  
     bridge rectifier 8.45  
     full-wave 8.43–8.46

half-wave 8.42  
 refractive index 11.1  
 relativistic correction 4.14  
 relaxation time 5.5  
 repulsive forces 1.5  
 repulsive potential energy 1.6  
 requirements of insulators 6.21  
 resonance 13.9  
 reverberation 13.1, 13.2  
 reverberation time 13.2  
 rhombohedral crystal system 2.7  
 Rochelle salt 6.17, 6.18  
 root mean square velocity 5.2, 5.5  
 ruby laser 10.10–10.11

**S**

Sabine's empirical formula 13.2  
 Sabine's reverberation theory 13.2–13.7  
 scanning tunneling microscope 14.1, 14.7, 14.8  
 scattered electrons 4.23  
 scattering power 5.16  
 Schottky defect 3.7  
 Schrödinger's wave equation 4.25–4.28  
 secondary bonds 1.1, 1.3  
 semiconductor lasers 10.12  
 semiconductors  
     conductivity double 8.13  
     direct band gap 8.31  
     electrical conductivity 8.10  
     energy gap 8.12  
     extrinsic 8.14  
     intrinsic 8.1  
     indirect band gap 8.31  
 sensing applications of fibre 11.13–11.15  
 sensors 11.13–11.15  
     displacement 11.13  
     liquid level 11.14  
     pressure 11.14  
     temperature 11.14  
 separation between planes 3.4–3.6  
 silencer 13.12–13.13  
 silicon 8.1  
 simple cubic structure 2.8  
 single hetero structure laser 10.13  
 smart windows 14.14  
 sodium chloride structure 2.13  
 soft magnetic materials 7.20  
 sol-gel method 14.10  
 sound proofing 13.13  
 source of electrical resistance 5.11

space elevators 14.13

space lattice 2.2

SQUIDS 9.21

stacking sequence 2.14

step index fibre 11.5–11.7

    multi mode 11.6

    single mode 11.5

stimulated emission 10.2–10.3

Stirling's theorem 4.3, 4.4, 4.6

superconducting

    breaker 9.19

    fuse 9.19

    magnets 9.18

superconducting sensitive magnetometer 9.21

superconductivity 9.1

    applications 9.18–9.21

    general features 9.3–9.7

superconductors in medicine 9.21

super paramagnetic 14.5

surface defects A-5–A-8

## T

target 4.12

temperature sensor 11.14

tetragonal crystal system 2.5

thermal conductivity 9.5

thermal properties 14.4

thermal vibrations 5.12

thermo nuclear fusion 10.19

threshold current 11.12

tourmaline crystal 6.17

transition temperature 9.1

transmitter 11.11

triclinic crystal system 2.7

trigonal crystal system 2.7

tunneling microscope 14.1, 14.7, 14.8

type-I and type-II superconductors 9.7–9.9

## U

unit cell 2.3

## V

valence band 8.1

void 2.13

## W

wave function 4.25, 4.30

    physical significance of 4.30

wave guides 11.1

waves and particles 4.12

Weiss 7.13

Wiedmann–Franz law 5.1

## X

x-cut quartz crystal 6.18

xenon lamp 10.10

x-ray diffraction 3.14

## Y

y-cut quartz crystal 6.18

## Z

zig-zag carbon nanotubes 14.11

zinc sulphide structure 2.14

