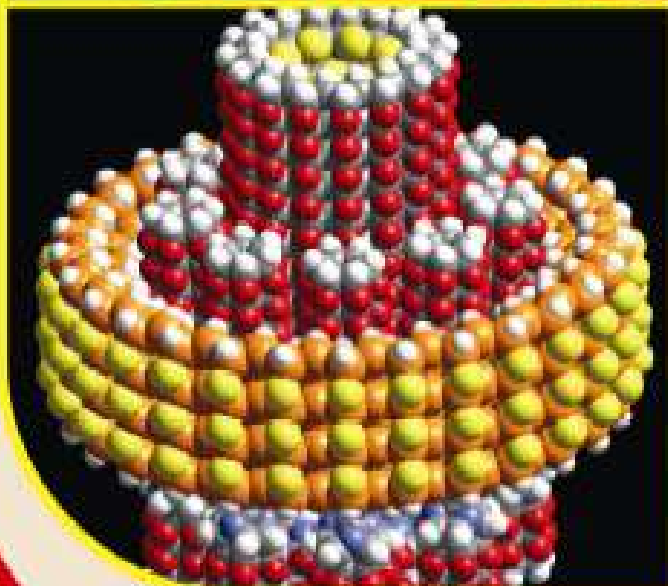
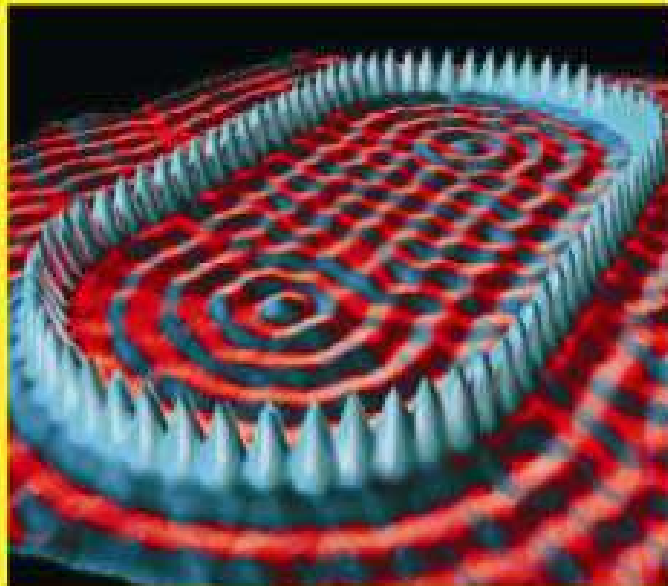


TEXTBOOK OF ENGINEERING PHYSICS



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Textbook of Engineering Physics

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Preface

The purpose of this book is to provide an in-depth information on fundamentals of Engineering Physics to the student community to improve their general understanding on the subject. The book has been designed as a textbook for the beginners in all branches of Engineering according to the latest syllabus of Visvesvaraya Technological University, Belgaum, Karnataka. The emphasis is given on basic concepts & fundamental aspects of modern physics.

The book has been divided into eight Chapters. The first Chapter is **Modern Physics**, which contains Blackbody radiation spectrum, Photo-electric effect, Compton effect, Wave particle Dualism, de-Broglie hypothesis - de-Broglie wavelength, extension to electron particle, Davisson and Germer Experiment, Matter waves and their Characteristic properties, and Expression for de-Broglie wavelength using group velocity. The second Chapter is **Quantum Mechanics**, which involves Heisenberg's uncertainty principle and its physical significance, Wave function, Time independent Schrödinger wave equation, Application of Schrödinger wave equation - Energy eigen values for a free particle, and Energy eigen values of a particle in a potential well of infinite depth. The third Chapter focuses on **Electrical Conductivity in Metals**, which includes Free-electron concept, Classical free-electron theory, Expression for drift velocity, Expression for electrical conductivity in metals, Failure of classical free-electron theory, Quantum free-electron theory, Fermi - Dirac Statistics, Expression for electrical resistivity/conductivity, and Temperature dependence of resistivity of metals. The fourth Chapter is on **Dielectric & Magnetic Properties of Materials**, which includes Dielectric constant and polarization of dielectric materials. Types of polarization. Equation for internal fields in liquids and solids, Clausius - Mossotti equation, Ferro and Piezo - electricity, Frequency dependence of dielectric constant, Classification of dia, para and ferro-magnetic materials, Hysteresis in ferromagnetic materials, and Soft and Hard magnetic materials.

The fifth Chapter focus on **Lasers**, which includes Principle and production, Einstein's coefficients, Condition for Laser action, Principle, Construction and working of He-Ne and semiconductor Laser, Applications of Laser, and Holography - Principle of Recording and reconstruction of 3-D images. The sixth Chapter is on **Optical Fibers & Superconductivity**, which contains Propagation mechanism in optical fibers, Types of optical fibers and modes of propagation, Applications of optical fibers, Temperature dependence of resistivity in superconducting materials, Effect of magnetic field, Type I and Type II superconductors, BCS theory, High temperature superconductors, and Applications of superconductors. The seventh Chapter is on **Crystal Structures**, which contains Crystal systems, Miller indices, Expression for inter-planar spacing, Atomic packing factor, and Determination of crystal structure by Bragg's X-ray spectrometer. The last Chapter is on **Material Science**, which focuses on Nano-science and Nano-technology, Shapes of nano-materials, Methods of preparation of nano-materials, Ultrasonic non-destructive testing of materials, and Measurements of velocity in solids and liquids.

Every attempt has been made to make this book error free and useful for the students. Two sample question papers are included at the end of the book. Each Chapter begins with objective and ends with unit questions, objective type questions and assignment problems. Any constructive suggestion and criticism regarding the improvement of this book will be acknowledged.

— Authors

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In conclusion, we thank all those who have helped us directly or indirectly during the preparation of this book.

We also whole heartedly grateful to the Publisher of Acme Learning Private Limited, New Delhi, for bringing out this book on time.

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MODERN PHYSICS

OBJECTIVES

This Chapter contains the detailed discussion on the origin of modern physics and introduces to the subject of failures of classical mechanics and how the quantum theory consolidated the answer for the problems which were remained unanswered by classical theory. The duality of light and the hypothetical argument given by de-Broglie to explore the wave nature of moving particle and evidence for existence of matter waves are discussed. The main objectives of this chapter are to study:

- The failures of classical mechanics and origin of Quantum Mechanical Theory
- The application of quantum idea to explain black body radiation spectrum, photoelectric effect, and Compton effect
- The de-Broglie hypothesis (matter waves) and experimental evidence given by Davison and Germer
- The relation between the group velocity, phase velocity, particle velocity and velocity of light
- Characteristics of matter waves

1.1 INTRODUCTION TO PHYSICS

The word science comes from a Latin word “scientia” which means ‘to know’. Science is the knowledge gained through the systematic observations and experiments. Scientific methods include the systematic observations, reasoning, modeling and theoretical prediction. Science is divided into two broad categories as *natural science* and *philosophical science*. Natural Science has many disciplines, physics being one of them.

The word physics has its origin in a Greek word ‘physis’ meaning ‘nature’. Physics is the most basic science, which deals with the study of nature and natural phenomena, especially, properties of matter, energy and their interactions. Understanding of science begins with understanding of physics. Physics is an empirical study. Everything we know about physical world and about the principles that govern its behaviour has been learned through observations of the phenomena of nature. The ultimate test of any physical theory is its agreement with observations and measurements of physical phenomena.

Technology is the application of the doctrines in physics for practical purposes. The invention of steam engine had a great impact on human civilization. Till 1933, Rutherford did not believe that

energy could be tapped from atoms. But in 1938, Hann and Meitner discovered neutron-induced fission reaction of uranium. This is the basis of nuclear weapons and nuclear reactors. The contribution of physics in the development of alternative resources of energy is significant. We are consuming the fossil fuels at such a very fast rate that there is an urgent need to discover new sources of energy which are cheap. Production of electricity from solar energy and geothermal energy is a reality now, but we have a long way to go. Another example of physics giving rise to technology is the integrated chip, popularly called as IC. The development of newer ICs and faster processors made the computer industry to grow leaps and bounds in the last three decades. Computers have become affordable now due to improved production techniques and low production costs.

The legitimate purpose of technology is to serve people. Our society is becoming more and more science-oriented. We can contribute better to the science and society if we develop a deeper understanding of the basic laws of physics.

1.2 INTRODUCTION TO BLACKBODY RADIATION SPECTRUM

1.2.1 Introduction to Modern Physics

At the end of nineteenth century, the physics consisted of mainly Newton's laws of motion and universal gravitation, the laws of conservation of energy and momentum, the laws of thermodynamics, and Maxwell's equations for electricity and magnetism were all more or less nearly complete and were used to describe the machines that launched two waves of industrial revolution—the first one powered by steam and the second one powered by electric current. Most of the people believed that there is nothing new to discover in physics now. All that remains is more and more precise measurement. But **Lord Kelvin** (1824-1907) identified two problems with the physics at that time. They were: (1) Theory of luminiferous ether to explain light wave propagation in space (Wave theory of light) and (2) The inability of electromagnetic theory of light to adequately predict the characteristics of thermal radiation.

In the beginning of the 20th century, the first problem was solved by **Albert Einstein**, by means of **theory of relativity**. The major revelations of this theory were that there is no ether, there is no absolute space, there is no absolute time, mass is not conserved, energy is not conserved, and nothing travels faster than light. For awhile, this was the most revolutionary theory in all of physics. The second problem was solved by **Max Karl Planck** (1858-1947) by means of **quantum mechanical theory**. The major revelations of this theory are that all things are both particles and waves at the same time and that nothing can be predicted or known with absolute certainty.

The arrival of these two revolutionary theories divided physics up into two domains. All theories developed before the arrival of relativity and quantum mechanics and any work derived from them are called **Classical physics**. All theories derived from the basic principles of relativity and quantum mechanics are called **Modern physics**. The quantum mechanics principle initially could able to explain the following phenomenon successfully:

- Blackbody radiation and the ultraviolet catastrophe
- Photoelectric effect

- Discrete atomic spectra and the problem of how atoms manage to exist
- Radioactive decay

1.2.2 Blackbody Radiation

All objects radiate electro-magnetic energy in the form of heat continuously whatever is their temperature, though which frequencies predominates depends on the temperature. At room temperature most of the radiation emitted by an object is in the infrared part of the spectrum and hence the emitted radiations are invisible.

A *blackbody* is defined as an object that absorbs all the frequencies of electromagnetic radiation falling on it and consequently appears black. A blackbody or perfect absorber is also an ideal radiator which emits radiation in all frequencies. Such a radiation emitted/radiated by a blackbody is called **blackbody radiation**. In practice, a small opening in any heated cavity, such as a port in an oven, behaves like a blackbody because such an opening traps all incident radiation (Fig. 1.1). The opening to the cavity inside a body is a good approximation of a blackbody. Light entering the small opening strikes the far wall, where some of it is absorbed but some is reflected at a random angle. The light continues to be reflected, and at each reflection a portion of the light is absorbed by the cavity walls. After many reflections essentially all of the incident energy is absorbed. If the direction of the radiation is reversed in Fig. 1.1, the light emitted by a small opening is in thermal equilibrium with the walls, because it has been absorbed and re-emitted many times.

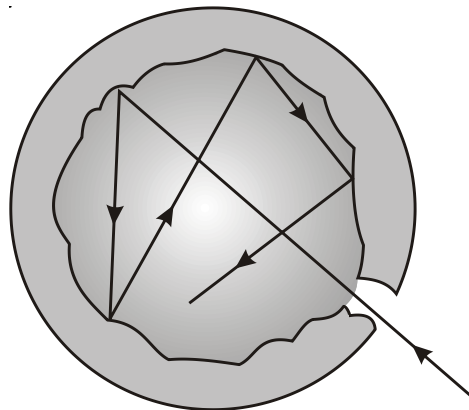


Figure 1.1 The opening to the cavity inside a body is a good approximation of a blackbody

1.2.3 Blackbody Radiation Spectrum

To study the distribution of radiant energy over different frequencies, the black body is maintained at a constant temperature. By means of an infrared spectrometer and a bolometer/photodetector the emissive powers of the black body for different frequencies are measured. The results of the experiment is shown

in Fig. 1.2 as blackbody radiation spectrum. In the spectrum, at a given temperature, the radiation intensity (energy density) initially increases with frequency, then peaks at around a particular frequency and after that decreases, finally reaches to zero at very high frequencies.

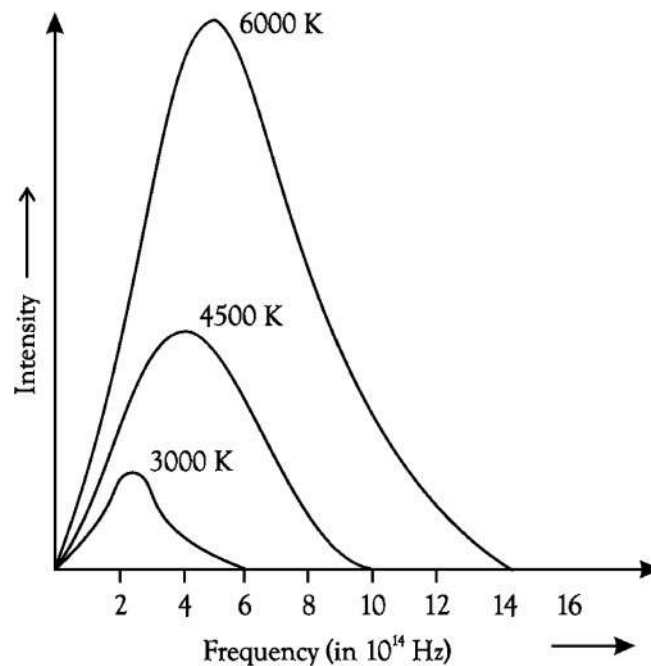


Figure 1.2 *Blackbody radiation spectrum*

1.2.4 Energy Distribution in Blackbody Radiation Spectrum

Based on the study of the blackbody radiation spectrum, following observations can be made:

1. The energy is not uniformly distributed with frequency.
2. At a given temperature, the energy density initially increases with increase in frequency reaches a maximum value and then decreases with further increase in frequency.
3. The frequency corresponding to the maximum energy density (peak of the curve) shifts towards higher frequency side with increase in temperature.

1.2.5 Laws of Blackbody Radiation

1. Stefan's Law

In 1879, an Austrian physicist **Josef Stefan** (1835-1893) found experimentally that the total power

per unit area emitted at all frequencies by a hot solid, e_{total} , is proportional to the fourth power of its absolute temperature. Therefore, Stefan's law may be written as

$$e_{\text{total}} = \int_0^{\infty} e_f df = \sigma T^4 \quad \dots (1.1)$$

where e_{total} is the power per unit area emitted at the surface of the blackbody at all frequencies, e_f is the power per unit area per unit frequency emitted by the blackbody, T is the absolute temperature of the body, and σ is the Stefan-Boltzmann constant, given by $5.67 \times 10^{-8} \text{ W.m}^{-2}.\text{K}^{-4}$. A body that is not an ideal radiator will obey the same general law but with a coefficient, α , which has value less than 1:

$$e_{\text{total}} = \alpha \sigma T^4 \quad \dots (1.2)$$

2. Wein's Distribution Law

In 1893, **Wilhelm Wien** proposed a general form for the blackbody distribution law that gave the correct experimental behavior of λ_{max} with temperature. This law is called *Wien's displacement law* and may be written as:

$$\lambda_{\text{max}} T = 2.898 \times 10^{-3} \text{ m.K} \quad \dots (1.3)$$

where λ_{max} is the wavelength in meters corresponding to the blackbody's maximum intensity and T is the absolute temperature of the surface of the object emitting the radiation. Assuming that the peak sensitivity of the human eye (which occurs at about 500 nm—blue-green light) coincides with λ_{max} for the Sun (a blackbody), we can check the consistency of Wien's displacement law with Stefan's law by calculating the Sun's surface temperature:

$$T = \frac{2.898 \times 10^{-3} \text{ m.K}}{500 \times 10^{-9} \text{ m}} = 5800 \text{ K} \quad \dots (1.4)$$

3. Wein's Exponential Law

In 1893, **Wein** also calculated the energy per unit volume at frequency range f and $f + df$ of the radiation within the blackbody cavity, $u(f, T)$ as:

$$u(f, T) df = A f^3 e^{-\beta f/T} df \quad \dots (1.5)$$

where A and β are Wien's constants. This result was known as Wien's exponential law.

Limitations of Wein's Law:

Experiments show that Wein's law holds good for shorter wavelength (higher frequency) region of the spectrum and at higher temperature of the blackbody. It fails to explain the gradual drop of the energy density at longer wavelengths (lower frequency) after the peak value as shown in Fig. 1.3.

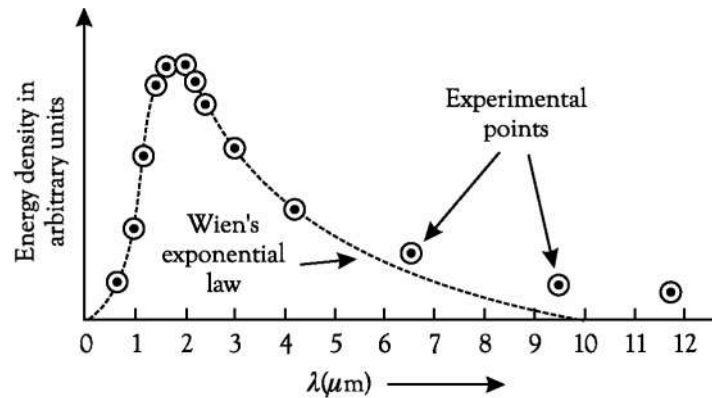


Figure 1.3 Discrepancy between Wien's law and experimental data for a blackbody at 1500 K

4. Rayleigh-Jeans Law

According to **Lord Rayleigh** and **James Jeans**, the spectral energy density at frequency range f and $f + df$ is simply the density of modes multiplied by $k_B T$,

$$\text{or} \quad u(f, T)df = \frac{8\pi f^2 k_B T}{c^3} df \quad \dots (1.6)$$

where k_B is Boltzmann's constant = 1.380×10^{-23} J/K.

Limitations of Rayleigh-Jeans Law: The Ultraviolet Catastrophe

A blackbody is an idealized object which absorbs and emits all frequencies of radiation. Classical physics can be used to derive an equation which describes the intensity of blackbody radiation as a function of frequency for a fixed temperature—the result is known as the Rayleigh-Jeans law. Although the Rayleigh-Jeans law works for low frequencies, it diverges as f^2 ; this divergence for high frequencies (ultraviolet frequencies) is called the **Ultraviolet catastrophe**.

5. The Planck's Radiation Law

In 1900, **Max Planck** was working on the problem of how the radiation an object emits is related to its temperature. He came up with a formula that agreed very closely with experimental data, but the formula only made sense if he assumed that the energy of a vibrating molecule was **quantized**—that is, it could only take on certain values. The energy would have to be proportional to the frequency of vibration, and it seemed to come in little “chunks” of the frequency multiplied by a certain constant. This constant came to be known as **Planck's constant**, or h , and it has the value $h = 6.626 \times 10^{-34}$ J.s. He has been honoured by Nobel Prize in the year 1918.

Max Planck discovered the famous blackbody formula, which used the quantum theory. Accordingly, $u(f, T)$, is given by:

$$u(f, T) df = \frac{8\pi hf^3}{c^3} \left(\frac{1}{e^{hf/k_B T} - 1} \right) df \quad \dots (1.7)$$

where h is Planck's constant = 6.626×10^{-34} J.s. and k_B is Boltzmann's constant = 1.380×10^{-23} J/K.

Since Wien's law holds good in the higher frequency region and Rayleigh-Jeans law in the lower frequency region and if Planks law could able to explain the energy distribution in entire region of blackbody radiation spectrum then one should able to deduce Wien's and Rayleigh-Jeans law from Plank's law.

For higher frequency region $e^{hf/k_B T}$ is very large

$$\Rightarrow e^{hf/k_B T} \gg 1$$

$$\therefore (e^{hf/k_B T} - 1) \approx e^{hf/k_B T}$$

Substitute the above approximation in (1.7) we get

$$u(f, T) df = \frac{8\pi hf^3}{c^3} e^{-hf/k_B T} df$$

Compare the above equation with the Wien's law we get $A = 8\pi h / c^3$ and $\beta = h/k_B$

Similarly for lower frequency region

f is small implies $\frac{hf}{k_B T}$ is very small and expand $e^{hf/k_B T}$ as power series, we have

$$e^{hf/k_B T} = 1 + \frac{hf}{k_B T} + \frac{1}{2!} \left(\frac{hf}{k_B T} \right)^2 + \frac{1}{3!} \left(\frac{hf}{k_B T} \right)^3 + \dots$$

Since $\frac{hf}{k_B T}$ is very small and the higher power terms are very small and can be neglected

$$\therefore (e^{hf/k_B T} - 1) = \frac{hf}{k_B T}$$

Substitute the above result in Eqn (1.7) we get the Eqn (1.6) which is the Rayleigh-Jeans law. Hence the expression given by Plank valid in the entire frequency region of blackbody radiation spectrum.

1.3 PHOTO-ELECTRIC EFFECT

1.3.1 Definition

The phenomenon of emission of electrons from a metal surface when illuminated by light of suitable frequency is called the **photoelectric effect**. Photoelectric effect was discovered by **H. Hertz** in 1887.

The photoelectric effect involves conversion of light energy into electrical energy. The electrons emitted during photoelectric effect are called **photoelectrons** and the current constituted by photoelectrons is called the photoelectric current.

The minimum frequency of the incident radiation required for the emission of electrons from the surface of a metal is called the threshold frequency of the metal. Threshold frequency varies from metal to metal.

It has been observed that metals like zinc, cadmium, magnesium etc. shows photoelectric effect only for ultraviolet light. But some alkali metals like lithium, sodium, potassium, caesium and rubidium shows photoelectric effect even for visible light.

1.3.2 Experimental Study

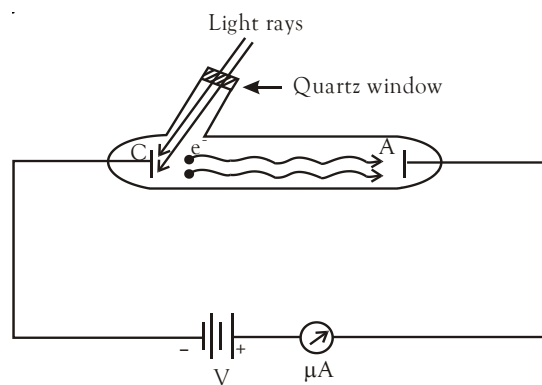


Figure 1.4 Experimental study of photoelectric effect

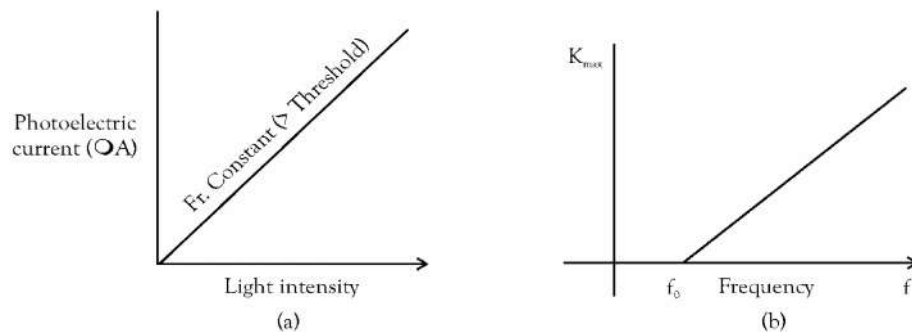


Figure 1.5 (a) Graph of photoelectric current versus intensity of light (b) Graph of kinetic energy of electrons versus frequency of incident light

The experimental set-up consists of an evacuated glass tube which contains two electrodes, a cathode C and an anode A, which are sealed inside the tube (Fig. 1.4). The tube contains a side window of quartz which allows light of reasonably short wavelength to pass through and allows to falls on cathode C. The electrons emitted from cathode C will move towards the anode A. This will constitutes the photoelectrons and causes photoelectric current to flow in the circuit and measured using a micro ammeter connected in the circuit.

The photoelectric current can be increased or decreased by varying the magnitude and sign of the anode potential with respect to the cathode. It is observed that there is a certain minimum negative (retarding) potential at anode which will reduce the photoelectric current to be zero and is referred as stopping potential or retarding potential or cut-off potential, represented as V_s . Therefore the stopping potential is defined as the minimum negative potential required at the anode so as to completely suppress the photoelectrons reaching the anode and hence the current to zero in the circuit.

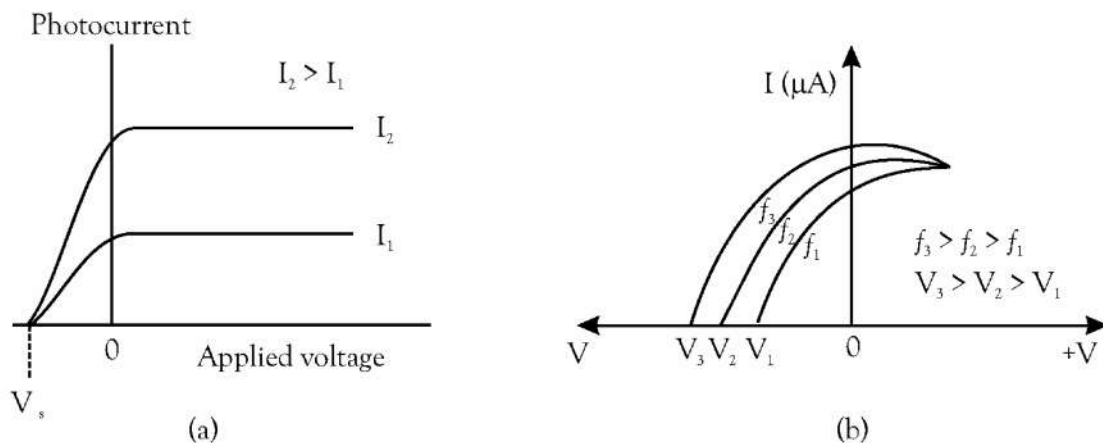


Figure 1.6 (a) Plot of photoelectric current versus applied potential between electrodes at two different intensity of incident light (b) Plot of photoelectric current versus applied potential between electrodes at three different frequencies of incident light

Experimental Observations:

1. Photoelectric effect is an instantaneous process. Photoelectrons will ejected out within 10^{-9} s (very small time) after light irradiation on the metal surface.
2. For a given photosensitive material, there exist a certain minimum frequency called the **cut-off** or **threshold frequency** below which no photoelectric effect takes place.
3. For a given photosensitive material and frequency of incident radiation (more than threshold frequency) the photoelectric current is directly proportional to the **intensity** of incident light, as shown in Fig. 1.5 (a).
4. **Effect of potential at anode:** The graph of photoelectric current and the voltage applied between

the electrodes (cathode C and anode A) shows that initially the photoelectric current increases with the increasing potential. For a certain potential, the current becomes maximum. For further increase in potential, the graph shows saturation of current (Horizontal portion).

5. The value of stopping potential increases with increase in frequency of the incident radiation which is shown in Fig. 1.6 (b).
6. The kinetic energy of the photoelectrons increases linearly with the frequency of the incident radiations [Fig. 1.5 (b)]. It is independent of the intensity of the incident radiations which is as shown Fig. 1.6 (a).

1.3.3 Laws of Photoelectric Effect

On the basis of the above experiment, **Lenard and Millikan** gave the following laws regarding photoelectric effect:

1. The number of photoelectrons emitted per second from the metal surface is directly proportional to the intensity of incident light.
2. The maximum Kinetic Energy of emitted photoelectrons does not depend upon the intensity of incident light.
3. The maximum Kinetic Energy of emitted photoelectrons increases linearly with increase in frequency of incident light.
4. If the frequency of incident light is less than certain minimum value, then no photoelectrons emitted from the metal surface whatever may be the intensity of incident light. This minimum frequency (threshold frequency) is different for different metals.
5. Photoelectric process is instantaneous i.e., there is no time-lag between incidence of light and emission of photoelectrons.

Classical physics failed to explain the observed laws on the basis of electromagnetic theory.

1.3.4 Einstein's Photoelectric Equation

To explain the experimental observations of photoelectric effect, Einstein used Plank's Quantum Theory of light (light beam consists of photons). He introduced a concept of work function and is nothing but the minimum energy required to make the electron to come out of the metal surface, represented by ϕ . Work function is measured in eV (electron volt). Work function depends on the properties of the metal and the nature of the surface.

According to Einstein, whenever a photon of energy hf is incident on a metal, an electron absorbs it instantaneously and if the absorbed energy hf by the electron is greater than the work function (binding energy of electron), it will come out of the metal **surface** and then acquire some kinetic energy to move out with a velocity v .

The energy of a photon absorbed by the electron is used in two ways.

- (i) The part of absorbed photon energy is used in releasing the electron from the metal surface
- (ii) The remaining energy appears as the kinetic energy of the electron.

Thus we can write: Energy of incident photon = *Binding energy* of electron + *K.E.* of electron

$$\text{Then, } hf = \phi + \frac{1}{2} mv_{\max}^2 \quad \dots (1.8)$$

Eqn. 1.8 is the Einstein's photoelectric equation where ϕ is called the work function of the given metal. Work function of a metal is the minimum energy needed to liberate an electron from the surface of the metal.

Here, $\frac{1}{2} mv_{\max}^2$ represents the kinetic energy (KE.) imparted to the electron.

$$\text{K.E.} = \frac{1}{2} mv_{\max}^2 = hf - \phi \quad \dots (1.9)$$

Work function is different for different metals.

$$\text{If } f_0 \text{ is the threshold frequency then } \phi = hf_0 \quad \dots (1.10)$$

$$\text{K.E.} = \frac{1}{2} mv_{\max}^2 = hf - \phi = hf - hf_0 = h(f - f_0) \quad \dots (1.11)$$

Explanation of experimental observations using Einstein's Photoelectric equation:

1. Photoelectric effect is instantaneous process because of collision between two micro particles namely an electron and a photon.
2. Kinetic energy of the electron depends on the term $(f-f_0)$ as seen from equation (1.11). For frequency $f = f_0$, kinetic energy of the electron equal to zero. This frequency f_0 represents the threshold frequency. Photoelectrons are not emitted if $f < f_0$.
3. If intense light radiation is incident on a metal surface, then it implies that more photons are incident on more electrons and hence making more photoelectrons to be emitted which increases the photoelectric current.
4. An increase in frequency of the incident radiation increases the energy of the emitted electrons as given by Einstein's equation. The increase in frequency has no effect on the magnitude of photo current.
5. As the kinetic energy of the photoelectrons increases with frequency; it requires large value of retarding potential to stop the electrons. If m is the mass and e is the charge of the electron emitted with velocity v and V is the stopping potential, then $eV = \frac{1}{2} mv^2$.

Thus, Einstein explained photoelectric effect successfully on the basis of *particle nature of light* and got Nobel Prize in 1921.

1.4 COMPTON EFFECT

In the year 1916, **Einstein** extended his photon concept and proposed that when light interacts with matter, not only energy but also linear momentum of photon gets transferred in discrete amounts and both law of conservation of energy and law of conservation of momentum holds good. The magnitude of momentum transferred with each photon of frequency f is given by:

$$p = hf/c = h/\lambda \quad \dots (1.12)$$

In 1923, Arthur Compton at Washington University carried out an experiment that gave support to the views of Einstein. Compton arranged for a beam of X-rays of wavelength λ to fall on a target made of graphite and measured the wavelengths and intensities of X-rays scattered in various directions from the target. The observed phenomena is called as Compton effect. He received Nobel Prize in 1927.

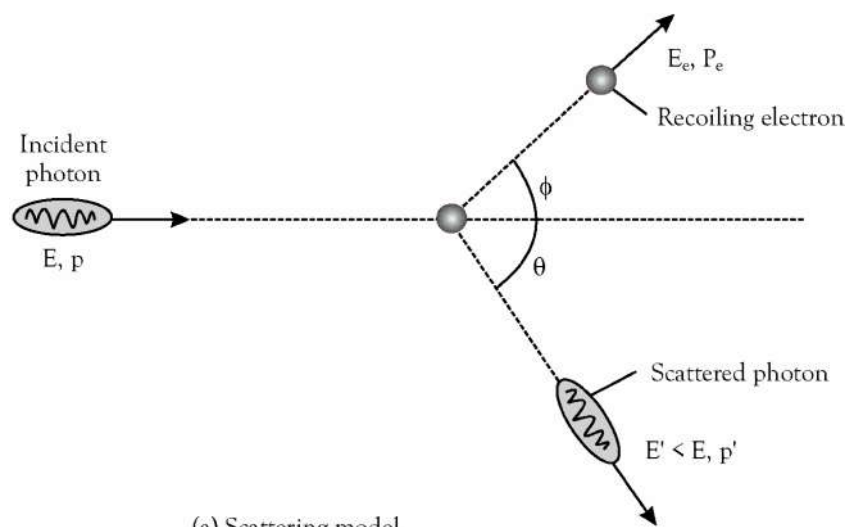
1.4.1 Definition

When X-rays of sharply defined frequency are incident on a material of low atomic number like carbon, they suffer a change of frequency on scattering. The scattered beam contains two wavelengths. In addition to the expected incident wavelength, there exists a component of longer wavelength. This phenomenon is called **Compton effect**. The change in wavelength ($\Delta\lambda$) from incident wavelength (λ) to scattered X-ray wavelength (λ') is called **Compton shift**.

Explanation: The classical electromagnetic theory failed to explain Compton shift but Compton successfully used Quantum Theory of Radiation to explain the phenomena. Accordingly, the whole process is treated as a particle collision event between X-ray photon and a loosely bound electron of the scatterer. In this process, both momentum and energy are conserved. In this photon-electron collision, a portion of the energy of the photon is transferred to the electron. As a result, the X-ray proceeds with less than the original energy and therefore gains lower frequency or higher wavelength.

1.4.2 Expression for Compton Shift

The incident photon with an energy hf and momentum hf/c strikes an electron at rest. The initial momentum of the electron is zero and its initial energy is only the rest mass energy m_0c^2 . The scattered photon of energy hf' and momentum hf'/c moves away in a direction inclined at an angle θ to the original direction as shown in Fig. 1.7. After scattering, the electron acquires a momentum mv and moves at an angle ϕ to the original direction. The energy of this recoil electron is mc^2 .



(a) Scattering model

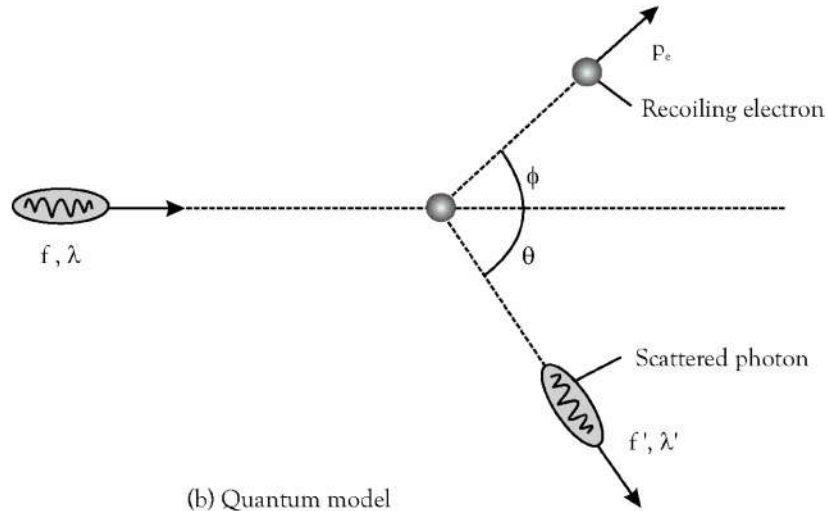


Figure 1.7 Scattering of photon by electron of an atom

According to the principle of conservation of energy,

$$hf + m_0c^2 = hf' + mc^2 \quad \dots (1.13)$$

Considering x and y components of the momentum and applying the principle of conservation of momentum gives :

$$hf/c + 0 = (hf'/c) \cos \theta + mv \cos \phi \quad \dots (1.14)$$

$$\text{and} \quad 0 = (hf'/c) \sin \theta - mv \sin \phi \quad \dots (1.15)$$

Here, m is the mass associated with moving electron related to its rest mass by the following relation as given by Einstein Relativistic equation,

$$m = \frac{m_0}{\sqrt{1 - \left(\frac{v^2}{c^2}\right)}} \quad \dots (1.16)$$

From Eqn. (1.14) and (1.15) we have

$$hf - hf' \cos \theta = mvc \cos \phi \quad \dots (1.17)$$

$$hf' \sin \theta = mvc \sin \phi \quad \dots (1.18)$$

Squaring and adding Eqn. (1.17) and (1.18),

$$h^2f^2 + h^2f'^2 - 2h^2ff' \cos \theta = m^2v^2c^2 \quad \dots (1.19)$$

From Eqn. (1.13),

$$hf - hf' + m_0c^2 = mc^2 \quad \dots (1.20)$$

Squaring Eqn. (1.20) gives

$$(hf - hf')^2 + m_0^2 c^4 + 2 m_0 c^2 h(f - f') = m^2 c^4$$

$$\text{or } h^2 f^2 - h^2 f'^2 - 2h^2 ff' + m_0^2 c^4 + 2 m_0 c^2 h(f - f') = m^2 c^4 \quad \dots (1.21)$$

Subtracting Eqn. (1.19) from Eqn. (1.21) we get,

$$\begin{aligned} m^2 c^2 (c^2 - v^2) &= -2h^2 ff' + 2 m_0 c^2 h(f - f') + 2h^2 ff' \cos \theta + m_0^2 c^4 \\ m^2 c^2 (c^2 - v^2) &= -2h^2 ff' (1 - \cos \theta) + 2 m_0 c^2 h(f - f') + m_0^2 c^4 \end{aligned} \quad \dots (1.22)$$

From Eqn. (1.16) we get, $m^2 = m_0^2 c^2 / (c^2 - v^2)$

$$\text{or } m^2 (c^2 - v^2) = m_0^2 c^2 \quad \dots (1.23)$$

Using Eqn. (1.23) in Eqn. (1.22), we get

$$m_0^2 c^4 = -2h^2 ff' (1 - \cos \theta) + 2 h(f - f') m_0 c^2 + m_0^2 c^4$$

$$\text{or } 2 h(f - f') m_0 c^2 = 2h^2 ff' (1 - \cos \theta)$$

$$\text{or } (f - f') / ff' = (h/m_0 c^2) (1 - \cos \theta)$$

$$\text{or } 1/f' - 1/f = (h/m_0 c^2) (1 - \cos \theta)$$

$$\text{or } c/f' - c/f = (h/m_0 c) (1 - \cos \theta)$$

$$\text{or } \lambda' - \lambda = (h/m_0 c) (1 - \cos \theta)$$

$$\text{or } \lambda' = \lambda + (h/m_0 c) (1 - \cos \theta) \quad \dots (1.24)$$

$$\text{Therefore the change in wavelength} = \Delta\lambda = \lambda' - \lambda = (h/m_0 c) (1 - \cos \theta) \quad \dots (1.25)$$

Eqn. (1.25) shows that:

1. Compton shift $\Delta\lambda$ is independent of the wavelength of incident radiation.
2. Compton shift $\Delta\lambda$ is independent of the nature of scattering substance.
3. Compton shift $\Delta\lambda$ depends only on the angle of scattering θ .
4. The wavelength of scattered light is always greater than the wavelength of incident light.

Based on angle of scattered light, three cases can be considered:

Case (1): When $\theta = 0^\circ$: $\Delta\lambda = 0$, i.e., there is no scattering of photon along the incident direction.

Case (2): When $\theta = 90^\circ$: $\Delta\lambda = h/m_0 c = 0.02426 \text{ \AA}$, This is known as **Compton wavelength**.

Case (3): When $\theta = 180^\circ$: $\Delta\lambda = 2 h/m_0 c = 0.04852 \text{ \AA}$, This is twice of Compton wavelength.

1.4.3 Experimental Verification of Compton Shift

Monochromatic X-rays of wavelength λ are allowed to fall on a scattering material like a small block of carbon. The scattered X-rays are received by a Bragg spectrometer and their wavelength is determined (Fig. 1.8). The spectrometer can freely swing in an arc about the scatterer. The wavelength of the scattered X-rays is measured for different values of the scattering angle. The experimental results obtained by Compton are shown in Fig. 1.9. In the scattered radiation, in addition to the incident wavelength (λ),

there exists a line of longer wavelength (λ'). The Compton shift $\Delta\lambda$ is found to vary with the angle at which the scattered rays are observed.

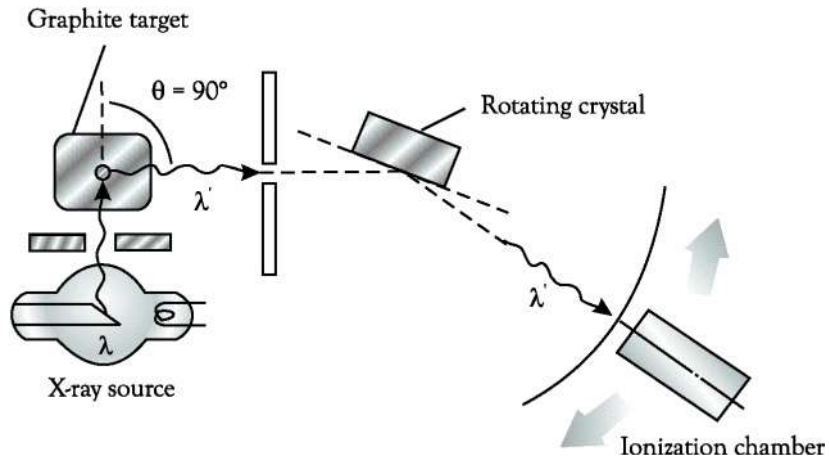


Figure 1.8 Schematic diagram of Compton's apparatus

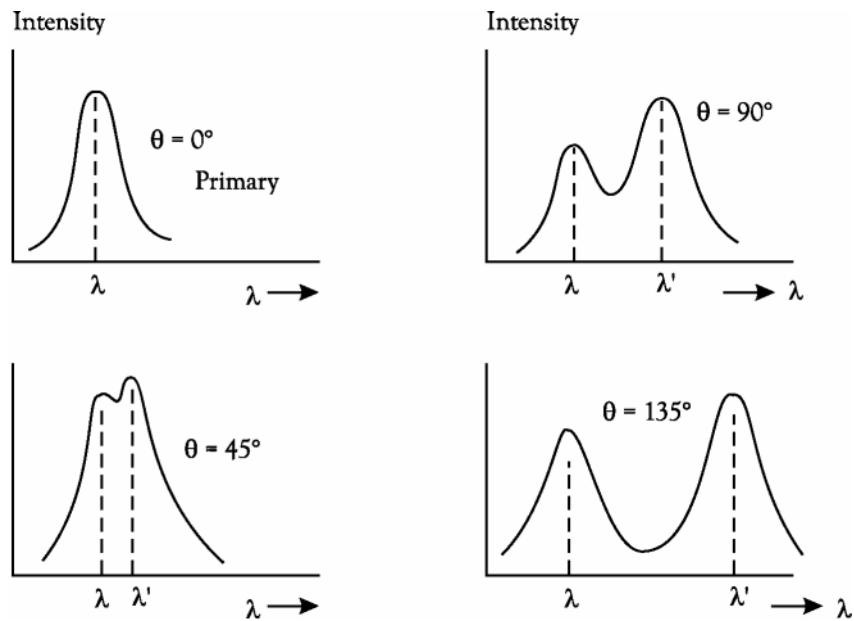


Figure 1.9 Scattered X-ray intensity versus wavelength of Compton scattering at 0° , 45° , 90° , and 135°

1.5 WAVE PARTICLE DUALISM

Various optical phenomena like reflection, refraction, interference, diffraction and polarization of light can be easily explained by wave theory of light. But, the wave theory of light failed to explain the blackbody radiation, photoelectric effect, and Compton effect. These phenomena can be easily explained by quantum theory of light. This shows light appears in both form as to support wave theory at one hand and quantum theory on the other hand. This complex nature of light is said to be dual nature. In quantum theory of light, the energy is thought to be in the form of energy packet, called photons. The energy carrying particle 'photon' itself exhibits diffraction effects, thereby showing wave like characters. But this leads to an important conclusion that light possesses dual characters, i.e., at the same time it behaves like wave and particle.

1.5.1 de-Broglie Hypothesis

In 1923, **Louis de-Broglie** (pronounced broylee) proposed that matter, like radiation, has **dual nature**. That means, the matter, which is made up of discrete particles (atoms, protons, electrons etc.), may exhibit wavelike properties under appropriate conditions. de-Broglie named these waves associated with material particles as **matter waves**. In his Ph.D. thesis, de-Broglie postulated that because photons have wave and particle characteristics, perhaps all forms of matter have wave as well as particle properties. He has been honoured by Nobel Prize in the year 1929 for unfolding the existence of wave nature of moving particles.

He proposed following similarities for his hypothesis of matter waves:

1. **Nature loves symmetry:** The two forms in which nature manifests herself are matter and radiation. We know that radiation possess dual nature so that matter also may show dual nature. Physicists have rarely gone wrong by assuming the symmetry of nature. A changing magnetic field produces an electric field in nature, and due to symmetry, it is also found that a changing electric field produces magnetic field.
2. **The close parallelism between mechanics and optics:** The principle of least action in mechanics states that a moving particle always chooses minimum action path. Similarly, the Fermat's principle in optics states that light always chooses a path where the time of transit is minimum.
3. **Bohr's theory of atomic structure:** According to Bohr's theory, the stable states of electrons in the atom are governed by integer rule. The only phenomena involving integers in Physics are those of interference and modes of vibration of stretched strings, both of which imply wave motion. Hence de-Broglie thought that the electrons may also be characterized by a periodicity like waves.

The above similarities suggested that an electron or any other material particle must exhibit wave-like properties in addition to particle-like properties. These waves, associated with a material particle, are called **matter waves**.

1.5.2 de-Broglie's Wavelength

The expression for de-Broglie's matter wave can be obtained by considering Einstein's mass-energy relationship and Max Planck's energy equation.

According to Einstein, the relationship between mass and energy of photon moving at a velocity c is given by

$$E = mc^2 \quad \dots (1.26)$$

According to Max. Plank, the energy associated with a photon of frequency f is given by

$$E = hf = hc/\lambda \quad \dots (1.27)$$

Comparing Eqn. (1.26) and (1.27), $mc^2 = hc/\lambda$

$$\text{or} \quad \lambda = h/mc \quad \dots (1.28)$$

Eqn. (1.28) gives the expression for the wavelength of a photon wave that moves through a medium when photon travels with a velocity equal to velocity of light (c).

Similarly, when any material particle having mass m and moving with velocity v must possess a de-Broglie wavelength given by

$$\lambda = h/mv \quad \dots (1.29)$$

If the material particle moves with kinetic energy $E = \frac{1}{2} mv^2$, then de-Broglie wavelength can be written as

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} \quad \dots (1.30)$$

1.5.3 de-Broglie's Wavelength-Extension to electron Particle

Consider an electron of rest mass m_0 and charge e accelerated by a potential of V volts from rest to a velocity v . Then we write:

$$\frac{1}{2} m_0 v^2 = eV$$

$$\text{or} \quad v = \sqrt{\frac{2eV}{m_0}} \quad \dots (1.31)$$

$$\text{We also know that the wavelength of matter wave as } \lambda = h/m_0 v \quad \dots (1.32)$$

Using Eqn. (1.31) and (1.32), we write:

$$\lambda = \frac{h}{\sqrt{2m_0 eV}} \quad \dots (1.33)$$

Putting $m_0 = 9.11 \times 10^{-31}$ kg; $h = 6.62 \times 10^{-34}$ J/s and $e = 1.602 \times 10^{-19}$ C, we get Eqn. (1.33) as

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ \AA} \quad \dots (1.34)$$

If the accelerating voltage $V = 100$ volts, then the wavelength of electron becomes $\lambda = 1.226 \text{ \AA}$. Since this wavelength is comparable with the wavelength of X-rays, the de-Broglie waves should be capable of being diffracted by a crystal, just like X-rays.

1.5.4 Davison and Germer Experiment

de-Broglie's predictions of the existence of matter waves is first verified experimentally in 1927, by **C. J. Davison** and **L.H. Germer** of Bell Telephone Laboratories in New York.

Experimental Setup :

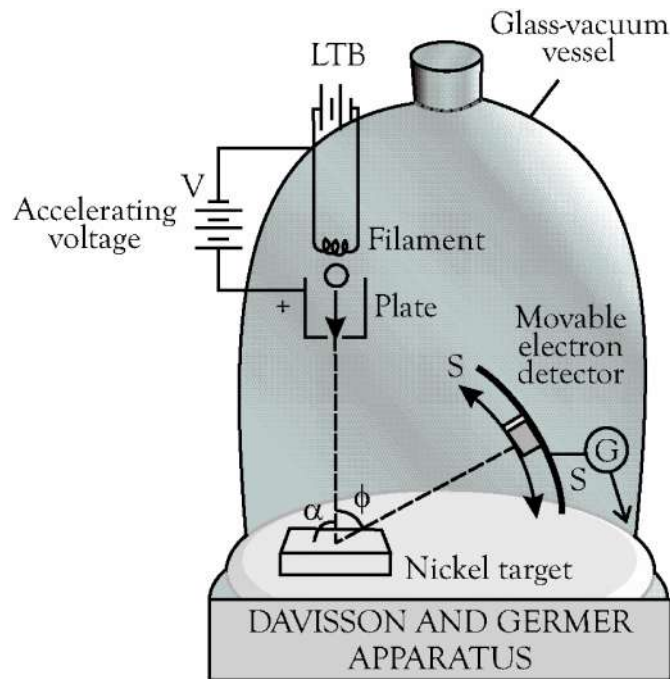


Figure 1.10 A schematic diagram of the Davison–Germer apparatus

The experimental setup is shown in Fig. 1.10. Electrons are produced by heating a filament (F) by a low tension battery (LTB). These electrons are accelerated and focused to nickel crystal by applying accelerating voltage V . The diffracted beam is collected by means of a movable detector. The whole experimental setup is placed inside a vacuum chamber.

Experimental Procedure

The beam of electron is allowed to fall normally on the surface of the crystal. Due to normal incidence, the nickel crystal acts like diffraction grating and the diffracted beam is collected by means of a detector which can be moved to positions on a circular scale S and the intensity of electron beam is measured by means of a galvanometer G . The galvanometer deflection is plotted against the angle between incident beam and the beam entering the detector. The experiment is repeated for different accelerating voltages and resulting curves are drawn. A typical curve obtained for accelerating potential of 54 V is shown in Fig. 1.11.

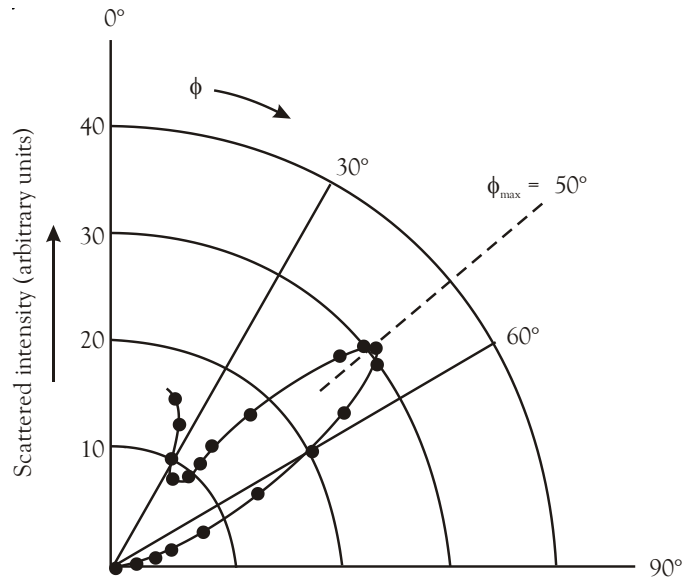


Figure 1.11 Graph of intensity of diffracted beam versus the angle between incident and diffracted beam for 54 V

Experimental Result

The graph remains fairly smooth till the accelerating voltage becomes 44 volts. At 44 volts, a spur appears in the graph and as the accelerating voltage is increased, the length of the spur increases, till the accelerating voltage reaches 54 volts at an angle of 50°. With further increase in accelerating voltage, the spur decreases in length and finally disappears at 68 volts.

Inference

The occurrence of a pronounced spur at 50° with the electron accelerated through 54 volts can be explained as due to constructive interference of the electron waves, scattered in this direction, from the regularly spaced parallel planes in the Nickel crystal. According to de-Broglie's theory, the wavelength of the electron accelerated through a potential of 54 volts is given by:

$$\lambda = \frac{12.26}{\sqrt{54}} \text{ \AA} = 1.66 \text{ \AA}.$$

According to the experiment, a diffracted beam at co-latitude of 50° corresponds to the electron beam glancing angle of $\theta = 65^\circ$ with respect to the crystal plane is observed. For nickel, the interplanar distance, d is found to be 0.91 Å from the X-ray diffraction studies. The order of diffraction is taken to be 1 in this case and applying the Bragg's equation $n\lambda = 2d \sin \theta$, where n refers to order of diffraction. By simplifying, we get, $\lambda = 2 \times 0.91 \text{ \AA} \times \sin 50^\circ = 1.65 \text{ \AA}$. Thus the experimental value is in close agreement with the theoretical value. This shows that a beam of electrons behaves like X-rays, suffers diffraction at reflecting surfaces and thus has wave-like characteristics.

1.6 MATTER WAVES AND THEIR CHARACTERISTIC PROPERTIES

Unlike electromagnetic waves, the matter waves have following properties:

1. The wavelength of matter wave is inversely proportional to mass of the particle. Hence larger the mass of the particle, shorter will be the wavelength and vice versa.
2. The wavelength of matter wave is inversely proportional to velocity of the particle. Hence greater the velocity of the particle, smaller will be the wavelength and vice versa.
3. The amplitude of the de-Broglie wave varies with likelihood of detecting the particle at a particular position. Hence the matter wave is termed as probability wave.
4. When a particle is in motion, two different velocities are associated with it. They are mechanical motion of particle (v_{particle}) and motion of associated matter wave (v_{phase}). These two are connected by a relation $v_{\text{phase}} = c^2/v_{\text{particle}}$. Now, the particle velocity $v_{\text{particle}} < c$. Hence, the velocity of propagation of matter wave $v_{\text{phase}} > c$. Thus matter wave can travel greater than velocity of light!.

1.6.1 Phase Velocity, Group Velocity and Particle Velocity

According to de-Broglie, each particle of matter (like electron, proton etc.) may be regarded as consisting of group of waves or a wave packet. Each component wave propagates with a definite velocity called **phase velocity** or **wave velocity**. But when a disturbance consists of a number of component waves, each travelling with slightly different velocity, the resultant velocity will be that of a periodicity. The velocity of advance of this periodicity is called the **group velocity**.

Phase velocity

The equation for a wave travelling in positive x-direction is given by

$$y = A \sin(\omega t - kx) \quad \dots(1.35)$$

Where y is the displacement along y-direction at the instant t , ω is the angular frequency, k is the propagation constant and x is the displacement along x-axis at the instant t . In the above equation, $(\omega t - kx)$ gives the phase of the vibrating particle. The phase quantity $(\omega t - kx)$ is same for the particles which are in the same state of vibration (same phase). Therefore for those particles which are in the same phase, the rate of change of $(\omega t - kx)$ with respect to time is zero i.e.,

$$\frac{d}{dt}(\omega t - kx) = 0 \quad \text{or} \quad \omega - k \left(\frac{dx}{dt} \right) = 0$$

or
$$\frac{dx}{dt} = \frac{\omega}{k}$$

The velocity with which the phase of the vibrating particle propagates as the wave progresses is called phase velocity. Here the dx/dt is taken as phase velocity.

$$v_{\text{phase}} = \frac{\omega}{k}$$

Group velocity

Definition: The velocity with which the wave packet, formed due to the superposition of two or more travelling waves of slightly different frequency, is transported is called group velocity.

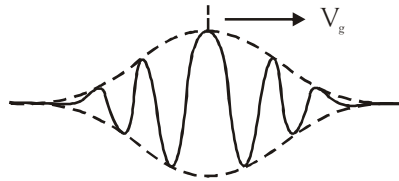


Figure 1.12 Illustration on group velocity

Consider two travelling waves y_1 and y_2 of same amplitude with slightly difference in their wavelengths and are given by

$$y_1 = A \sin(\omega_1 t - k_1 x)$$

$$y_2 = A \sin(\omega_2 t - k_2 x)$$

The resultant displacement y due to the superposition of two waves is given by

$$y = y_1 + y_2$$

$$y = A [\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

Using the identity $\sin a + \sin b = 2 \cos\left(\frac{a-b}{2}\right) \sin\left(\frac{a+b}{2}\right)$ we get

$$y = 2A \cos\left(\frac{(\omega_1 - \omega_2)t - (k_1 - k_2)x}{2}\right) \sin\left(\frac{(\omega_1 + \omega_2)t - (k_1 + k_2)x}{2}\right)$$

$$y = 2A \cos\left(\frac{\Delta\omega t - \Delta k x}{2}\right) \sin(\omega t - kx) \quad \dots(1.36)$$

where $\omega = (\omega_1 + \omega_2)/2$, $k = (k_1 + k_2)/2$, $\Delta\omega = (\omega_1 - \omega_2)$ and $\Delta k = (k_1 - k_2)$

Compare Eqn (1.35) with Eqn (1.36). In Eqn (1.35) 'A' is the amplitude but in Eqn (1.36) the amplitude is

$$2A \cos\left(\frac{\Delta\omega t}{2} - \frac{\Delta kx}{2}\right)$$

The above resultant wave amplitude is not constant but varies as a cosine function. The velocity with which the variation in amplitude is transmitted in the resultant wave is referred as group velocity. The group velocity is given by

$$v_{\text{group}} = \frac{\Delta\omega}{\Delta k} \quad \dots(1.37)$$

1.6.2 Relation between Phase Velocity and Group Velocity

The expression for group velocity is given by $v_{\text{group}} = d\omega/dk$... (1.38)

The expression for phase velocity is given by $v_{\text{phase}} = \omega/k$... (1.39)

where ω is the angular frequency of the wave, and k is the wave vector.

Eqn. (1.39) can be written as $\omega = kv_{\text{phase}}$

Then,
$$v_{\text{group}} = \frac{d\omega}{dk} = \frac{d}{dk}(kv_{\text{phase}}) = v_{\text{phase}} + k \frac{dv_{\text{phase}}}{dk}$$

Hence,
$$v_{\text{group}} = v_{\text{phase}} + k \left(\frac{dv_{\text{phase}}}{d\lambda} \right) \frac{d\lambda}{dk} \quad \dots (1.40)$$

But, we know that $k = 2\pi/\lambda$

Differentiating we get, $dk/d\lambda = -2\pi/\lambda^2$,

or $d\lambda/dk = -\lambda^2/2\pi$

Then we can write $k(d\lambda/dk) = (2\pi/\lambda)(-\lambda^2/2\pi) = -\lambda$

Substituting the above Eqn. in Eqn. (1.40), we get,

$$v_{\text{group}} = v_{\text{phase}} - \lambda \left(\frac{dv_{\text{phase}}}{d\lambda} \right) \quad \dots (1.41)$$

Eqn. (1.41) gives the relationship between group velocity and phase velocity.

1.6.3 Relation between Group Velocity and Particle Velocity

The expression for group velocity is given by

$$v_{\text{group}} = d\omega/dk \quad \dots(1.42)$$

But $\omega = 2\pi f = 2\pi (E/h)$... (1.43)

$$d\omega = (2\pi/h) dE \quad \dots (1.44)$$

Also we have $k = 2\pi/\lambda = 2\pi (p/h)$... (1.45)

$$dk = (2\pi/h) dp \quad \dots (1.46)$$

Dividing Eqn. (1.44) by Eqn. (1.46) gives

$$d\omega/dk = dE/dp \quad \dots (1.47)$$

But we know that the kinetic energy of particle is $E = p^2/2m$, where p is momentum of the particle.

Then,
$$dE/dp = 2p/2m = p/m \quad \dots (1.48)$$

Using Eqn. (1.48) in Eqn. (1.47) we get, $d\omega/dk = p/m$

But $p = mv_{\text{particle}}$ where v_{particle} is the velocity of the particle.

Then,
$$d\omega/dk = mv_{\text{particle}}/m = v_{\text{particle}} \quad \dots (1.49)$$

From Eqn. (1.42) and (1.49), we get,

$$v_{\text{group}} = v_{\text{particle}} \quad \dots (1.50)$$

Thus the de-Broglie wave group associated with a particle travels with a velocity equal to the velocity of the particle itself.

1.6.4 Expression for de-Broglie Wavelength using Group Velocity

The expression for group velocity is given by

$$v_{\text{group}} = d\omega/dk \quad \dots (1.51)$$

But $\omega = 2\pi f$ and $k = 2\pi/\lambda$

Then $d\omega = 2\pi df$ and $dk = 2\pi d(1/\lambda)$

Then Eqn. (1.51) becomes
$$v_{\text{group}} = d\omega/dk = df/d(1/\lambda) \quad \dots (1.52)$$

We can consider the particle velocity is same as group velocity. Hence

$$v = df/d(1/\lambda) \quad \text{or} \quad d(1/\lambda) = df/v \quad \dots (1.53)$$

Using total energy of the particle, we can write $hf = \frac{1}{2}mv^2 + V \quad \dots (1.54)$

Let the particle is moving in a field of constant potential V , then by differentiating Eqn. 1.54 gives:

$$h df = mv.dv \quad \text{or} \quad df/v = (m/h)dv \quad \dots (1.55)$$

From Eqn. (1.53) and (1.55), we get, $d(1/\lambda) = (m/h)dv$

Integrating,
$$1/\lambda = (m/h)v + \text{constant} \quad \dots (1.56)$$

Let the momentum of the particle be p and $p = mv$. Also by substituting the constant of integration is zero, we get,

$$1/\lambda = p/h \quad \text{or} \quad \lambda = h/p \quad \dots (1.57)$$

The above Eqn. (1.57) is the de-Broglie's equation.

1.6.5 Relation between Group Velocity, Phase Velocity and Velocity of Light

We know that the expression for phase velocity is given by $v_{\text{phase}} = \omega/k$

Also
$$\omega = 2\pi f = 2\pi \frac{E}{h} \quad \dots(1.58)$$

Also
$$k = \frac{2\pi}{\lambda} = 2\pi \frac{p}{h} \quad \dots(1.59)$$

Then
$$v_{\text{phase}} = \frac{\omega}{k} = \frac{E}{p} = \frac{mc^2}{mv_{\text{particle}}} = \frac{c^2}{v_{\text{particle}}} \quad \dots(1.60)$$

But, from Eqn. (1.50),
$$v_{\text{group}} = v_{\text{particle}}$$

Using Eqn. (1.60) and (1.50), we can write as

$$v_{\text{phase}} \cdot v_{\text{group}} = c^2 \quad \dots(1.61)$$

SOLVED PROBLEMS

Photoelectric Effect

1. Calculate the velocity of the ejected photoelectron for the incident photon energy of 5eV. The threshold energy for the photosensitive metal is given by 3.2eV.

Given data,

$$\text{Photon energy } E = hf = 5 \text{ eV}$$

$$\text{Work function of photosensitive metal } \phi = 3.2 \text{ eV}$$

From the Einstein Photoelectric equation

$$hf = \phi + \frac{1}{2}mv^2$$

Therefore,
$$\frac{1}{2}mv^2 = hf - \phi$$

$$\frac{1}{2}mv^2 = 5\text{eV} - 3.2\text{eV}$$

$$= 1.8 \text{ eV}$$

$$= 1.8 \times 1.6 \times 10^{-19} \text{ J} \quad (\because 1\text{eV} = 1.6 \times 10^{-19} \text{ J})$$

$$= 2.88 \times 10^{-19} \text{ J}$$

Therefore,
$$v = \sqrt{\frac{2 \times 2.88 \times 10^{-19}}{9.11 \times 10^{-31}}}$$

$$= 7.95 \times 10^5 \text{ m/s}$$

The maximum velocity of the photoelectron ejected due to the incident radiation energy of 5 eV on the metal surface is $7.95 \times 10^5 \text{ m/s}$.

2. Electrons are ejected out of the photosensitive metal surface when a radiation of wavelength 210 nm falls on it. Given that the limiting wavelength for the photosensitive metal is 325 nm. Calculate the kinetic energy, stopping potential and velocity of the photoelectron.

Given data:

Incident wavelength $\lambda = 210 \text{ nm}$

The corresponding photon energy is

$$E = hf = \frac{hc}{\lambda} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{210 \times 10^{-9}} = 9.64 \times 10^{-19} \text{ J}$$

Threshold (limiting) wavelength $\lambda_0 = 325 \text{ nm}$

The threshold energy (work function) is

$$\phi = hf_0 = \frac{hc}{\lambda_0} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{325 \times 10^{-9}} = 6.12 \times 10^{-19} \text{ J}$$

- (i) The kinetic energy of the photoelectron is

$$\frac{1}{2}mv^2 = hf - \phi$$

$$\frac{1}{2}mv^2 = 9.64 \times 10^{-19} \text{ J} - 6.12 \times 10^{-19} \text{ J}$$

$$\frac{1}{2}mv^2 = 3.34 \times 10^{-19} \text{ J}$$

Therefore,

$$v = \sqrt{\frac{2 \times 3.34 \times 10^{-19}}{m}}$$

$$v = \sqrt{\frac{2 \times 3.34 \times 10^{-19}}{9.11 \times 10^{-31}}}$$

$$v = 8.56 \times 10^5 \text{ m/s}$$

- (ii) Stopping potential

$$K.E = eV = 3.34 \times 10^{-19} \text{ J}$$

$$V = \frac{3.34 \times 10^{-19} \text{ J}}{e}$$

$$V = \frac{3.34 \times 10^{-19}}{1.6 \times 10^{-19}}$$

$$V = 2.087 \text{ volts}$$

Therefore the stopping potential $V = 2.087$ volts

Compton Effect

3. The wavelength of the incident X-ray is 1.54 \AA . Calculate the maximum wavelength of the scattered X-ray by the target material in a Compton scattering process and hence calculate the energy and velocity of the recoiling electron.

Given data:

The incident X-ray wavelength $\lambda = 1.54 \text{ \AA} = 1.54 \times 10^{-10} \text{ m}$

The scattered X-ray wavelength is maximum for $\theta = 180^\circ$

- (i) To calculate maximum wavelength

We have from Compton shift expression

$$\Delta\lambda = (\lambda^i - \lambda) = \frac{h}{m_0c}(1 - \cos\theta)$$

or

$$\lambda^i = \lambda + \frac{h}{m_0c}(1 - \cos\theta)$$

$$\lambda^i = 1.54 \times 10^{-10} + \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-31} \times 3 \times 10^8}(1 - \cos 180)$$

$$\lambda^i = 1.54 \times 10^{-10} + \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-31} \times 3 \times 10^8}(1 - \cos 180)$$

$$\lambda^i = 1.588 \times 10^{-10} \text{ m}$$

- (ii) To calculate Kinetic energy of recoiling electron

The kinetic energy of the recoiling electron = incident photon energy - scattered photon energy

$$K.E. = E - E^i = hf - hf^i = hc \left[\frac{1}{\lambda} - \frac{1}{\lambda^i} \right]$$

$$K.E. = 6.625 \times 10^{-34} \times 3 \times 10^8 \left[\frac{1}{1.54 \times 10^{-10}} - \frac{1}{1.588 \times 10^{-10}} \right] \text{ J}$$

$$K.E. = 3.9 \times 10^{-17} \text{ J}$$

(iii) To calculate the velocity of the recoiling electron

$$\frac{1}{2}mv^2 = 3.9 \times 10^{-17} \text{ J}$$

Therefore,

$$v = \sqrt{\frac{2 \times 3.9 \times 10^{-17}}{m}}$$

$$v = \sqrt{\frac{2 \times 3.9 \times 10^{-17}}{9.11 \times 10^{-31}}}$$

$$v = 9.25 \times 10^6 \text{ m/s}$$

The maximum wavelength of scattered X-ray is $\lambda' = 1.588 \times 10^{-10} \text{ m}$, the kinetic energy of recoiling electron is $K.E. = 3.9 \times 10^{-17} \text{ J}$ and the velocity of the recoiling electron is $v = 9.25 \times 10^6 \text{ m/s}$

de-Broglie hypothesis

4. Calculate the velocity of the electron whose de-Broglie wavelength is 4.52 \AA .

Given data:

$$\lambda = 4.52 \text{ \AA} = 4.52 \times 10^{-10} \text{ m}$$

To calculate velocity of the electron $v = ?$

The expression for de-Broglie wavelength is

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

Therefore,

$$v = \frac{h}{m\lambda} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-31} \times 4.52 \times 10^{-10}}$$

$$v = 1.61 \times 10^6 \text{ m/s}$$

The velocity of the accelerated electron is $v = 1.61 \times 10^6 \text{ m/s}$

Davison and Germer Experiment

5. In a Davison and Germer experiment the second order diffraction resulting in a constructive interference was observed at an angle of 40° with respect to incident electron beam direction for the wavelength of electron waves 2.5 \AA . Calculate the interplanar distance of the experimental crystal.

Given data:

$$n = 2$$

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

$\phi = 40^\circ$ is the angle made by the scattered electron waves with respect to incident electron waves

To calculate

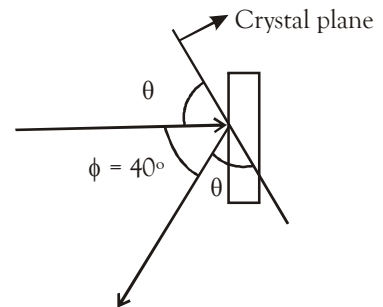
Interplanar distance, $d = ?$

The glancing angle can be calculated as follows

$$180^\circ = 40^\circ + 2\theta$$

$$2\theta = 180^\circ - 40^\circ$$

$$\theta = \frac{180^\circ - 40^\circ}{2} = 70^\circ$$



The Bragg's equation is

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

Therefore,

$$d = \frac{n\lambda}{2\sin\theta} = \frac{2 \times 2.5 \times 10^{-10}}{2\sin 70^\circ} = 2.66 \text{ \AA}$$

The interplanar spacing for the given crystal is 2.66 \AA

Group velocity and Phase velocity

6. The particle of mass $3.5 \times 10^{-30} \text{ kg}$ is accelerated it attains a steady kinetic energy of 25 eV. Calculate the wavelength associated with the moving particle and also the phase velocity of the matter wave.

Given Data:

$$\text{Mass of the particle } m = 3.5 \times 10^{-30} \text{ kg}$$

$$\text{Kinetic energy of the particle, K.E.} = 25 \text{ eV} = 25 \times 1.6 \times 10^{-19} \text{ J} = 40 \times 10^{-19} \text{ J}$$

To calculate

$$\text{de-Broglie (matter waves) wavelength } \lambda = ?$$

$$\text{Phase velocity of the matter waves } v_{\text{phase}} = ?$$

The de-Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2 \times m \times \text{K.E.}}} = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 3.5 \times 10^{-30} \times 40 \times 10^{-19}}} = 1.25 \text{ \AA}$$

The particle velocity is

$$v_{\text{particle}} = \frac{h}{m\lambda}$$

Therefore,

$$v_{\text{particle}} = \frac{h}{m\lambda} = \frac{6.625 \times 10^{-34}}{3.5 \times 10^{-30} \times 1.25 \times 10^{-10}} = 1.51 \times 10^6 \text{ m/s}$$

The phase velocity of a de-Broglie wave is given by

$$v_{\text{particle}} v_{\text{phase}} = c^2$$

Therefore,

$$v_{\text{phase}} = \frac{c^2}{v_{\text{particle}}} = \frac{(3 \times 10^8)^2}{1.51 \times 10^6} = 5.96 \times 10^{10} \text{ m/s}$$

The wavelength associated with the moving particle is 1.25 \AA and the phase velocity is $5.96 \times 10^{10} \text{ m/s}$

EXERCISES

I. Descriptive Type Questions

1. What is a blackbody? What are the characteristics of black body radiation spectrum?
2. What are the drawbacks of Wein's law and Rayleigh-Jeans law?
3. Write a note on Planck's law of blackbody radiation.
4. Write a note on Einstein theory of photoelectric effect.
5. Explain why the wave theory of light failed to explain Compton Effect and Photoelectric Effect and how the quantum theory explained these phenomena?
6. What is Compton Effect? Derive an expression for the Compton shift.
7. Write a note on de-Broglie hypothesis and explain why this hypothesis is insignificant for macroscopic world with examples.
8. Derive an expression for de-Broglie wavelength of a accelerated particle and also for the particles at thermal equilibrium.
9. Describe the experimental setup and results which gave the proof for existence of matter waves or de-Broglie waves.
10. What is group velocity and phase velocity? Derive an expression relating them.
11. Prove that the particle velocity is nothing but group velocity of the resultant de-Broglie wave itself.
12. Derive an expression for the de-Broglie wavelength from group velocity.
13. What are matter waves? What are the characteristics of matter waves?
14. Describe Davisson and Germer experiment for confirmation of de-Broglie hypothesis.
(VTU June 2009)
15. Define Phase velocity and Group velocity. Show that Group velocity is same as particle velocity.
(VTU Jan 2009)
16. Derive de-Broglie wavelength using Group velocity.
(VTU Jan 2009)
17. Explain the energy distribution in the spectrum of a block body. Give an account of the attempts made through various laws to explain the spectrum.
(VTU Jan 2008)
18. Define phase velocity and group velocity. Derive an expression for de-Broglie wavelength from group Velocity.
(VTU Jan 2008)
19. What is Planck's radiation law? Show how Wien's law and Rayleigh-Jeans's law can be derived from it.
(VTU June 2008)
20. Explain phase velocity and group velocity. Derive the expression for de-Broglie wave length using the concept of group velocity.
(VTU June 2008)

21. Give a brief account of black body radiation and Planck's radiation law; leading to quantization of energy. (VTU June 2007)
22. Explain phase velocity, group velocity and particle Velocity and write down the relation between them. (VTU June 2007)
23. From the concept of group velocity, obtain an expression for de-Broglie wavelength. (VTU June 2007)
24. Discuss Planck's radiation law. (VTU Jan 2007)
25. Explain the duality of matter waves from the inferences drawn from photoelectric effect and Davisson-Germer effect. (VTU Jan 2007)
26. Define group velocity and obtain an expression for the same. (VTU Jan 2007)
27. What is Planck's radiation law? Show how Wien's law and Rayleigh-Lean's law can be derived from it. (VTU Jan 2010)
28. Define group velocity. Derive relation between group velocity and phase velocity. (VTU Jan 2010)

II. Multiple Choice Questions

1. An electron and a proton are accelerated through same potential. The ratio of de-Broglie wave length λ_e/λ_p is
 - (a) 1
 - (b) m_e/m_p
 - (c) m_p/m_e
 - (d) $\sqrt{\frac{m_p}{m_e}}$
2. Wave function associated with a material particle is :
 - (a) Single valued
 - (b) Finite
 - (c) Continuous
 - (d) All the above
3. In a black body radiation Spectrum, the maximum energy peaks shifts towards the shorter wave length side with the increase in temperature. This confirms
 - (a) Stefan's law
 - (b) Wein's law
 - (c) Rayleigh-Jean's law
 - (d) Planck's law .
4. The group velocity of the particle is 3×10^6 m/s, whose Phase velocity is
 - (a) 6.06×10^6 m/s
 - (b) 3×10^{10} m/s
 - (c) 30 m/s
 - (d) 1.5×10^{10} m/s

5. The de-Broglie wave length associated with an electron of mass m and accelerated by a potential V is
- (a) $\frac{h}{\sqrt{2meV}}$ (b) $\frac{\sqrt{2mVe}}{h}$
(c) $\frac{h}{Vem}$ (d) $\frac{h}{2Vem}$
6. Davisson and Germer were the first to demonstrate:
- (a) The straight line propagation of light (b) The diffraction of Photons
(c) The effective mass of electron (d) None of the these.
7. Electrons behaves as waves because they can be:
- (a) Deflected by an electric field (b) Diffracted by a crystal
(c) Deflected by magnetic field (d) They ionize a gas.
8. In Davisson -Germer experiment the hump is most prominent when the electron is accelerated by
- (a) 34 volts (b) 54 volts
(c) 60 volts (d) 80 volts
9. In a blackbody radiation spectrum, the Wein's distribution law is applicable only for
- (a) Longer wavelength (b) Shorter wavelength
(c) Entire wavelength (d) None of these.
10. The de-Broglie wavelength associated with the particles in thermal equilibrium at temperature T is given by
- (a) $\frac{h}{2Vem}$ (b) $\frac{\sqrt{2mVe}}{2kTm}$
(c) $\frac{h}{\sqrt{3mkT}}$ (d) $\frac{h}{\sqrt{2mVe}}$
11. In a Davison and Germer experiment the spur is prominent for the scattering angle of
- (a) 35° (b) 90°
(c) 50° (d) none of these
12. If the group velocity of de Broglie wave is 4×10^7 m/sec, its phase velocity is
- (a) 12×10^8 m/sec (b) 2.25×10^9 m/sec
(c) 5.33×10^8 m/sec (d) 1.33×10^9 m/sec
13. Wien's law is deduced from Planck's radiation formula under the condition of
- (a) Very small wavelength and temperature

- (b) Large wavelength and temperature
 (c) Small wavelength and high temperature
 (d) Large wavelength and small temperature
14. The Compton wavelength is given by
- (a) $\frac{h}{m_0 c^2}$ (b) $\frac{h^2}{m_0 c^2}$
 (c) $\frac{h}{m_0 c}$ (d) $\frac{h^2}{2m_0 c}$
15. Which of the following relations can be used to determine de Broglie wavelength associated with a particle?
- (a) $\frac{h}{\sqrt{2mE}}$ (b) $\frac{h}{mv}$
 (c) $\frac{h}{\sqrt{2meV}}$ (d) All of these
16. If the group velocity of a particle is $3 \times 10^5 \text{m/s}$, its phase velocity is
- (a) 100m/s (b) $3 \times 10^6 \text{m/s}$
 (c) $3 \times 10^8 \text{m/s}$ (d) $3 \times 10^{11} \text{m/s}$
17. If the momentum of a particle is increased by four times, the de-Broglie Wave length
- (a) become twice (b) become four times
 (c) become one-fourth (d) Zero
18. In a black body radiation spectrum, maximum intensity is shifting towards
- (a) shorter wavelength (b) longer wavelength
 (c) no change (d) None of these
19. Group velocity of wave is equal to
- (a) V_{phase} (b) V_{particle}
 (c) Velocity of light (d) None of these
20. de-Broglie wave length of an electron accelerated through a potential difference of 54V is
- (a) 1.85 \AA (b) 1.58 \AA
 (c) 1.589 \AA (d) 1.66 \AA

21. The wave property of large, massive objects is not observed because _____
 - (a) their acceleration is too small
 - (b) their momenta are too small
 - (c) their speeds are too small
 - (d) none of these
22. The wavelength associated with a moving particle _____
 - (a) depends upon charge associated with it
 - (b) does not depend on charge associated with it
 - (c) depends upon the medium in which the particle travels
 - (d) none of these
23. In Compton effect, the wavelength of incident wave _____
 - (a) remains constant
 - (b) shifts towards longer wavelength
 - (c) shifts towards shorter wavelength
 - (d) shifts towards both longer and shorter wavelength
24. Which of the following statement is correct for matter waves
 - (a) Matter waves travel faster than velocity of light
 - (b) Matter waves travel slower than velocity of light
 - (c) Matter waves travel at velocity of light
 - (d) Matter waves can not travel
25. Which of the following is correct for Compton shift
 - (a) Compton shift is independent of the wavelength of incident radiation.
 - (b) Compton shift is independent of the nature of scattering substance.
 - (c) Compton shift depends only on the angle of scattering θ .
 - (d) All the above.

III. Numerical Problems

1. In a Compton scattering process, the scattered X-ray wavelength becomes twice that of the incident X-ray wavelength only when the Compton shift is maximum. Calculate (i) incident X-ray wavelength, (ii) scattered X-ray wavelength and (iii) velocity of the recoiling electron.
2. Prove that the De-Broglie wavelength of a particle in thermal equilibrium at temperature T is
$$\frac{h}{\sqrt{2mK_B T}}$$
3. Calculate the potential difference through which an electron should be accelerated so that its De-Broglie wavelength becomes 10\AA .
4. When an electron is accelerated through some potential difference, it attains a steady velocity and this accelerated electron crosses two points separated by a distance of 250 cm in a 10^{-4} second.

- Calculate (i) de-Broglie wavelength of the accelerated electron and hence calculate the potential difference through which it has to be accelerated to obtain the calculated de-Broglie wavelength.
5. In a Davison and Germer experiment the electron accelerated through a potential difference of 100 V are impinged on a crystal X. It is observed that the first order diffraction maximum was observed at an angle of 65° with respect to incident electron beam direction. Calculate the interplanar distance of the crystal X.
 6. The second order diffraction resulting in maximum intensity was observed for the incident electrons energy of 75 eV at a glancing angle of 60° with respect to crystal plane. Calculate (i) angle by which the diffracted electron beam makes with respect to incident direction on the crystal (ii) calculate the interplanar distance of the crystal planes.
 7. Explain phase and group velocity. Calculate the de-Broglie wavelength of a bullet of mass 5 gm moving with velocity 20 km/h. (VTU June 2009)
 8. Compare the energy of a photon with that of a neutron when both are associated with wave length of 1 \AA given that the mass of neutron is $1.678 \times 10^{-27} \text{ kg}$ (VTU Jan 2009)
 9. A particle of mass $0.65 \text{ MeV}/c^2$ has a kinetic energy 80 eV. Calculate the deBroglie, wave length, group velocity and phase velocity of the de-Broglie wave. (VTU Jan 2008)
 10. A particle of mass $0.65 \text{ MeV}/c^2$ has free energy 120 eV. Find its de-Broglie wavelength, c is the velocity of light. (VTU June 2008)
 11. Calculate the de-Broglie wavelength of a 0.3 kg cricket ball moving with a speed of 120 km/hr. (VTU June 2007)
 12. A particle of mass $0.5 \text{ MeV}/c^2$ has kinetic energy 100 eV. Find its de-Broglie wavelength, where c is the velocity of light. (VTU Jan 2007)
 13. A fast moving neutron is found to have a associated de-Broglie wavelength of 2 \AA , find its kinetic energy and group velocity of the de-Broglie waves. (VTU Jan 2010)

Answers to Multiple Choice Questions

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

QUANTUM MECHANICS

OBJECTIVES

In the previous chapter we have seen that the wave associated with any particle in motion is a matter wave and the mathematical function which describes the motion of particle is referred as quantum mechanical wave function. How this wave function affects our description of a particle and its behavior is the subject of this section. The work carried out by Schrödinger, Heisenberg, and others, makes it possible to understand most of the phenomena involving elementary particles, atoms, molecules, and solids. In this section, we shall describe the basic features of wave mechanics and its application to simple systems. The main goal of this unit is to study

- Uncertainty principle, its application to prove non-existence of free electron inside the nucleus and physical significance
- Fundamental properties of wave function and its significance
- Probability density and normalization of wave function
- Schrödinger wave equation and its application to electron confined in one dimensional box of finite width with infinite height
- Eigen energy value and Eigen function for the particle in one dimensional box
- Application of wave equation to free particle

2.1 INTRODUCTION

Before the beginning of 20th century two theories dominated the world of physics namely Newton's laws of motion and Maxwell's laws of electromagnetism. At the end of the nineteenth century, physicists distinguished between two entities in physical phenomena : matter and radiation. To explain the phenomenon related to matter and radiation completely different laws were used for each one. For predicting the motion of material bodies, the laws of Newtonian mechanics were utilized whereas to explain the radiation, the theory of electromagnetic waves developed by Maxwell's was utilized. The Maxwell theory had produced a unified interpretation of a set of phenomena which had previously been considered as belonging to different domains: electricity, magnetism and optics. Finally, interactions between radiation and matter were well explained by the Lorentz force. This set of laws had brought physics to a point which could be considered satisfactory, in view of the experimental data at that time.

However, at the beginning of the 20th century, many experimental results reported remain unexplained by classical theory. This failure of Classical physics marked tremendous changes in the

conceptual ideas and led to the introduction of Relativistic Mechanics and Quantum Mechanics. The relativistic mechanics take care of the material bodies travelling at very high speeds, comparable to that of light (relativistic domain) and where as the Quantum theory treats the material particles and radiation on the same footing.

In the beginning of 20th century, to explain the energy distribution in the black body radiation spectrum Max Planck introduced a concept of “quantum”. Using this quantum concept Einstein successfully explained the photoelectric effect. The same concept was used later by Compton to explain Compton Effect. Quantum mechanics was further developed by Heisenberg, Schrödinger, Pauli, Dirac and many others. Quantum mechanics plays a fundamental role in the description and understanding of natural phenomena. In this section, a brief conceptual overview of the quantum mechanics which is most relevant for undergraduate level students is provided.

2.2 HEISENBERG’S UNCERTAINTY PRINCIPLE

In 1927, Werner Heisenberg at Max Planck Institute of Physics, West Germany, developed a principle on uncertainty in measurement of physical quantities and received Nobel prize in 1932.

2.2.1 Statement of Heisenberg’s Uncertainty Principle

Heisenberg’s uncertainty principle states that it is impossible to determine precisely and simultaneously the values of both the members of a pair of physical variables which describe the motion of an atomic system. Such pairs of variables are called canonically conjugate variables. Example: Position and momentum, Energy and time.

2.2.2 Heisenberg’s Uncertainty Principle Applied to Position and Momentum

According to Heisenberg, it is impossible to determine simultaneously and precisely both position and momentum of a moving particle. If Δx is the error in determining the position and Δp is the error in determining its momentum at the same instant, then these errors are related as:

$$\Delta x. \Delta p \geq \hbar / 2 \quad \dots (2.1)$$

where $\hbar = h / 2\pi$

The product of two errors is approximately of the order of Plank’s constant. If Δx is small, Δp will be large and vice versa. It means that if one quantity is measured accurately, the other quantity becomes less accurate. Thus any physical instrument cannot measure the quantities more accurately than predicted by Heisenberg’s principle.

2.2.3 Heisenberg’s Uncertainty Principle Applied to Energy and Time

According to Heisenberg, it is impossible to determine simultaneously and precisely both energy of a wave packet and time taken to measure that energy. If ΔE is the error in determining the Energy and Δt is the error in the time, then these errors are related as:

$$\Delta E. \Delta t \geq \hbar / 2 \quad \dots (2.2)$$

where $\hbar = h / 2\pi$

Heisenberg's principle implies that, in any physical measurement, probability takes the place of exactness.

2.2.4 Illustration: Heisenberg Microscope

Let us consider an idealized experiment (referred as *thought experiment*) and show that it is impossible to carry out an experiment that allows one to measure the position and momentum of a particle simultaneously and with an accuracy that violates the uncertainty principle. The thought experiment was introduced by Heisenberg himself and involves the measurement of an electron's position by means of a microscope (Fig. 2.1), which forms an image of the electron on the retina of the eye. Suppose we try to measure the position and linear momentum of an electron using this imaginary microscope with a very high resolving power (Fig 2.1), the electron can be observed if an electron scatters the photon into the microscope lens. According to physical optics, the limit of resolution of the microscope is given by the relation

$$\Delta x = \lambda/2\sin\theta \quad \dots (i)$$

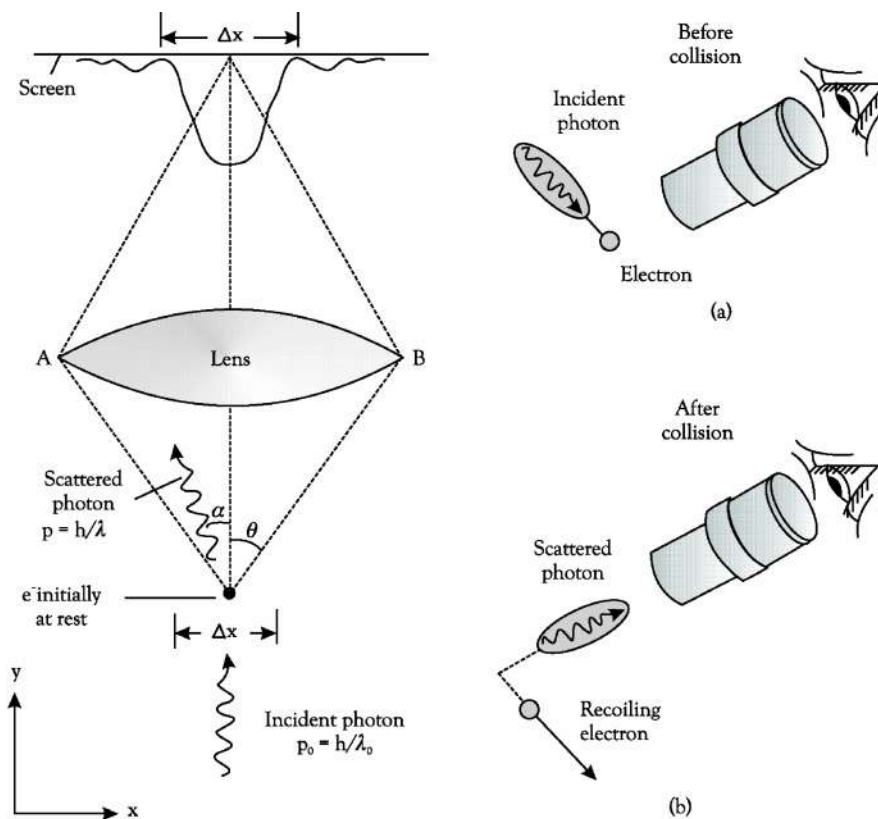


Figure 2.1 Experimental set-up to measure the position and linear momentum of an electron using an imaginary microscope

where Δx is the distance between the two points which can be just resolved by the microscope lens. This is the range in which the electron would be visible when disturbed by the photon. Hence Δx is the uncertainty involved in the position measurement of the electron.

In order to see the electron, the scattered photon must enter the microscope within the angle 2θ . The momentum imparted by the photon to the electron during the impact is of the order of h/λ . The component of this momentum along OA is $-(h/\lambda) \sin\theta$ and that along OB is $(h/\lambda) \sin\theta$. Hence, the uncertainty in the momentum measurement in the x-direction is:

$$\Delta p_x = [(h/\lambda) \sin\theta] - [-(h/\lambda) \sin\theta] = (2h/\lambda) \sin\theta \quad \dots \text{(ii)}$$

$$\Delta x \cdot \Delta p_x = [\lambda/2\sin\theta] \cdot [(2h/\lambda) \sin\theta] = h \quad \dots \text{(iii)}$$

$$\text{A more sophisticated approach will lead to } \Delta x \cdot \Delta p_x \geq \hbar/2 \quad \dots \text{(iv)}$$

2.2.5 Physical Significance

1. As per uncertainty principle, instead of trying to find the exact position or momentum of micro-particle like photon, electron or atom, one should think of probability of finding the particles at a certain positions or probable value of the momentum of the particle.
2. The uncertainty principle has no practical importance for Macro particles where de-Broglie wavelength is negligibly small.

2.3 APPLICATION OF UNCERTAINTY PRINCIPLE

2.3.1 Why Electron cannot be Present inside the Nucleus?

The typical size of nucleus is of the order of 5×10^{-15} m. Suppose if the electron exists inside a nucleus, the uncertainty in its position Δx may not exceed 5×10^{-15} m. Using Heisenberg's Uncertainty principle, uncertainty in electron's momentum is:

$$\Delta p \geq \hbar/2\Delta x \geq (1.055 \times 10^{-34})/2 \times (5 \times 10^{-15}) \geq 1.055 \times 10^{-20} \text{ Kg. m.s}^{-1}$$

An electron whose momentum is $1.055 \times 10^{-20} \text{ Kg. m.s}^{-1}$ has a kinetic energy (K.E.) many times greater than its rest mass m_0c^2 . That means $\text{K.E.} \gg m_0c^2$. Hence we can use relativistic formula $\text{K.E.} = pc$ to find kinetic energy.

$$\begin{aligned} \text{Hence,} \quad \text{K.E.} &= (1.055 \times 10^{-20})(3 \times 10^8) \\ &= 3.2 \times 10^{-12} \text{ J} \\ &= (3.2 \times 10^{-12}/1.6 \times 10^{-19}) \text{ eV} \\ &= 20 \text{ MeV} \end{aligned}$$

This shows that if an electron exists in the nucleus, the kinetic energy of electron must be more than 20 MeV. But, electrons of such large energy have never found to be emitted during β -decay. The maximum energy of β particle emitted is only of 2 to 3 MeV. Hence, we conclude that electrons can not be present within nucleus and the electrons observed in β -decay are actually created at the instant of decay.

2.4 WAVE FUNCTION, PROPERTIES AND PHYSICAL SIGNIFICANCE

2.4.1 Wave Function

The probability that a particle found at a given place in space at a given instant of time is characterized by the function $\psi(x, y, z, t)$, and is called the wave function. Wave function can be either real or complex.

2.4.2 Properties of Wave Function

1. The wave function ψ is in general is a complex function. ψ^* is its complex conjugate.
2. The wave function must be well defined, i.e., it must be single valued and continuous everywhere.
3. It is used to describe the motion of an atomic particle and is a function of both position and time.
4. ψ represents probability amplitude, $|\psi|^2$ represents probability density i.e., is probability per unit length in one dimension and probability per unit volume in three dimension.

2.4.3 Physical Significance

The wave function ψ has no physical significance by itself. The only quantity having a physical meaning is the square of its magnitude P called probability density. $P = |\psi|^2 = \psi\psi^*$ where ψ^* is the complex conjugate of ψ . The probability of finding a particle in a volume dx, dy, dz is $|\psi|^2 dx dy dz$. Further, since the particle (say electron or photon) is certainly to be found somewhere in space, the triple integral extending over all possible values of x, y, z .

$$\iiint |\psi|^2 dx dy dz = 1 \quad \dots (2.3)$$

A wave function ψ satisfying the above relation is called a normalized wave function.

2.5 PROBABILITY DENSITY AND NORMALIZATION OF WAVE FUNCTION

The probability of finding a particle in a given volume dV is given by $\psi\psi^* dV$. Using Eqn. (2.3) the total probability of finding a particle in the entire space is always unity. i.e., $\int |\psi|^2 dV = 1$, where the integration extends over all space. The above equation can be also written as $\int \psi\psi^* dV = 1$. Any wave function satisfying this equation is said to be **normalized to unity** or simply **normalized function**. Max Born in 1926 interpreted the wave function as a probability density and got Nobel Prize in 1954 for this discovery.

2.6 SETTING UP OF A ONE DIMENSIONAL, TIME INDEPENDENT, SCHRÖDINGER WAVE EQUATION

2.6.1 Schrödinger Wave Equation

In 1925, Erwin Schrödinger, an Austrian physicist used de-Broglie's ideas to set-up a rigorous mathematical theory to describe the dual (wave and particle) nature of matter. The essential feature of this theory is the incorporation of de-Broglie wavelength expression ($\lambda = h/mv$) in to the classical wave equation. Thus, he derived a wave equation for a single moving particle along one-dimension in the steady state (time - independent) as:

$$(d^2\psi/dx^2) + (8\pi^2m/h^2) (E - U)\psi = 0 \quad \dots (2.4)$$

2.6.2 Derivation

Let us assume that a particle of mass m is in motion along the x -direction. Let the wave function ψ of this wave is a function of the coordinates x and t . Analogous to classical wave, ψ is a function of $(x - vt)$. Since $v = \omega/k$, ψ may be written as a function of $(kx - \omega t)$.

$$\psi = f(kx - \omega t) \quad \dots (2.5)$$

Taking the help of Euler's identity, we can write Eqn. (2.5) in exponential form as follows:

$$\psi = A \exp(kx - \omega t) \quad \dots (2.6)$$

where A is a constant.

Differentiating Eqn. (2.6), twice with respect to t , we get

$$(d^2\psi/dt^2) = -\omega^2\psi \quad \dots (2.7)$$

The expression for a travelling wave along one direction can be written as

$$(d^2y/dx^2) = (1/v^2) (d^2y/dt^2) \quad \dots (2.8)$$

where y is the displacement and v is the velocity of the wave.

In the above travelling wave equation, by replacing y by ψ , we get

$$(d^2\psi/dx^2) = (1/v^2) (d^2\psi/dt^2) \quad \dots (2.9)$$

From Eqn (2.7) and Eqn. (2.9), we get

$$(d^2\psi/dx^2) = -(\omega^2/v^2)\psi \quad \dots (2.10)$$

But we know that $\omega = 2\pi f$ and $v = \lambda f$.

Hence,

$$(d^2\psi/dx^2) = -(4\pi^2/\lambda^2)\psi \quad \dots (2.11)$$

We also know that the Total energy of a particle = Kinetic energy + Potential energy.

or Kinetic energy = Total energy - Potential energy

$$p^2/2m = (E - U) \quad \dots (2.12)$$

[Since $K.E. = \frac{1}{2} mv^2 = m^2v^2/2m = p^2/2m$]

Using $\lambda = h/p$, we get $p = h/\lambda$. Then Eqn. (2.12) becomes

$$h^2/2m\lambda^2 = (E - U) \quad \dots (2.13)$$

or

$$1/\lambda^2 = (2m/h^2) (E - U) \quad \dots (2.14)$$

Using Eqn. (2.14) in Eqn. (2.11), we get,

$$(d^2\psi/dx^2) = -(8\pi^2m/h^2)(E - U)\psi$$

or

$$(d^2\psi/dx^2) + (8\pi^2m/h^2)(E - U)\psi = 0 \quad \dots (2.15)$$

This is a one-dimension time-independent Schrödinger's wave equation. For this discovery, Erwin Schrödinger, has been honoured by Nobel Prize in the year 1933.

2.6.3 Eigen Values and Eigen Function

While solving time-independent Schrödinger's wave equation, we get possible set of acceptable solutions only for certain specified values of energy. These discrete values of energy $E_1, E_2, E_3, \dots, E_n$ are called **Eigen values** or **allowed values** of the energy of the particle. The solutions $\psi_1, \psi_2, \psi_3, \dots, \psi_n$ corresponding to the **Eigen values** E_n are called the **Eigen functions**. The quantization of energy thus appears as a natural element of the wave equation.

2.7 APPLICATION OF SCHRÖDINGER WAVE EQUATION

2.7.1 The Particle in a Box of Infinite Depth

Consider a particle moving inside a box of infinite depth with finite width along the x -direction. The particle is bouncing back and forth between the walls of the box. The box is supposed to have walls of infinite height at $x = 0$ and $x = L$ as shown in the Fig. 2.2. The particle has a mass m and its position x at any instant of time is given by $0 < x < L$.

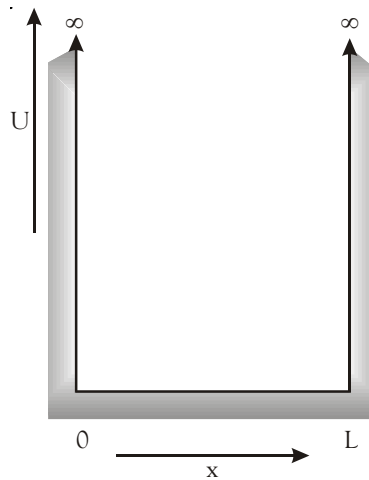


Figure 2.2 Particle in a box of infinite potential depth

The potential energy U of the particle is infinite on both sides of the box and is assumed to be zero within the box between $x = 0$ and $x = L$. In terms of boundary conditions imposed by the problem, the potential function is $U = 0$ for $0 < x < L$; $U = \infty$ for $x \leq 0$ and $U = \infty$ for $x \geq L$.

The particle can not exist outside the box and so its wave function $\psi = 0$ for $x \leq 0$ and for $x \geq L$. Our objective is to find the value of ψ within the box.

Within the box, the Schrodinger's equation for the wave function becomes

$$(d^2\psi/dx^2) + (8\pi^2m/h^2)(E)\psi = 0 \quad \dots (2.16)$$

Substituting $(8\pi^2m/h^2)(E) = k^2$ we can write Eqn. (2.16) as

$$(d^2\psi/dx^2) + k^2\psi = 0 \quad \dots (2.17)$$

The general solution of this equation is of the form

$$\psi = A \sin kx + B \cos kx \quad \dots (2.18)$$

The boundary conditions can be used to evaluate the constants A and B in Eqn (2.18).

$$\psi = 0 \text{ at } x = 0 \text{ and hence } B = 0$$

$$\psi = 0 \text{ at } x = L \text{ and hence } 0 = A \sin kL$$

Since $A \neq 0$, $kL = n\pi$ where n is an integer or $k = n\pi/L$.

Thus,

$$\psi_n(x) = A \sin (n\pi x/L) \quad \dots (2.19)$$

The energy of the particle = $E_n = k^2 h^2 / 8\pi^2 m = (h^2 n^2 \pi^2) / (L^2 8\pi^2 m)$

$$\therefore E_n = (n^2 h^2) / (8mL^2) \quad \dots (2.20)$$

2.7.2 Energy Eigen Values and Functions of a Particle in a Potential Box of Infinite Depth

In Eqns. (2.19) and (2.20), for each value of n , there is a Energy level E_n and corresponding wave function ψ_n . Each value of E_n is called an **Eigen value** and the corresponding wave function ψ_n is called **Eigen function**. Thus inside the box, the particle can only have the discrete energy values (quantization of energy) as shown in Fig. 2.3.

(i) Eigen Values of a particle :

Using Eqn. (2.20), the allowed energy states are given by :

First energy level $E_1 = (h^2)/(8mL^2)$

Second energy level $E_2 = (4h^2)/(8mL^2)$ or $E_2 = (h^2)/(2mL^2)$

Third energy level $E_3 = (9h^2)/(8mL^2)$ and so on.

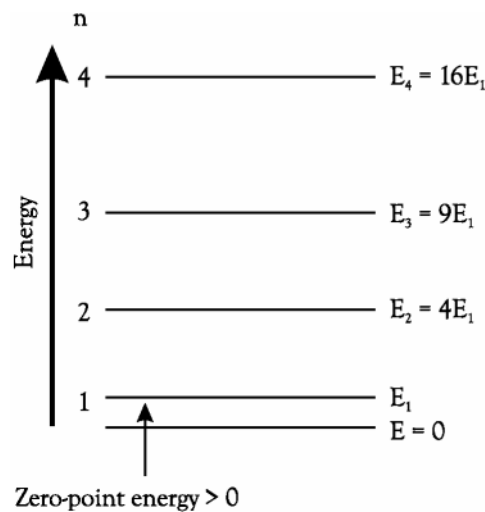


Figure 2.3 Energy eigen values of a particle in a one dimensional box of infinite height

It can be noted that the particle cannot have zero energy. The lowest energy allowed for the particle is $E_1 = (h^2)/(8mL^2)$. A particle can not possess energy less than this in one dimensional potential well. The minimum possible energy for a particle in a box is E_1 and is called **zero-point energy**.

The zero-point energy is a consequence of **Uncertainty** principle. In case if the energy of the particle is zero, its momentum in the box would be zero, and as per uncertainty principle, the wavelength of the particle will become infinite. In such case, the particle cannot be confined within the well. This leads to the argument that the particle should have some minimum energy (zero-point energy).

(ii) **Eigen Functions of a Particle**

Since the particle is somewhere inside the box, the normalized wave function becomes :

$$1 = \int_{-\infty}^{\infty} |\Psi_n(x)|^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx$$

The integral is evaluated with the help of the trigonometric identity $2\sin^2\theta = 1 - \cos 2\theta$

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{1}{2} \int_0^L [1 - \cos(2n\pi x/L)] dx$$

Only the first term contributes to the integral, because the cosine integrates to $\sin(2n\pi x/L)$, which vanishes at the limits 0 and L. Thus, normalization requires $1 = A^2 L/2$

or
$$A = \sqrt{\frac{2}{L}}$$

\therefore The normalized wave function of the particle $\Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$... (2.21)

The normalized wave functions Ψ_1 , Ψ_2 , and Ψ_3 are plotted in Fig. 2.4.

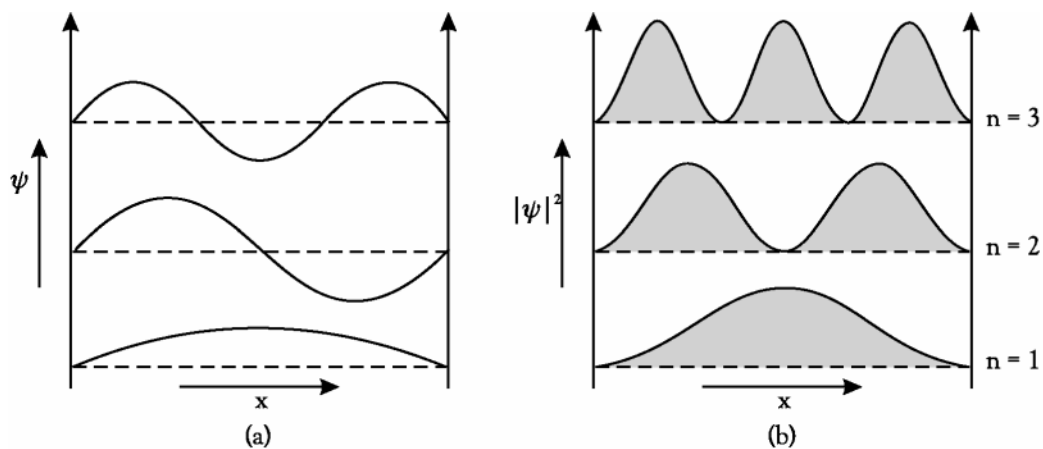


Figure 2.4 The first three allowed stationary states for a particle confined to a one dimensional box. (a) The wave functions for $n = 1, 2,$ and 3 (b) The probability distributions for $n = 1, 2,$ and 3

2.7.3 Energy Eigen Values for a Free Particle

A particle is said to be free when it is moving in space without any external force and when its potential energy is constant everywhere ($U = \text{constant}$). Consider a particle moving along positive x-axis in one dimensional space. As the particle is freely moving in space without any external force, the potential energy of the particle is constant. For convenience, we consider the constant potential to be zero. Then the time-independent Schrodinger wave equation for free particle can be written as

$$(d^2\psi/dx^2) + (8\pi^2m/h^2)(E)\psi = 0 \quad \dots (2.22)$$

Since the particle is moving freely with zero potential energy, its total energy will be kinetic energy and is given by

$$E = p_x^2/2m \quad \dots (2.23)$$

where p_x is the momentum of the particle along the x-direction.

Eqn. (2.22) can be re-written as

$$(d^2\psi/dx^2) + k^2\psi = 0 \quad \dots (2.24)$$

where $(8\pi^2mE/h^2) = k^2 \dots (2.25)$

(a) Wave function :

The general solution of the Eqn (2.24) is of the form

$$\psi_n(x) = Ae^{ikx} + Be^{-ikx} \quad \dots (2.26)$$

where A and B are constants and $\psi_n(x)$ is called wave function.

(b) Energy :

Using Eqn. (2.25), the energy of the particle is given by

$$E = (k^2 h^2) / 8\pi^2 m \quad \dots (2.27)$$

From the above Eqn. (2.27), it is clear that the particle is permitted to have any value of energy and is not **quantized**. This means the freely moving particle possesses a continuous energy spectrum.

SOLVED PROBLEMS

Uncertainty Principle

1. Electrons moving with a velocity of $3.32 \times 10^5 \text{ m/s}$ if this velocity is measured with an inaccuracy of 0.53% then estimate the uncertainty in the position of an electron.

Given that:

$$\text{Velocity of the electron is } v = 3.32 \times 10^5 \text{ m/s}$$

$$\text{Inaccuracy in the measurement of velocity} = 0.53 \%$$

To find,

$$\Delta x = ?$$

Uncertainty in the velocity is $\Delta v = \frac{3.32 \times 10^5 \times 0.53}{100} = 1.76 \times 10^3 \text{ m/s}$

Therefore, the uncertainty in the electron momentum

$$\Delta p = m\Delta v$$

$$\Delta p = m\Delta v = 9.11 \times 10^{-31} \times 1.76 \times 10^3 = 16.03 \times 10^{-28} \text{ kg.m/s}$$

From the Heisenberg Uncertainty principle we have,

$$\Delta x \Delta p_x \geq \frac{h}{4\pi}$$

or
$$\Delta x \geq \frac{h}{4\pi\Delta p_x} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 16.03 \times 10^{-28}} = 32.8 \times 10^{-9} \text{ m}$$

Therefore, the uncertainty in position is greater than or equal to $32.8 \times 10^{-9} \text{ m}$

2. In an experimental determination of displacement of an electron in 10^{-6} second is 3.6m. Calculate the uncertainty involved in the determination of position if the inherent error involved in the measurement of displacement of the electron in given time is 0.23%.

Given that:

The displacement of an electron in 10^{-6} second = 3.6 m

The error in the displacement measurement = 0.23%

Therefore, uncertainty in the displacement Δd is

$$\Delta d = \frac{3.6 \times 0.23}{100} = 8.28 \times 10^{-3} \text{ m}$$

The uncertainty in the velocity of the electron Δv is

$$\Delta v = \frac{\Delta d}{t} = \frac{8.28 \times 10^{-3}}{10^{-6}} = 8.28 \times 10^3 \text{ m/s}$$

Therefore, the uncertainty in the momentum Δp is

$$\Delta p = m\Delta v = 9.11 \times 10^{-31} \times 8.28 \times 10^3 = 75.43 \times 10^{-28} \text{ kg.m/s}$$

The uncertainty in the electron position Δx is

$$\Delta x \geq \frac{h}{4\pi\Delta p_x} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 75.43 \times 10^{-28}} = 6.97 \times 10^{-9} \text{ m}$$

The minimum uncertainty in the position of electron is $6.97 \times 10^{-9} \text{ m}$

Particle in a Box

3. The velocity of an electron confined in an infinite potential well is found to be $3 \times 10^4 \text{ m/s}$ for the ground state. Calculate the velocity of the electron in first and second excited state.

Given that:

$$\text{Velocity of the electron in ground state } v_g = 3 \times 10^4 \text{ m/s}$$

To calculate:

$$\text{Velocity of the electron in first excited state } v_f = ?$$

$$\text{Velocity of the electron in the second excited state } v_s = ?$$

The energy of an electron confined to one dimensional infinite potential well of finite width for an n^{th} state is given by

$$E_{n-1} = \frac{n^2 h^2}{8ma^2}$$

Where $a = L$ in Eqn (2.20). For ground state $n = 1$

$$E_o = \frac{h^2}{8ma^2} \quad \dots(1)$$

For first and second excited state $n = 2$ and $n = 3$ respectively

Therefore energy of an electron in the respective energy state is given by

$$E_1 = \frac{4h^2}{8ma^2} \quad \text{and} \quad E_2 = \frac{9h^2}{8ma^2} \quad \dots(2)$$

Form equation (1) and (2)

$$E_1 = \frac{4h^2}{8ma^2} = 4E_o \quad \text{and} \quad E_2 = \frac{9h^2}{8ma^2} = 9E_o$$

Therefore the velocity of the electron in the first excited state can be calculated as follows

$$E_1 = 4E_o$$

$$\frac{1}{2} m v_f^2 = 4 \times \frac{1}{2} m v_g^2$$

$$v_f^2 = 4 v_g^2$$

i.e. $v_f = 2v_g = 2 \times 3 \times 10^4 = 6 \times 10^4 \text{ m/s}$

Similarly,

$$v_s^2 = 9 v_g^2$$

i.e. $v_s = 3v_g = 3 \times 3 \times 10^4 = 9 \times 10^4 \text{ m/s}$

Therefore, the velocity of the electron confined in a one dimensional potential well of infinite height for the first and second excited state is 6×10^4 m/s and 9×10^4 m/s, respectively.

4. An electron is bound in one dimensional potential well of width 0.18nm. Find the energy value in eV of the second excited state. (VTU may/June 2010)

Given that:

$$\text{Width of the potential well } a = 0.18 \text{ nm} = 0.18 \times 10^{-9} \text{ m}$$

To calculate:

$$\text{Second excited state energy} = ? \text{ eV}$$

For second excited state $n = 3$

Energy of an electron in an n^{th} state is given by

$$E_{n-1} = \frac{n^2 h^2}{8ma^2}$$

Therefore, the energy of the electron in second excited state is

$$E_2 = \frac{9h^2}{8ma^2}$$

$$E_2 = \frac{9h^2}{8ma^2} = \frac{9 \times (6.625 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (0.18 \times 10^{-9})^2} \text{ J}$$

$$E_2 = 1.67 \times 10^{-17} \text{ J}$$

$$E_2 = \frac{1.67 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV} = 104.5 \text{ eV}$$

The energy, in eV, of an electron in second excited state confined to potential well of 0.18 nm width is 104.5 eV

5. Compute the first three permitted energy values for an electron in a box of width 4\AA . (Model Q.P)

Given that:

$$\text{The width of the Box, } a = 4 \text{\AA} = 4 \times 10^{-10} \text{ m.}$$

To calculate

$$\text{Ground state energy } E_0 = ?,$$

$$\text{First excited state energy } E_1 = ?$$

$$\text{and second excited state energy } E_2 = ?$$

We have,

$$E_{n-1} = \frac{n^2 h^2}{8ma^2}$$

For ground state $n = 1$

$$E_0 = \frac{h^2}{8ma^2} = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (4 \times 10^{-10})^2} J$$

$$E_0 = 3.76 \times 10^{-19} J$$

$$E_0 = \frac{3.76 \times 10^{-19}}{1.6 \times 10^{-19}} eV = 2.35 eV$$

For first excited state $n = 2$

We have,

$$E_{n-1} = n^2 E_0$$

$$E_1 = 2^2 E_0 = 4 \times 2.35 eV = 9.41 eV$$

For second excited state $n = 3$

$$E_2 = 3^2 E_0 = 9 \times 2.35 eV = 21.17 eV$$

The energies of the electron in first three allowed states are 2.35 eV, 9.41 eV and 21.17 eV, respectively.

6. A particle limited to the x -axis has the wave function $\Psi = ax$ between $x = 0$ and $x = 1$; $\Psi = 0$ elsewhere. Find the probability that the particle can be found between $x = 0.25$ and $x = 0.50$.

Given that:

Wave function of the particle defined in the region $x = 0$ and $x = 1$ is

$$\Psi = ax$$

To find:

The probability of finding the particle in the region $x = 0.2$ to $x = 0.7$, $P = ?$

Probability

$$P = \int_{x=0.2}^{x=0.7} \Psi \Psi^* dx = \int_{x=0.2}^{x=0.7} a^2 x^2 dx = a^2 \int_{x=0.2}^{x=0.7} x^2 dx = \frac{1}{3} a^2 [x^3]_{x=0.2}^{x=0.7}$$

$$P = \frac{1}{3} a^2 [0.7^3 - 0.2^3]$$

$$P = 0.1116a^2$$

EXERCISES**I. Descriptive Type Questions**

1. Write a note on Heisenberg uncertainty principle and its significance.
2. Write a note on probability density and normalization of wave function.
3. Prove that a free electron cannot exist inside a nucleus using the Heisenberg uncertainty principle.
4. Derive Schrödinger wave equation.
5. What is Eigen value and Eigen function? Derive the expression for Eigen function and Eigen energy values for a particle in a infinite potential well of finite width.
6. Derive an expression for the energy Eigen values of a free particle.
7. Discuss the wave functions and probability density for particle in an infinite potential well for first three allowed states.
8. State Heisenberg's uncertainty principle and discuss its physical significance. (VTU Jan 2010)
9. Solve the Schrödinger's wave equation for allowed energy values in case of a particle in a potential box. (VTU Jan 2010)
10. Set up time independent wave equation.
11. What are eigen values ?
12. Show that electrons cannot exist in the nucleus of an atom. (VTU Jan 2007)
13. Discuss the wave functions, probability densities and energy levels for a particle in a box. (VTU Jan 2007)
14. State and explain Heisenberg's uncertainty principle and prove that nuclei do not contain electron. (VTU June 2010)
15. Discuss the wave functions and probability density for particle in an infinite potential well, for first two states. (VTU June 2010)
16. What are the properties of Wave functions? (VTU June 2007)
17. Find the eigen functions and eigen values for a particle in one dimensional potential well of infinite height discuss the solutions. (VTU June 2007)
18. Show that electrons cannot exist in the nucleus of an atom. (VTU June 2008)
19. Discuss the Eigen function, Eigen values and probability density for a particle in a potential well of infinite depth. (VTU June 2008)
20. Assuming the time independent Schrödinger wave equation, discuss the solution for a particle in one dimensional potential well of infinite height. Hence obtain the normalized wave function. (VTU Jan 2008)

21. Explain Heisenberg's uncertainty principle. Based on this, show the non-existence of electrons inside the nucleus. (VTU Jan 2008)
22. Set-up time independent Schrodinger wave equation. (VTU Jan 2009)
23. Write the physical significance of wave function. (VTU Jan 2009)
24. Explain Heisenberg's uncertainty principle. Give its physical significance. (VTU June 2009)
25. Set up Time-independent one-dimensional Schrodinger's wave equation. (VTU June 2009)

II. Multiple Choice Questions

1. The normalization of wave function is always possible, if
 - (a) $\int_{-\infty}^{\infty} \Psi \Psi^* dx = \text{infinite}$
 - (b) $\int_{-\infty}^{\infty} \Psi \Psi^* dx = \text{finite}$
 - (c) $\int_{-\infty}^{\infty} \Psi \Psi^* dx = 0$
 - (d) All of these
2. Schrödinger's time independent equation is applicable for the particles with
 - (a) Constant energy
 - (b) Variable energy
 - (c) Only constant potential energy
 - (d) All of these
3. The ground state energy of an electron in an infinite well is 5.6 meV. If the width of the well is doubled, the ground state energy is
 - (a) $9.92 \times 10^{-23} \text{J}$
 - (b) $4.48 \times 10^{-22} \text{J}$
 - (c) $2.24 \times 10^{-22} \text{J}$
 - (d) None of these
4. The wave function is acceptable wave function if it is
 - (a) Finite everywhere
 - (b) Continuous everywhere
 - (c) Single valued everywhere
 - (d) All of these.
5. The product of uncertainty between energy and time
 - (a) $\geq h/2\pi$
 - (b) $\geq h/4\pi$
 - (c) $= h/2\pi$
 - (d) None of these
6. According to Max Born Approximation wave function is interpreted as _____
 - (a) Energy density
 - (b) Particle density
 - (c) Probability density
 - (d) Charge density
7. The first permitted energy level is also referred as
 - (a) Excited energy
 - (b) Zero point energy
 - (c) Potential energy
 - (d) None of these

8. The energy associated with a particle in infinite well of finite width is
 (a) Finite (b) Continuous
 (c) Discrete (d) all the above
9. If free electron exists in a nucleus, its energy value must have a minimum energy of about
 (a) 4 MeV (b) 20 MeV
 (c) 20 KeV (d) 10 KeV
10. According to Max Born approximation $\psi\psi^*$ represents
 (a) Charge Density (b) Particle Density
 (c) Energy Density (d) Probability density
11. If E_1 is the energy of the lowest state of a one dimensional potential box of length 'a' and E_2 is the energy of the lowest state when the length of the box is halved, then
 (a) $E_2 = E_1$ (b) $E_2 = 2E_1$
 (c) $E_2 = E_1/2$ (d) $E_2 = 4E_1$
12. The wave function for the motion of the particle in a one dimensional potential box of length 'a' is given by ' $\Psi_n = A \cdot \sin\left(\frac{n\pi x}{a}\right)$ ' where A is normalization constant. The value of A is
 (a) $\frac{1}{\sqrt{a}}$ (b) $\frac{2}{\sqrt{a}}$
 (c) $\sqrt{\frac{2}{a}}$ (d) $\sqrt{\frac{a}{2}}$
13. The product of uncertainty between angular momentum and angular displacement is
 (a) $\geq \frac{h}{2\pi}$ (b) $\geq \frac{h}{4\pi}$
 (c) $= \frac{h}{2\pi}$ (d) $\leq \frac{h}{4\pi}$
14. Kinetic energy of electron accelerated by a voltage 50 Volts.
 (a) 50 eV (b) 10 eV
 (c) 5e V (d) 15 eV
15. The energy of the lowest state in one dimensional potential box of length is
 (a) Zero (b) $\frac{2h^2}{8ma^2}$
 (c) $\frac{h^2}{8ma^2}$ (d) $\frac{h}{8ma^2}$

16. The velocity of the electron in ground and first excited state, confined one dimensional potential well is given by
- (a) $v_f = 4v_g$ (b) $v_f = v_g$
 (c) $v_f = 2v_g$ (d) None of these
17. According to Max Born approximation $|\psi|^2$ represents
- (a) Energy density (b) Particle density
 (c) Probability density (d) Charge density
18. An electron has a speed of 100 m/s, accurate to 0.005%. The uncertainty in its position is
- (a) 0.01m (b) 0.0115m
 (c) 0.024m (d) 0.04m
19. An electron moving in a box of length 'a'. If ψ_1 is the wave function at $x = \frac{a}{4}$ with $n=1$ and ψ_2 at $x = a$ for $n=2$, then $\frac{\psi_2}{\psi_1}$ is
- (a) $\frac{\sqrt{2}}{a}$ (b) $\sqrt{\frac{a}{2}}$
 (c) 0 (d) ∞
20. The first excited state energy of a particle of mass m in a box of length L is given by
- (a) zero (b) $h^2/8mL^2$
 (c) $\frac{2h^2}{8mL^2}$ (d) $\frac{h^2}{2mL^2}$
21. Uncertainty principle is developed by _____
- (a) Max Born (b) Max Plank
 (c) de-Broglie (d) Heisenberg
22. Which of the following is not a pair of canonically conjugate variables?
- (a) Position and Momentum (b) Position and energy
 (c) Energy and Time (d) All of these
23. Uncertainty principle has no practical importance for
- (a) Macro particles (b) Atomic particles
 (c) Both of them (d) None of them

24. Wave function is a _____
- (a) Linear function (b) Exponential function
(c) Quadratic function (d) Complex function
25. Zero point energy is _____
- (a) Minimum possible energy of a particle in side a box
(b) First eigen energy
(c) Consequence of Uncertainty Principle
(d) All of these

III. Numerical Problems

- The distance of separation between two rigid walls of infinite height is 3.15\AA . Calculate the energies of the electron in second, third and fourth excited state.
- The de-Broglie wavelength associated with the electron moving back and forth in the infinite potential well in the first excited state is 3×10^{-8} m. Calculate the de-Broglie wavelength associated with the electron in ground, second, and third excited state.
- Calculate the first four permitted energy values of an electron in an infinite potential well with width 2.75\AA .
- Calculate the first four permitted energy values of an electron in an infinite potential well of finite width. Given that the velocity of the electron in the first excited state is 4.35×10^6 m/s.
- Calculate the first five permitted energy values of an electron in an infinite potential well of finite width. Given that the de-Broglie wavelength associated with an electron in the second excited state is 7.45×10^{-9} m.
- Compute the first 4 permitted energy levels of an electron in a box of width 4\AA
- An electron has a speed of 6×10^5 m/s with an inaccuracy of 0.01%. With what fundamental accuracy can we locate the position of the electron? (VTU Jan 2007)
- An electron is bound in one dimensional potential well of width 0.18 nm. Find the energy value in eV of the second excited state. (VTU June 2010)
- A spectral line of-wavelength 4000\AA , has a Width $8 \times 10^{-5} \text{\AA}$. Evaluate the minimum time spent by the electrons in the upper energy state between the excitation and de-excitation processes. (VTU June 2007)
- An electron is bound in one dimensional infinite well of width 0.12 nm. Find the energy values, and de Broglie wavelength in the ground state and first excited state. (VTU June 2008)
- An electron is bond in one dimensional potential well of width 0.12 nm. Find the energy values in the ground state and also the first two excited states in eV. (VTU Jan 2008)

12. A quantum particle confined to one dimensional box of width 'a' is in its first excited state. What is the probability of finding the particle over an interval of $(a/2)$ marked symmetrically at the centre of the box? (VTU Jan 2009)
13. A particle confined to one dimensional box of width in its first excited state. What is the probability of finding particle at interval of $\frac{a}{2}$ marked symmetrically at the centre of the box? (VTU June 2009)
14. An electron has a speed of 600 m/s with an accuracy of 0.005 %. Calculate the certainty with which we can locate the position of the electron. Given : $h = 6.6 \times 10^{-34}$ J.s., and $m = 9.1 \times 10^{-31}$ Kg. (Ans : $\Delta x \approx 0.003846$ m)
15. A particle is moving in one dimensional potential box of infinite height. What is the probability of finding the particle in a small interval Δx at the centre of the box when it is in the energy state, next to the least energy state ? (Hint : (i) $\Psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$; At the centre of the box, $x = \frac{L}{2}$ and $\Psi_2 = 0$. (ii) Probability of finding the particle in an interval at the centre of the box = $(\Psi_2^2 \cdot \Delta x = 0)$.
16. A particle is moving in one dimensional potential box of infinite height and width 10 \AA .. Calculate the probability of finding the particle within an interval of 1 \AA at the centre of the box, when it is in the state of least energy ? [Hint : (i) $\Psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$; (ii) $P = \Psi_1^2 = \frac{2}{L}$; (iii) $W = \Psi_1^2 \cdot \Delta x = 0.2$. = 0.2. Since $L = 10 \times 10^{-10}$, $\Delta x = 1 \times 10^{-10}$]

Answers to Multiple Choice Questions

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

ELECTRICAL CONDUCTIVITY IN METALS

OBJECTIVES

This section is dedicated to discuss the fundamental aspects of solid state physics (or condensed matter physics) and the discussion is confined to electrical conductivity in metals. The theories put forward by various scientists to explain the phenomenon observed in metals are described. This chapter is mainly allocated to study

- Fundamental properties of metals
- Assumption of classical theory, merits and demerits of classical free electron theory
- Electrical conductivity, effect of impurities and temperature on the electrical resistivity
- Basic assumption of Quantum free electron theory, merits of this theory over classical free electron theory
- Fermi-Dirac statistics, Fermi energy, Fermi factor and Temperature dependence of resistivity

3.1 INTRODUCTION

The matter generally exist in four states namely solid, liquid, gas and plasma state. The branch of physics which deals the phenomenon related to solids is classified as solid state physics. Learning solid state physics requires a certain degree of knowledge regarding diverse concepts from many areas of physics. The objective is to understand, in a most fundamental way, how solid materials behave. The solid state physics (also referred as condensed matter physics) is defined as the study of the physical (e.g. the electrical, dielectric, magnetic, elastic, thermal etc.) properties of solids in terms of basic physical laws. The emphasis of the solid state physics is to give better correlation between the physical properties that are linked to the electronic structure of the materials. The development of solid state physics impacted tremendously on the technology. It is very difficult to imagine the world without solid state devices. From the past several decades the solid state physics witnessed a tremendous growth leading to the improved devices and their performance. As the time goes, the devices becoming smaller and smaller due to the success and deeper understanding and application of solid state physics. It is very difficult to accommodate the development, all the phenomenon and related theory that noticed in the solid state physics. This section gives consolidated information regarding few topics related to solids which are relevant for under graduate students.

3.2 PROPERTIES OF METALS

Metals show following outstanding physical properties:

1. High electrical and thermal conductivity.
2. Obey Ohm's law. i.e., steady state current (I) is proportional to applied voltage E . ($I \propto E$).
3. At low temperature, resistivity is proportional to fifth power of absolute temperature. ($\rho \propto T^5$).
4. At high temperature, above room temperature, the resistivity is linearly proportional to absolute temperature. ($\rho \propto T$).
5. In many metals, resistivity is inversely proportional to the pressure. ($\rho \propto 1/P$).
6. Near absolute zero temperature, resistivity of metals tends towards zero leads to superconductivity.
7. Wiedemann-Franz law : For most of the metals, the ratio of thermal conductivity to electrical conductivity is proportional to absolute temperature.
8. The specific heat capacity of metals increases with the increase in temperature.
9. The paramagnetism of metals is nearly independent of temperature.

3.3 CLASSICAL FREE ELECTRON THEORY

3.3.1 Free Electron Concept

After the discovery of electron in 1897 by J. J. Thomson, many theories were proposed to explain the properties of electrons. Out of them, Drude-Lorentz free electrons theory was widely accepted and could able to explain many observed behaviors of the electrons in metals.

According to Drude-Lorentz free electrons theory, all metal atoms are consists of valence electrons which are outermost orbit electrons which can become free during the formation of metal and can move freely throughout the metal. Such electrons are called free electrons. Due to the loss of free electrons from the valence orbit the atoms of the metals become positive ions. Such immovable metal ions form the metal structure and is called lattice. Thus, a metal piece contains immobile **lattice ions** and randomly moving electrons called **free electrons**.

When we apply external electric field to the metal piece, the randomly moving electrons displaces in a direction opposite to the direction of the applied electric field. This displacement/unit time is called **drift velocity**. As a result, electrons are tend to accelerate in the direction opposite to applied electric field and constitute **electric current**. At room temperatures due to thermal agitation the lattice points vibrate about their mean position in the metal and tend to scatter the electrons accelerated by the applied electric field. Finally a balance occurs between accelerated electrons and scattering leads to electrical current. This scattering due to lattice ions vibration leads to resistance of the metal.

3.3.2 Assumptions of Classical Free Electron Theory

1. In a metal, there are freely moving valence electrons called free electrons. When we apply an external electric field, electric current flows due to drift velocity of electrons.

2. In absence of external electric field, free electrons moves **randomly** with a kinetic energy ($\frac{1}{2}mv_{th}^2$) equal to $(3/2)k_B T$, and collide with stationary lattice ions and lose most of their kinetic energy in each collision, where T is absolute temperature, m is mass of electrons, k_B is Boltzmann constant and v_{th} is thermal velocity of electrons. Thus there is no net movement of valence electrons in absence of an applied electric field.
3. The electric potential due to lattice ions is taken to be constant throughout the metal.
4. The repulsion between free electrons and the attraction between free electrons and lattice ions are considered insignificant.
5. The average distance travelled by the free electrons between successive collisions with the lattice ions is called **mean free path** (λ) and the average time elapsed between two consecutive collisions of an electron with the lattice points is called **mean collision time** (τ). Here, $\tau = \lambda/v_{th}$, where v_{th} is thermal velocity of electrons.
6. When electric field is applied across the metal, the electrons are accelerated/drifted in the direction opposite to the applied field, gains **mobility** (μ) and the velocity acquired by these electrons is called **drift velocity** (v_d). This accounts for a current in the direction of applied field.
7. When the external applied electric field is switched off, the drift velocity of the electrons decreases to thermal velocity (v_{th}). The time required to decay the velocity of electrons ($1/e$) times the initial constant drift velocity before switching off the field is called **relaxation time** (τ_r).

3.3.3 Expression for Drift Velocity

When the electric field E is applied across the metal, the free electron acquires a constant velocity in steady state is called drift velocity. If m is the mass, v_d is drift velocity and τ is the mean collision time of electron, then the resistance force F_r offered to its motion can be written as:

$$F_r = mv_d/\tau \quad \dots (3.1)$$

The driving force acting on the electron due to applied electric field is

$$F = eE \quad \dots (3.2)$$

In the steady state,

$$F_r = F \Rightarrow mv_d/\tau = eE$$

or

$$v_d = eE\tau/m \quad \dots (3.3)$$

Eqn. (3.3) gives an expression for drift velocity.

The mobility of electrons under applied electric field is given by

$$\mu = v_d/E = e\tau/m \quad \dots (3.4)$$

Therefore the mobility is defined as the magnitude of the drift velocity gained by the free electrons in an applied unit electric field.

3.3.4 Expression for Electrical Conductivity in Metals

Consider the motion of free electrons in a conductor due to applied electric field E . Then the force F on the electrons is given by

$$F = eE \quad \dots (3.5)$$

Using Newton's second law of motion, the force on the electron of mass m is given by

$$F = m(dv/dt) \quad \dots (3.6)$$

From Eqn. (3.5) and (3.6), we write

$$eE = m(dv/dt) \quad \dots (3.7)$$

or

$$dv = (eE/m)dt \quad \dots (3.8)$$

Integrating both sides we get,

$$\int dv = \int (eE/m)dt \quad \dots (3.9)$$

or

$$v = eEt/m \quad \dots (3.10)$$

where t is time of traverse.

When the traverse time t is equal to the collision time τ , the velocity of electron becomes the average velocity \bar{v} . Hence Eqn. (3.10) can be re-written as

$$\bar{v} = eE\tau/m \quad \dots (3.11)$$

Let the area of cross-section of the conductor is A and the current flowing is I due to applied electric field E . Then the current density is given by $J = I/A$ and the expression for electrical conductivity is given by

$$\sigma = J/E \quad \dots (3.12)$$

or

$$\sigma = I/AE \quad \dots (3.13)$$

Now, the distance travelled by electrons in a unit time is numerically equal to average velocity \bar{v} . These electrons sweep a volume equal to $\bar{v}A$ in a unit time. If e is the charge of the electron, n is the number of electrons/unit volume, then the current flowing through the conductor is given by $I = (ne\bar{v}A)$. Substituting the value of current in Eqn. (3.13), we get,

$$\sigma = ne\bar{v}/E \quad \dots (3.14)$$

Substituting \bar{v} from Eqn (3.11) we get $\sigma = \frac{ne}{E} \left(\frac{eE\tau}{m} \right)$

or

$$\sigma = \frac{ne^2\tau}{m} \quad \dots (3.15)$$

Eqn. (3.15) is the expression for electrical conductivity in metals.

3.3.5 Effect of Impurity and Temperature on Electrical Resistivity of Metals

As per classical theory, the resistivity of metals is attributed to the scattering of conduction electrons which takes place under two mechanisms gives rise to two components of resistivity. They are residual resistivity (ρ_i) and ideal resistivity (ρ_{ph}). These two scattering mechanisms are acting independently and the total resistivity is the sum of individual resistivity.

i.e.,
$$\rho = \rho_{ph} + \rho_i \quad \dots (3.16)$$

(i) **Effect of Impurity on Electrical resistivity :**

The residual resistivity ρ_i is due to scattering of conduction electrons by the presence of impurities, and imperfections such as point defects, dislocation vacancies and grain boundaries. Residual resistivity is independent of temperature and present in the metal even at 0°K.

(ii) **Effect of Temperature on electrical resistivity :**

The ideal resistivity ρ_{ph} is due to scattering of conduction electrons by vibrating lattice ions called phonons which increases with increase in temperature. This resistivity is not affected by the presence of impurity in the metal.

The total resistivity of the metal given in Eqn. (3.16) is called **Matthiessen's Rule**. It states that the total resistivity of a metal is the sum of the resistivity due to scattering by impurities (residual resistivity) which is temperature independent and the resistivity due to phonon scattering (ideal resistivity) which is temperature dependent.

Since the resistivity $\rho = 1/\sigma$ and $\sigma = ne^2\tau/m$, we can write

$$\rho = m/ne^2\tau \quad \dots (3.17)$$

If τ_{ph} is the mean collision time of each electron in the metal assuming no scattering by impurities, then ideal resistivity is given by $\rho_{ph} = m/ne^2\tau_{ph} \quad \dots (a)$

Similarly, if τ_i is the mean collision time of each electron assuming no scattering by lattice, then residual resistivity is given by $\rho_i = m/ne^2\tau_i \quad \dots (b)$

Using Eqn. (3.16), the total resistivity of the metals is given by

$$\rho = \rho_{ph} + \rho_i = m/ne^2\tau_{ph} + m/ne^2\tau_i \quad \dots (3.18)$$

Fig. 3.1 shows the variation of resistivity of copper with temperature.

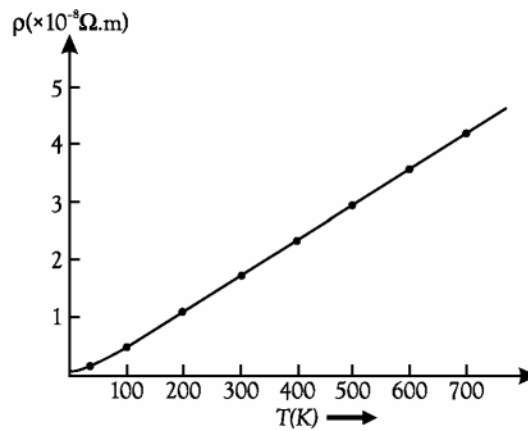


Figure 3.1 Variation of resistivity of copper with temperature

3.3.6 Failure of Classical Free Electron Theory

Even though the classical free electron theory satisfactorily explains Ohms law, Wiedemann-Franz law, variation of resistivity with temperature, and inverse relationship of resistivity with pressure, it fails to explain the following properties of the metals:

1. **Specific heat capacity:** As per classical theory, the specific heat is independent on temperature, but actually it increases with the increase in temperature.
2. **Paramagnetic susceptibility:** As per classical theory, the paramagnetic susceptibility is inversely proportional to temperature. But experiments show that it is nearly independent of temperature.
3. **Mean free path:** Classical free electron theory is failed to explain the occurrence of long electronic mean free paths of the order of 10^{-8} m in inter-atomic spacing.
4. **Classification of solids:** Classical theory failed to explain the distinction between conductors, semiconductors and insulators.
5. **Value of Hall coefficient:** Classical theory failed to explain the occurrence of positive value of Hall coefficient of metals.
6. **Ferromagnetism:** Classical theory failed to explain the ferromagnetism in iron, cobalt etc.
7. **Photoelectric & Compton effect:** Classical theory failed to explain the observed Photoelectric effect & Compton effect.
8. **Value of electrical conductivity:** According to classical theory, monovalent metals like Cu, Ag should have less electrical conductivity compared to divalent (Cd, Zn) and trivalent (Al, In) metals which is against the observation.

3.4 QUANTUM FREE ELECTRON THEORY

In 1928, Arnold Sommerfield modified classical free electron theory using Planks Quantum mechanical principles and Pauli Exclusion Principle. This theory could able to explain many drawbacks of classical free electron theory and known as **Quantum Free Electron Theory**.

3.4.1 Assumptions

1. The energy values of conduction electrons are quantized as various allowed energy levels.
2. The distribution of electrons in these allowed energy levels takes place as per Pauli exclusion principle.
3. The free electrons travel in a constant potential inside the metal but confined their stay within the metal.
4. The attractive force between free electrons and lattice ions and repulsive force between free electrons themselves are ignored.

In above assumptions, last two assumptions are borrowed from classical free electron theory and hence quantum free electron theory is an extension of classical free electron theory.

3.4.2 Fermi-Dirac Statistics

Based on the first assumption of quantum free electron theory, to answer a question—what are the possible energy levels and states available to the free electrons?, Fermi-Dirac Statistics is used to explain the behavior of particles called **fermions**, which are identical, indistinguishable, have half integral spins and obey Pauli's exclusion principle.

If N is the number of Fermions having total energy E , in which n_1 particles occupy the first energy level E_1 , n_2 particles occupy the second energy level E_2 , and so on, then according to Fermi-Dirac Statistics, the total number of ways in which n_i particles can be distributed in g_i cells having the same energy E_i is given by

$$n_i = g_i / [(e^{\alpha + \beta E_i}) + 1] \quad \dots(3.19)$$

where $\beta = 1/kT$ and $\alpha = -E_F/kT$ where E_F is called Fermi energy and is the maximum kinetic energy that the free electron can have at the absolute zero temperature. Eqn. (3.19) is called Fermi distribution function. Substituting the value of α and β , we can rewrite Eqn. (3.19) as:

$$n_i = g_i / [(e^{(E_i - E_F)/k_B T}) + 1] \quad \dots(3.20)$$

The examples of fermions are electrons, protons, and neutrons. According to Pauli exclusion principle, no more than one particle can be available in one quantum state, i.e., an energy level can accommodate at most two electrons, one with spin up and the other with spin down. Thus in filling the energy levels, two electrons occupy the lowest level, two more in the next level, and so forth, until all electrons in the metal have been accommodated as shown in Fig. 3.2.

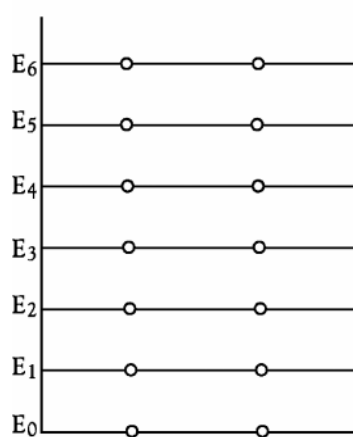


Figure 3.2 Energy levels in metals

3.4.3 Fermi-energy – Fermi Factor

The energy of highest occupied level at absolute zero temperature (0 K) is called the Fermi Energy or Fermi Level (E_F). It is constant for a particular metal.

According to Fermi-Dirac Statistics, the probability $F(E)$ of occupying a particular quantum state having energy E by an electron is governed by **Fermi-Dirac function** and is given by:

$$F(E) = 1/[\exp \{(E - E_F)/k_B T\} + 1] \quad \dots (3.21)$$

Here $F(E)$ is called the Fermi function or Fermi Factor, E is the energy of the level whose occupancy is being considered, E_F is the Fermi energy or Fermi level and it is constant for a particular metal. The variation of $F(E)$ with E depends on temperature as shown in Fig. 3.3.

- (i) At absolute zero, $F(E) = 0$ for $E > E_F$ and $F(E) = 1$ for $E < E_F$.
- (ii) At any other temperature $T > 0$ K, $F(E) = 1/2$ when $E = E_F$.

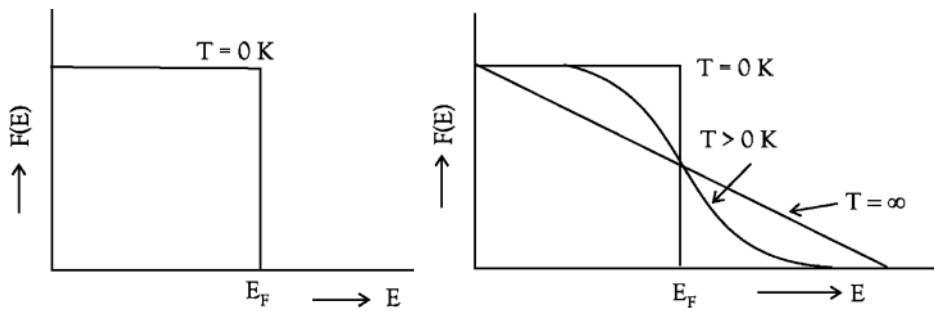


Figure 3.3 The Fermi distribution function at various temperatures

Thus the Fermi level is also defined as the energy level ($E = E_F$) for which the probability of occupation is **half** for $T > 0$ K. Thus the probability of finding an electron with energy equal to the Fermi-energy in a metal is $1/2$ at any temperature above absolute zero.

At very high temperature, $k_B T \gg E_F$, the electrons lose their quantum mechanical property and the Fermi distribution function reduces to classical free electron function.

This quantity E_F is called Fermi energy in honor of Enrico Fermi, who (along with Arnold Sommerfeld) did the most to apply quantum mechanics to calculate the properties of solids in the late 1920s.

3.4.4 Density of States

Density of Energy States $N(E) dE$

In a metal, since the electrons are confined inside, their wave properties will limit the energy values which they may have. Let $g(E) dE$ be the number of quantum states available to electrons with energies between E and $E + dE$. It can be shown that :

$$g(E)dE = \frac{4\pi}{h^3} V(2m)^{3/2} E^{1/2} dE \quad \dots(3.22)$$

where m is the mass of the electron, and V is the volume of the electron gas. We can calculate Fermi energy E_F by filling up the energy states in the metal sample with N free electrons it contains, in order of increasing energy, starting from $E = 0$. The highest state to be filled will then have the energy $E = E_F$ by definition of Fermi energy.

The number of electrons that can have the same energy E is equal to the number of states that have this energy, since each state is limited to one electron. Hence

$$N = \int_0^{E_F} g(E) dE$$

substituting the value of $g(E) dE$ from Eqn. (3.22), we get

$$N = \frac{4\pi}{h^3} V (2m)^{3/2} \int_0^{E_F} E^{1/2} dE \quad \dots(3.23)$$

$$= \frac{4\pi}{h^3} V (2m)^{3/2} \frac{2}{3} E_F^{3/2} \quad \dots(3.24)$$

Let the number of electrons per unit volume is n is equal to N/V . Then

$$n = \frac{N}{V} = \frac{8\pi}{3h^3} (2m)^{3/2} E_F^{3/2} \quad \dots(3.25)$$

Thus the expression for Fermi energy at $T = 0$ K, is given by

$$E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3} \quad \dots(3.26)$$

Substituting the values of h , m , π etc., we get

$$E_F = 3.65 \times 10^{-19} n^{2/3} \text{ eV} \quad \dots(3.27)$$

Thus Eqn (3.27) gives the value of Fermi energy as a function of density of valance electrons.

Average Energy of Electron at Absolute Zero

The average energy of an electron at $T = 0$ K is obtained by the following relation :

$$\bar{E} = \frac{1}{N} \int_0^{E_F} E N(E) dE$$

Using Eqn. (3.23),

$$\begin{aligned} \bar{E} &= \frac{4\pi}{Nh^3} V (2m)^{3/2} \int_0^{E_F} E^{3/2} dE \\ &= \frac{2}{5} \frac{4\pi}{Nh^3} V (2m)^{3/2} E_F^{5/2} \quad \dots(3.28) \end{aligned}$$

Using eqn. (3.24) in Eqn. (3.28) we get

$$\bar{E} = \frac{3}{5} E_F \quad \dots(3.29)$$

Eqn. (3.29) is used to estimate the average energy of an electron.

3.4.5 Expression for Electrical Resistivity/Conductivity

The momentum of free electrons in a metal when there is no applied electric field is given by

$$p = h/\lambda = (h/2\pi)k \quad \dots(3.30)$$

Since $\lambda = 2\pi/k$ and k is wave number.

As per quantum statistics, the Fermi surface separates the occupied states from unoccupied states and in metals, for every occupied state (+ k), there is an unoccupied state (- k), and hence the net momentum of electrons is zero. Therefore, there is no current flow across the metal.

When the external electric field E is applied, the electrons experience a force $F = (-eE)$ due to displacement of Fermi sphere opposite to the applied field direction. Then we get

$$F = dp/dt = -eE \quad \dots(3.31)$$

$$\text{or} \quad (h/2\pi) (dk/dt) = -eE \quad \dots(3.32)$$

$$\text{Integrating Eqn. (3.32), between } 0 \text{ \& } t \text{ we get} \quad k(t) - k(0) = -eEt/(h/2\pi) \quad \dots(3.33)$$

Thus the change in the centre of Fermi Sphere during a characteristic time, called Fermi time τ_F is given by

$$\Delta k = -eE\tau_F/(h/2\pi) \quad \dots(3.34)$$

Collisions of electrons with phonons and impurities opposes the displacement of Fermi sphere and tend to restore it back to its equilibrium position. Finally a steady state is reached. The steady state current density is given by

$$J = n(-e)v = -ne\Delta k (h/2\pi)/m^* = \sigma E \quad \dots(3.35)$$

where n is the number of electrons per unit volume of the conductor, m^* is effective mass of electrons under periodic potential ($m^* = 1.5 m$)

Using the value of Δk as Eqn. (3.34) in Eqn. (3.35) we get

$$J = -\frac{neh \Delta k}{2\pi m^*} = \sigma E \quad \dots(3.36)$$

$$\text{or} \quad J = -\frac{neh}{2\pi m^*} \left[-\frac{Eet_F}{h} \right] = \sigma E$$

$$\text{or} \quad \sigma = \frac{ne^2}{m^*} t_F \quad \text{or} \quad \sigma = \frac{ne^2}{m^*} \frac{\lambda_F}{v_F} \quad \dots(3.37)$$

where $\tau_F = \frac{\lambda_F}{v_F}$

Using Eqn. (3.36) and (3.37) we get

$$J = \sigma E = \left[\frac{ne^2}{m^*} \frac{\lambda_f}{v_f} \right] E \quad \dots(3.38)$$

and $\sigma = \left[\frac{ne^2}{m^*} \frac{\lambda_f}{v_f} \right] \quad \dots(3.39)$

The Eqn. (3.38) & (3.39) gives the expression for steady state current density and electrical conductivity respectively.

Unlike classical free electron theory where the electrical conduction is due to all the free electrons equally, each moving with average drift velocity v_d , in quantum free electron theory, the current is carried out by very few electrons only, all moving with a high velocity v_F . Both approaches gives same result but Quantum free electron theory is more accurate.

3.4.6 Temperature Dependence of Resistivity of Metals

As per quantum free electron theory, at absolute zero temperature, due to periodicity of lattice ions (phonons), electrons moves without any scattering during external applied electric field. As temperature increases, the periodicity of lattice ions get disturbed and they starts vibrating with larger amplitude. This increases the scattering of free electrons and hence in turn increases the resistivity of metals.

In Eqn. (3.39), the only a quantity which depends on temperature is the mean free path λ_f . Since this mean free path is inversely proportional to temperature, at high temperatures, we can conclude that conductivity $\sigma \propto \frac{1}{T}$ or resistivity $\rho \propto T$ which is in agreement with experimental observations.

3.4.7 Merits of Quantum Free-Electron Theory

Quantum free-electron theory proposed by Summerfield, which is based on the assumption that free electrons as Fermi gas, obeys Pauli's exclusion principle and Fermi-Dirac energy distribution, explains satisfactorily the phenomenon like, (1) electrical conductivity in metals, (2) specific heat of metals and (3) electron concentration in metals.

The important feature of quantum free electron theory is that it destroys the notion of classical theory that all free electrons are conduction electrons. It supports that only few electrons whose energies lie in the vicinity of Fermi energy level, contribute for conduction and only such free electrons are called conduction electrons.

One of the major failures of quantum free electron theory is that it could not explain why some solids are good conductors of electricity, some are semiconductors and others are insulators. Further development called **Band theory of solids** could able to explain these questions.

SOLVED PROBLEMS

Electrical conductivity in metals

1. A uniform silver wire has resistivity 1.54×10^{-8} ohm-m at room temperature for an electric field 2V/m. Calculate relaxation time and drift velocity of the electrons assuming that there are 5.8×10^{22} conduction electrons per cm^3 of the materials. (VTU May/June 2010)

Given that:

$$\rho = 1.54 \times 10^{-8} \text{ ohm-m}$$

$$E = 2 \text{ V/m}$$

$$n = 5.8 \times 10^{22} / \text{cm}^3$$

To calculate:

Relaxation time, $\tau = ?$

Drift velocity, $v_d = ?$

For isotropic solids the Relaxation time is equal to mean collision time

i.e., $\tau_r = \tau$

The expression for electrical resistivity is given by

$$\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$$

or

$$\tau = \frac{m}{ne^2\rho}$$

$$\tau = \frac{9.11 \times 10^{-31}}{5.8 \times 10^{22} \times (1.6 \times 10^{-19})^2 \times 1.54 \times 10^{-8}}$$

$$\tau = 3.98 \times 10^{-8} \text{ s}$$

The drift velocity of the electron is given by

$$v_d = \frac{eE\tau}{m}$$

$$v_d = \frac{1.6 \times 10^{-19} \times 2 \times 3.98 \times 10^{-8}}{9.11 \times 10^{-31}}$$

$$v_d = 1.4 \times 10^4 \text{ m/s}$$

The relaxation time and drift velocity of the electron in silver is $\tau = 3.98 \times 10^{-8}$ s and $v_d = 1.4 \times 10^4$ m/s respectively.

2. The experimentally measured resistivity of the silver (assuming only one electron per atom) is 1.64×10^{-8} ohm-m. Calculate the relaxation time, drift velocity and mobility of the electrons in silver for applied field strength of 2000V/m. (Given the density of silver is 10.5 g/cm^3 , atomic weight of silver is 107.82)

Given that:

$$\rho = 1.64 \times 10^{-8} \text{ ohm-m}$$

$$E = 2000 \text{ V/m}$$

$$D = 10.5 \text{ g/cm}^3 = 10500 \text{ kg/m}^3$$

$$M = 107.82$$

$$n = 1$$

To calculate:

$$\text{Mobility, } \mu = ?$$

$$\text{Drift velocity } v_d = ?$$

Each atom contributes only one electron and the electron concentration can be calculated as follows

n = no of electrons/unit volume

$$n = (\text{number of electrons per atom} \times N_A \times D) / M$$

$$n = \frac{N_A D}{M}$$

$$n = \frac{6.025 \times 10^{26} \times 10500}{107.82} = 5.87 \times 10^{28} / \text{m}^3$$

For isotropic materials $\tau_r = \tau$

The relaxation time is given by

$$\tau = \frac{m}{ne^2 \rho}$$

$$\tau = \frac{9.11 \times 10^{-31}}{5.87 \times 10^{28} \times (1.6 \times 10^{-19})^2 \times 1.64 \times 10^{-8}}$$

$$\tau = 3.7 \times 10^{-14} \text{ s}$$

Mobility, μ is given by

$$\mu = \frac{e\tau}{m} = \frac{1.6 \times 10^{-19} \times 3.7 \times 10^{-14}}{9.11 \times 10^{-31}} = 6.49 \times 10^{-3} \text{ m}^2 / \text{V.s}$$

Drift velocity V_d

$$v_d = \mu E = 6.49 \times 10^{-3} \times 2000$$

$$v_d = 12.99 \text{ m/s}$$

The relaxation time, mobility and drift velocity of the electron is, $3.7 \times 10^{-14} \text{ s}$, $6.49 \times 10^{-3} \text{ m}^2 / \text{V.s}$ and $v_d = 12.99 \text{ m/s}$ respectively.

3. The experimentally measured resistivity of the gold wire (assuming only one electron per atom) is $2.44 \times 10^{-8} \text{ ohm-m}$. Calculate the relaxation time, drift velocity and mobility of the electrons in gold (Given: applied field strength across the wire is 45 V/cm the density of gold is 19.3 g/cm^3 , atomic weight of gold is 196.96).

Given that:

$$\rho = 2.44 \times 10^{-8} \text{ ohm-m}$$

$$E = 45 \text{ V/cm} = 4500 \text{ V/m}$$

$$D = 19.3 \text{ g/cm}^3 = 19300 \text{ kg/m}^3$$

$$M = 196.96$$

$$n = 1$$

To calculate:

$$\text{Mobility, } \mu = ?$$

$$\text{Drift velocity } v_d = ?$$

The electron concentration n is

$n =$ no of electrons/unit volume

$$n = (\text{number of electrons per atom} \times N_A \times D) / M$$

$$n = \frac{N_A D}{M}$$

$$n = \frac{6.025 \times 10^{26} \times 19300}{196.96} = 5.9 \times 10^{28} / \text{m}^3$$

For isotropic materials $\tau_r = \tau$

The relaxation time is given by

$$\tau = \frac{m}{ne^2 \rho}$$

$$\tau = \frac{9.11 \times 10^{-31}}{5.9 \times 10^{28} \times (1.6 \times 10^{-19})^2 \times 2.44 \times 10^{-8}}$$

$$\tau = 2.47 \times 10^{-14} \text{ s}$$

Mobility, μ is given by

$$\mu = \frac{e\tau}{m} = \frac{1.6 \times 10^{-19} \times 2.47 \times 10^{-14}}{9.11 \times 10^{-31}} = 4.34 \times 10^{-3} \text{ m}^2/\text{V.s}$$

Drift velocity V_d

$$v_d = \mu E = 4.34 \times 10^{-3} \times 4500$$

$$v_d = 19.52 \text{ m/s}$$

The relaxation time, mobility and drift velocity of the electron is $\tau = 2.47 \times 10^{-14} \text{ s}$, $4.34 \times 10^{-3} \text{ m}^2/\text{V.s}$ and $v_d = 19.52 \text{ m/s}$, respectively.

Fermi Energy

4. Find the Fermi energy of copper by assuming that each copper atom contributes one free electron to the electron gas. The density of copper is $8.94 \times 10^3 \text{ kg/m}^3$.

Solution :

Given : $m = 9.11 \times 10^{-31} \text{ Kg}$;

$$n = N/V = N/(M/\rho) = 6.02 \times 10^{26} / (63.54 / 8.94 \times 10^3) = 8.48 \times 10^{28} \text{ electrons/m}^3;$$

Formula : The Fermi Energy $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$

$$E_F = \frac{(6.63 \times 10^{-34})^2}{2(9.11 \times 10^{-31})} \left(\frac{3}{8\pi} \times 8.48 \times 10^{28} \right)^{2/3} = 0.13 \times 10^{-18} \text{ J} = 7.04 \text{ eV}$$

5. Calculate the Fermi energy of Na assuming that it provides one free electron per atom.; Given $h = 6.625 \times 10^{-34} \text{ Js}$; mass of electron = $9 \times 10^{-31} \text{ kg}$; density of Na is 970 Kg/m^3 and atomic weight of sodium = 22.99.

Solution :

Given $h = 6.625 \times 10^{-34} \text{ Js}$; mass of electron = $9 \times 10^{-31} \text{ kg}$; density of Na is 970 Kg/m^3 and atomic weight of sodium = 22.99;

$$n = N/V = N/(M/\rho) = 6.02 \times 10^{26} / (22.99 / 970) = 2.54 \times 10^{28}$$

Formula : The Fermi Energy $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$

$$E_F = \frac{(6.625 \times 10^{-34})^2}{2(9.11 \times 10^{-31})} \left(\frac{3}{8\pi} \times 2.54 \times 10^{28} \right)^{2/3} = 5.11 \times 10^{-19} \text{ J} = 3.19 \text{ eV}$$

6. The density of zinc is $7.13 \times 10^3 \text{ kg.m}^{-3}$ and its atomic weight is 65.4. Calculate the Fermi energy and the mean energy at $T = 0 \text{ K}$. (assume two electron contributes for electrical conductivity)

Solution :

Given : $\rho = 7.13 \times 10^3 \text{ kg.m}^{-3}$; $M = 65.4$

Required : $E_F = ?$ & $\bar{E} = ?$

(i) $E_F = 3.65 \times 10^{-19} n^{2/3} \text{ eV}$

where $n = 2\rho N/M = [2 \times 7.13 \times 10^3 \times 6.023 \times 10^{26} / 65.4] = 1313 \times 10^{26}$

$E_F = 3.65 \times 10^{-19} \times (1313 \times 10^{26})^{2/3} \text{ eV} = 11.1 \text{ eV}$

(ii) $\bar{E} = \frac{3}{5} E_F = (3/5) E_F \frac{3}{5} \times 11.1 = 6.66 \text{ eV}$

7. Fermi energy of Silver is 5.51 eV. What is the average energy of a free electron at 0 K. ?

Solution : Given : $E_F = 5.51 \text{ eV}$

Required : Average energy = ?

Formula : $\bar{E} = \frac{3}{5} E_F$

$\bar{E} = \frac{3}{5} \times 5.51 \text{ eV} = 3.306 \text{ eV}$

8. Calculate the probability of an electron occupying an energy level 0.02 eV above the Fermi level at 200K, in a material. (VTU Dec. 09/Jan. 10)

Given that:

$E = E_F + 0.02 \text{ eV}$

$\Rightarrow E - E_F = 0.02 \text{ eV} = 0.02 \times 1.6 \times 10^{-19} \text{ J} = 0.032 \times 10^{-19} \text{ J}$

$T = 200 \text{ K}$

To calculate:

$f(E)$ at 200K = ?

The probability of occupation of electron at given temperature T is

$$f(E) = \frac{1}{e^{\left[\frac{E - E_F}{K_B T} \right]} + 1}$$

$$f(E) = \frac{1}{e^{\left[\frac{0.032 \times 10^{-19}}{1.38 \times 10^{-23} \times 200} \right]} + 1}$$

$$f(E) = 0.239$$

The probability of occupation of an electron 0.02eV above Fermi level at 200K is $f(E) = 0.239$

9. A metal has Fermi energy 6.23 eV. Determine the energy for which the probability of occupancy is 0.75 at 350 K.

Given that:

$$E_F = 6.23 \text{ eV} = 6.23 \times 1.6 \times 10^{-19} = 9.968 \times 10^{-19} \text{ J}$$

$$T = 350 \text{ K}$$

To calculate:

$$E = ?$$

The probability of occupancy at given temperature is

$$f(E) = \frac{1}{e^{\left[\frac{E-E_F}{K_B T}\right]} + 1}$$

$$f(E) \left[e^{\left[\frac{E-E_F}{K_B T}\right]} + 1 \right] = 1$$

$$f(E)e^{\left[\frac{E-E_F}{K_B T}\right]} + f(E) = 1$$

$$f(E)e^{\left[\frac{E-E_F}{K_B T}\right]} = 1 - f(E)$$

$$e^{\left[\frac{E-E_F}{K_B T}\right]} = \frac{1 - f(E)}{f(E)}$$

or

$$\left[\frac{E-E_F}{K_B T}\right] = \ln \left[\frac{1 - f(E)}{f(E)} \right]$$

$$E = E_F + K_B T \ln \left[\frac{1 - f(E)}{f(E)} \right]$$

$$E = 9.968 \times 10^{-19} + 1.38 \times 10^{-23} \times 350 \times \ln \left[\frac{1 - 0.75}{0.75} \right]$$

$$E = 9.915 \times 10^{-19} \text{ J}$$

$$E = 6.19 \text{ eV}$$

The energy for which the probability of occupancy is 0.75 at 350 K is 6.19 eV.

EXERCISES**I. Descriptive Type Questions**

1. What is a metal ? List various properties of metals ?
2. Give the expression for Density of states for conduction electron for unit volume of metal and obtain an expression for Fermi Energy. *(VTU June 2009)*
3. Discuss the various drawbacks of classical free electron theory of metals. What are the assumption made in quantum theory to over come. *(VTU June 2009)*
4. Explain classical free electron concept ? Write down the assumptions of classical free electron theory. *(VTU Jan 2009)*
5. Explain failure of classical free electron theory. *(VTU Jan 2009)*
6. Based on free electron theory, derive an expression for electrical conductivity of metals. How does electrical resistance change with impurity and temperature? *(VTU Jan 2008)*
7. Describe Fermi-Dirac distribution and discuss the same for different temperature conditions. *(VTU Jan 2008)*
8. Define drift velocity, mobility and relaxation time for free electron: derive the expression for conductivity in terms of mean collision time. *(VTU June 2008)*
9. Show that occupation probability at $E = E_F + \Delta E$ is same as non occupation probability at $E = E_F - \Delta E$, where E_F is the Fermi energy. *(VTU June 2008)*
10. Elucidate the difference, between classical free electron theory and quantum free electron theory. *(VTU June 2007)*
11. Explain Fermi energy and Fermi factor. Discuss the variation of Fermi factor with temperature and energy. *(VTU June 2007)*
12. Define relaxation time and discuss the dependence of electrical resistivity of metals with temperature and impurity. *(VTU June 2010)*
13. Explain how quantum free electron theory succeeds in overcoming the drawbacks of classical free electron theory. *(VTU June 2010)*
14. State Mathiessen's rule and give an account of the nature of total resistivity both at high and low temperatures. *(VTU Jan 2007)*
15. Using the free electron model derive an expression for electrical conductivity in metals. *(VTU Jan 2007)*
16. Explain density of states. *(VTU Jan 2007)*
17. Describe how quantum free electron theory has been successful in overcoming the failures of classical free electron theory. *(VTU Jan 2010)*

18. What is Fermi energy? Discuss variation of Fermi factor with energy and temperature.
(VTU Jan 2010)
19. Define Drift velocity, mean free path, mean collision time, relaxation time, and drift velocity and mobility?
20. Derive an expression for the drift velocity.
21. What is drift velocity? Derive an expression for the electrical conductivity in a metal.
22. What are the basic assumptions of classical free electron theory?
23. Define relaxation time and discuss the dependence of electrical resistivity of metals with temperature and impurity.
24. What are the similarities and difference between classical and quantum free electron theory.
25. Describe how quantum free electron theory has been successful in overcoming the failures of classical free electron theory.
26. What is Fermi energy? Discuss variation of Fermi factor with energy and temperature.
27. Derive an expression for Density of states for conduction electron for unit volume of metal.

II. Multiple Choice Questions

1. If the mobility of the electron is $7 \times 10^{-3} \text{ m}^2/\text{vs}$, when accelerated by a field $1\text{V}/\text{cm}$, the V_d is given by
- (a) $7 \times 10^{-3} \text{ m/s}$ (b) 0.7 m/s
(c) $7 \times 10^{-2} \text{ m/s}$ (d) 0.007 m/s
2. The temperature dependence for electrical resistivity of metal is
- (a) $\rho \propto \frac{1}{T}$ (b) $\rho \propto \frac{1}{\sqrt{T}}$
(c) $\rho \propto \sqrt{T}$ (d) $\rho \propto T$
3. The Fermi factor for $E = E_f$ at $T > 0\text{K}$ is
- (a) 1 (b) $\frac{1}{2}$
(c) 0 (d) 2
4. According to Quantum Free electron Theory, the energy level in a metal are
- (a) Continuous (b) Discrete
(c) Overlapping (d) None
5. If the mobility of electron in a metal increases with in the resistivity.
- (a) Decreases (b) Increases
(c) Remains constant (d) none of these

6. Ohms law relates to the electric field E, conductivity and current density J as
- (a) $J = E/\sigma$ (b) E^2
- (c) $J = \frac{\sigma}{E}$ (d) $J = \sigma.E$
7. The average drift velocity v_d of electrons in a metal is related to the electric field E, and collision time τ as
- (a) $\sqrt{\frac{eE\tau}{m}}$ (b) $\sqrt{\frac{m}{eE\tau}}$
- (c) $\frac{eE\tau}{m}$ (d) $\frac{E}{eM\tau}$
8. Experimentally specific heat at constant volume C_V is given by
- (a) $\frac{3}{2} R$ (b) $10^{-4}RT$
- (c) $\frac{2}{3} R$ (d) $10^{-4}R$
9. The collision time and root mean square velocity of an electron at room temperature are 3×10^{-14} sec and 1×10^5 m/s respectively. The classical value of mean free path of the electron is
- (a) 3×10^{-19} nm (b) 3 \AA
- (c) 3 nm (d) 17.3 nm
10. Mobility of electron is
- (a) Reciprocal of conductivity (b) Flow of electrons per unit time
- (c) Reciprocal of resistivity (d) Average electron drifts velocity per unit electric field.
11. The quantum mechanical expression for electrical conductivity is
- (a) $\sigma = \frac{m^* v_F}{ne^2 \lambda_F}$ (b) $\sigma = \frac{ne^2 \lambda_F}{m^* v_F}$
- (c) $\sigma = \frac{m^*}{n^2 e^2 \lambda_F}$ (d) $\sigma = \frac{m^*}{ne^2 \lambda_F}$
12. If the Fermi energy of metal at 0°K is 5 eV, $f(E)$ for Fermi energy at $T > 0^\circ\text{K}$ is
- (a) 0.5 eV (b) 1e V
- (c) 0.75 eV (d) 0 e V.

13. For ordinary metals, the resistivity versus temperature curve at $T = 0$,
- (a) has a positive intercept (b) has a negative intercept
(c) goes through the origin (d) none of these
14. Which one of the following relation is correct for current density?
- (a) $J = neAv_d$ (b) $J = \frac{neA}{v_d}$
(c) $J = nev_d$ (d) $J = \frac{1}{nev_d}$
15. The value of Fermi distribution function at absolute zero ($T = 0$ K) is 1, under the condition
- (a) $E = E_F$ (b) $E > E_F$
(c) $E \gg E_F$ (d) $E < E_F$
16. If the Fermi energy of silver is 5.5 eV, the Fermi velocity of conduction electron is
- (a) 0.98×10^6 m/s (b) 1.39×10^6 m/s
(c) 2.46×10^5 m/s (d) None of these.
17. The general expression for the Fermi energy of a metal at 0 K is _____
- (a) $3.65 \times 10^{-19} n^{2/3}$ eV (b) $3.65 \times 10^{19} n^{2/3}$ eV
(c) $3.65 \times 10^{19} n^{1/3}$ eV (d) $3.65 \times 10^{19} n^{3/2}$ eV
18. If the Fermi velocity of the electron is 1.3×10^6 m/s and the relaxation time is 3×10^{-13} s, then the mean free path is
- (a) 3.9×10^{-7} m (b) 12×10^{-7} m
(c) 3.9×10^7 m (d) 3×10^{-9} m
19. For most of the metals, the ratio of thermal conductivity to electrical conductivity is proportional to absolute temperature.
- (a) Wiedemann-Franz law (b) Ohm law
(c) Drude - Lorentz free electrons theory (d) Mathiessen's rule
20. Quantum free electron theory is developed by
- (a) Wiedemann-Franz (b) Arnold Sommerfield
(c) Drude - Lorentz (d) Mathiessen
21. Quantum free electron theory made use of _____
- (a) Planks quantum mechanical principle (b) Pauli exclusion principle
(c) Fermi-Dirac Statistics (d) All the above

22. The major failures of quantum free electron theory is _____
- (a) it fails to explain electrical conductivity in metals,
 - (b) it fails to explain specific heat of metals
 - (c) it fails to explain electron concentration in metals
 - (d) it fail to explain why some solids are good conductors, some are semiconductors and others are insulators
23. The example of fermions _____
- (a) Electrons
 - (b) Protons
 - (c) Neutrons
 - (d) All of these
24. According to Matthiessen's rule, the total resistivity of a metal is _____
- (a) resistivity due to phonon scattering
 - (b) resistivity due to scattering by impurities
 - (c) resistivity due to both phonon scattering and scattering by impurities
 - (d) resistivity due to collision of all electrons on lattice site
25. As per classical theory, Ideal resistivity of metal is _____
- (a) resistivity due to phonon scattering
 - (b) resistivity due to scattering by impurities
 - (c) temperature independent
 - (d) another name of residual resistivity

III. Numerical Problems

1. Find the temperature at which there is 1% probability that a state with an energy 0.5 eV above fermi energy is occupied. (VTU Jan 2009)
2. The Fermi level in potassium is 2.1 eV. What are the energies for which the probabilities of occupancy at 300 K are 0.99, 0.01 and 0.5? (VTU Jan 2008)
3. At what temperature we can expect 1% probability that an energy level 0.5 eV above Fermi, level will be occupied. (VTU June 2008)
4. Find the relaxation time of conduction electrons in a metal of resistivity $1.54 \times 10^{-8} \Omega - m$, if the metal has 5.8×10^{28} conduction, electrons per m^3 . (VTU June 2007)
5. A uniform silver wire has resistivity $1.54 \times 10^{-8} \text{ ohm-m}$ at room temperature for an electric field 2 V/m. Calculate relaxation time and drift velocity of the electrons, assuming that there are 5.8×10^{22} conduction electrons per cm^3 of the material. (VTU June 2010)
6. Calculate the drift velocity and thermal energy of electrons in a metal of thickness 1 mm across which a potential difference of 1 volt is applied, at the temperature of 300 K. The mobility of free electron is $40 \text{ cm}^2/\text{V.s}$. (VTU Jan 2007)

7. Calculate the probability of an electron occupying an energy level 0.02 eV above the Fermi level at 200 K, in a material. (VTU Jan 2010)
8. Calculate the Fermi energy of Aluminum at $T = 0$ K, if its free electron density is $1.81 \times 10^{29} \text{ m}^{-3}$ (Ans: 11.7 eV)
9. Calculate the relaxation time of conduction electron in a metal having resistivity $1.95 \times 10^{-8} \Omega\text{-m}$. [Given: number of electron per m^3 is 4.9×10^{28}]
10. The mobility of electron in certain metal is found to be $3.85 \times 10^{-3} \text{ m}^2\text{V}^{-1}\text{s}^{-1}$. Calculate Drift velocity of the electron [Given: Length of the wire is 3.2 m, Voltage across the wire is 25 V]
11. The resistance of the metal wire having length 40 cm is 0.3 Ω . If the relaxation time of the electron is 3×10^{-10} s, Calculate the drift velocity and mobility of the electron. [Given: current flowing through the metal wire is 2 Amp.]
12. The resistivity of the 98% pure gold wire (assuming only one electron per atom) is $2.52 \times 10^{-8} \text{ ohm-m}$. Calculate the relaxation time, drift velocity and mobility of the electrons in gold (Given: applied field strength across the wire is 23 V/mm the density of gold is 19.3 g/cm^3 , atomic weight of gold is 196.96).
13. The mobility of the electron in gold wire is found to be $4.3 \times 10^{-3} \text{ m}^2/\text{Vs}$. if the resistivity of the gold wire is $2.4 \times 10^{-8} \Omega\text{-m}$, calculate the electron concentration in the gold.
14. A metal has Fermi energy 5.6 eV. Determine the energy for which the probability of occupancy is 0.25 at 450 K.
15. The probability of occupancy is 2.5% for the energy 0.25 eV above Fermi energy. Determine the temperature for which the probability occupancy is 2.5% for the given energy.
16. The resistivity of the iron (assuming only one electron per atom) is $1.0 \times 10^{-7} \text{ ohm-m}$. Calculate the relaxation time, drift velocity and mobility of the electrons in Iron (Given: applied field strength across the wire is 5 V/mm the density of Iron is 7.86 g/cm^3 , atomic weight of Iron is 55.845)

Answers to Multiple Choice Questions

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

DIELECTRIC AND MAGNETIC PROPERTIES OF MATERIALS

OBJECTIVES

In previous chapter, our discussion was confined to electrical properties of metals. In this chapter, how the non-conducting material system behaves under the applied electric and magnetic field and the materials classification based on their dielectric and magnetic properties are discussed. The dielectric and magnetic materials find many applications including energy storage, memory devices, transducers, permanent magnets etc. in the day to day life. The main aim of this chapter is to introduce the basic concepts and phenomenon related to dielectric and magnetic materials and their applications in various industries. The objectives of this chapter are to study

- Classification of Dielectric materials, dielectric polarization, and dielectric susceptibility
- Different types of polarization
- Internal fields in liquids and solids and to derive the expression for the same for one dimensional array of molecular dipoles
- Clausius-Mossotti equation
- Frequency dependence of dielectric constant
- Ferro and Piezoelectric materials and Important applications of dielectric materials
- Magnetic materials and their classification
- Ferromagnetic materials and Hysteresis in ferromagnetic materials
- Properties and applications of Soft and Hard magnetic materials

4.1 INTRODUCTION

The materials can be classified into three major classes depending on their physical property and band structure as conductors, nonconductors (insulators) and semiconductors. The classification can be done either based on the conducting property, or resistivity, or the way in which the conduction and valence bands are arranged in materials. In the non-conducting materials the conduction and valence band is separated by large forbidden gap of several electron volts. As a consequence the electrons in the valence band cannot jump to conduction band easily and hence required to provide more energy to do so. The electrons in non-conducting materials are tightly bound to nucleus and abstract the flow of current due to unavailability of the electrons in the conduction band.

The non-conducting materials can be categorized depending on the purpose of usage, into two categories namely, insulators and dielectrics. If a non-conducting material is used for electrical insulation purpose then those materials are referred as insulators. Similarly, the non-conducting material is used for charge storage purpose (in capacitors) then those materials are known as dielectric materials. These materials play a crucial role in electronic industry. For instance, if a non-conducting material has to be used as dielectric media then these materials should be characterized by high dielectric constant with low dielectric loss. Specific applications require suitable property of material. In electronics industry several non-conducting materials are being used for insulation and charge storage applications.

4.2 DIELECTRIC CONSTANT AND POLARIZATION OF DIELECTRIC MATERIALS

4.2.1 Dielectric Material

Dielectrics are electrically non-conducting materials in which the valence band and the conduction band are separated by a forbidden energy gap of several electron volts. Examples of dielectrics are : Glass, wood, rubber etc. These materials are insulators and can be used to store electric charges by applying electric field.

4.2.2 Polarization of Dielectrics

When we apply some potential difference across a dielectric material, by means of a battery, the electrically charged components of atoms or molecules of dielectric undergoes displacement and forms positive and negative ions and gets polarized (Fig. 4.1). The process of charge separation in atoms/molecules due to applied electric field is called polarization of dielectrics. Such polarized dielectric behaves like big dipole.

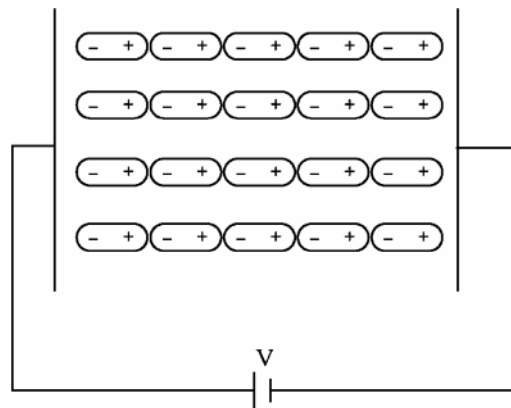


Figure 4.1 Polarization due to applied electric field

Based on the concept of polarization, dielectrics are classified into two categories namely polar and non-polar dielectrics. A **polar dielectric** is one in which the individual molecules possess a dipole moment even in the absence of applied electric field, i.e. the center of positive charge is displaced from the center of negative

charge. The polar dielectrics like water, hydrogen chloride, Polyvinyl chloride etc., have permanent molecular dipoles but arranged in random manner and hence the resultant dipole moment in any direction in a given volume may be zero. Under the influence of an external electric field, the dipoles of polar dielectrics are aligned in the direction of the field. This is known as orientation polarization. The non-polar dielectrics do not have any permanent dipole moment. When external electric field is applied, the molecules/atoms get polarized.

4.2.3 Dielectric Constant

Relative dielectric constant, ϵ_r , a non-dimensional material-dependent quantity that specifies the decrease in the electric field strength when a material (dielectric) is placed in an electric field. The relative permittivity of vacuum is $\epsilon_r = 1$. The relative permittivity of air is well approximated by unity. For most dielectrics, ϵ_r ranges from 1 to 100. There are dielectrics with ϵ_r up to 10,000.

The dielectric constant of a dielectric medium is defined as the ratio between the capacitance of a capacitor containing that dielectric medium (C) to the capacitance of the same capacitor with air as dielectric medium (C_0).

$$\epsilon_r = C/C_0 \quad \dots(4.1)$$

where ϵ_r is called the dielectric constant and is describes the ability of the dielectric material to store electric charges. Also, $\epsilon_r = \epsilon/\epsilon_0$ where ϵ_0 is permittivity of free space and ϵ is permittivity of the medium.

4.2.4 Dielectric Susceptibility

In dielectric medium, the magnitude of polarization (P) is directly proportional to the intensity of applied electric field (E).

$$P \propto \epsilon_0 E \quad \text{or} \quad P = \chi \epsilon_0 E \quad \dots(4.2)$$

χ is proportionality constant called dielectric susceptibility of the material. Hence dielectric susceptibility is characterized by ease with which the dielectric material can be polarized by an external electric field. Dielectric susceptibility χ is a unitless quantity and related with dielectric constant ϵ_r as $\chi = (\epsilon_r - 1)$.

4.2.5 Polarizability

In most of the dielectric materials, the electric dipole moment (μ) acquired is directly proportional to the intensity of applied electric field E.

$\mu \propto E$ or $\mu = \alpha E$, where the proportionality constant α is called polarizability of the molecule of the dielectrics. The Polarizability is a property of individual atom and the unit of polarizability is Fm^2 .

4.2.6 Relation between Dielectric Constant and Polarization

When an dielectric medium is placed in an electric field, the opposite charges present in the dielectrics get separated by small distance hence dipoles are created inside the dielectrics. Two charges separated by distance results in dipole moment. Total dipole moment occurring in a unit volume of the material gives the measure of magnitude of polarization.

Using Eqn. (4.2) we can write that $P = \chi \epsilon_0 \cdot E$ or $\epsilon_0 = P / (\chi \cdot E)$... (4.3)

We have $\epsilon_r = \chi + 1$... (4.4)

From Eqn. (4.3) and (4.4)

$$P = \epsilon_0 (\epsilon_r - 1) E \quad \dots(4.5)$$

4.3 TYPES OF POLARIZATION

There are several mechanisms by which the electrical polarization may occur in a dielectric material due to the applied external electric field. The type of the mechanism decides the magnitude of polarization. For a dielectric kept in external electric field, there is always possibility that one or more polarization mechanism may exist which mainly depends on the type of the dielectric material and magnitude and frequency of the applied electric field.

There are four basic types of polarization mechanisms. They are

- Electronic polarization
- Ionic polarization
- Orientational polarization and
- Space charge polarization.

4.3.1 Electronic Polarization (Optical polarization)

When an atom is placed in an external electric field, the electron cloud and positive charges displaced by small distance. The polarization that occurs due to the displacement of electron clouds of atoms relative to core nucleus in a dielectric material is known as electronic polarization. As electrons are very light, they have a rapid response to the field changes; they may even follow the field at optical frequencies. The electronic polarization does not depend on the temperature of the dielectric materials. The polarization occurs in a material within a very short period of time ($\sim 10^{-14}$ s) and electronic polarization gives very fast response and relatively weak in magnitude (Fig. 4.2).

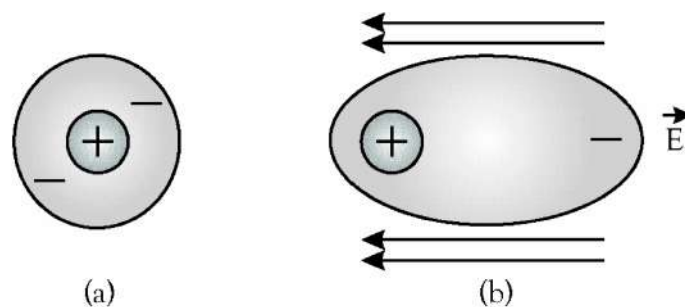


Figure 4.2 (a) Charge distribution in an atom in the absence of external electric field (b) Charge redistribution in the presence of applied external field

4.3.2 Ionic Polarization

Ionic polarization occurs due to the displacement of the ions from their mean position in dielectrics due to the applied electric field. The ionic polarization usually occurs in ionic crystals like NaCl. When an external field is applied across such ionic crystals the positive ions and negative ions get displaced in opposite direction as shown in Fig. 4.3. The positive ions move in the direction of applied field whereas the negative ions move in the opposite direction to external field direction. Such a separation of ions occurs throughout the ionic crystal and resulting polarization is referred to as ionic polarization. The response time or time required to set ionic polarization is slightly larger compared to electronic polarization. The magnitude of the electric field required to set the ionic polarization is much larger compared to electronic polarization and depends on the type of the materials.

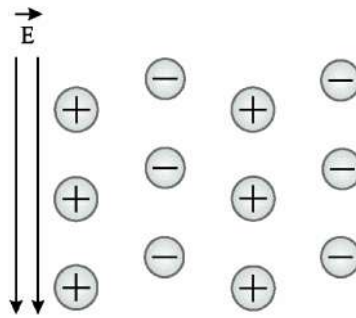


Figure 4.3 Ionic polarization

4.3.3 Orientational Polarization

The orientational polarization occurs in dielectric materials which are polar. The polar dielectrics have permanent dipole moment. The orientation of these molecules will be random due to thermal agitation and hence the net dipole moment is zero. Under an external field, these dipoles align themselves in the direction of the applied external field and undergo polarization. The magnitude of orientational polarization strongly depends on the temperature (decreases with increase in temperature) and magnitude of the field applied. In solids the atoms are fixed at definite positions and the orientation of dipole due to the external field is abstracted. But in the case of gases and liquids this polarization mechanism is common. Orientational polarization process requires longer time to set (Fig. 4.4).

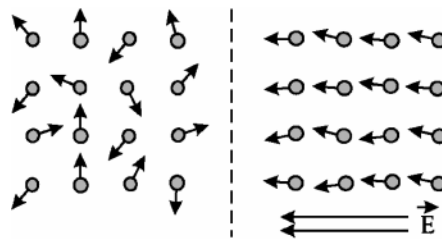


Figure 4.4 Orientational polarization in a polar dielectrics : (a) random alignment of dipole in the absence of the field (b) parallel alignment of dipole due to applied external field

4.3.4 Space Charge Polarization

The space charge polarization is also known as Migrational or interfacial polarization. This type of polarization mechanism are observed in heterogeneous dielectrics or *multiphase dielectric materials* and also in the homogeneous dielectrics which contain impurities, inclusion etc. The Migrational polarization takes longer time and is therefore occurs at low frequency. The space charge polarization in a dielectric occurs when charge carriers migrate to an appreciable distance through the dielectrics due to applied electric field and accumulate with opposite polarity on the interfaces, becomes trapped or cannot discharge at an electrode as shown in Fig. 4.5.

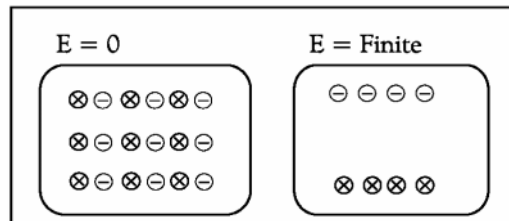


Figure 4.5 Space charge polarization

4.3.5 Frequency and Temperature Dependence of Polarization

Among all these mechanism of polarization, the molecular polarization (orientational and space charge polarizations) sets slowly and has large polarization magnitude compared to ionic and electronic polarization. The magnitude of the electronic polarization is less compared to other two polarization mechanism but the response time or switching is extremely fast. The Fig. 4.6 shows the various types of polarization mechanism and their frequency dependence.

The total polarizability, α , is given by

$$\alpha = \alpha_e + \alpha_i + \alpha_o$$

where α_e , α_i and α_o are the electronic, ionic and orientational polarizability, respectively.

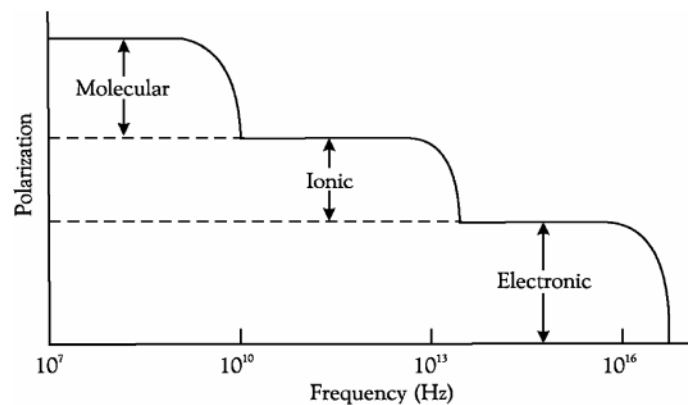


Figure 4.6 Frequency dependence of polarization

When a material is heated, the electronic distribution in the constituent molecules is hardly affected i.e. no influence on the electronic and ionic polarization mechanisms. The increase in temperature causes higher degree of randomness in the molecular orientation in the material. Therefore increase in temperature affects the orderliness in the dipolar arrangement that is established by the applied electric field. The orientational polarization varies inversely with the temperature. The thermal energy facilitates the ion diffusion i.e increase in temperature increases space charge polarization.

4.4 EQUATION FOR INTERNAL FIELDS IN LIQUIDS AND SOLIDS

4.4.1 Internal Fields in Liquids and Solids

The internal field is the electric field that acts at the site of any given atom of a solid or liquid dielectric subject to an external electric field and is the resultant of the applied field and the field due to all the surrounding dipoles.

4.4.2 Expression for One-dimensional Internal Field

Consider a dielectric which is kept in an external uniform electric field strength E . In the dielectric, an array of atomic dipoles aligns parallel to the direction of the applied electric field.

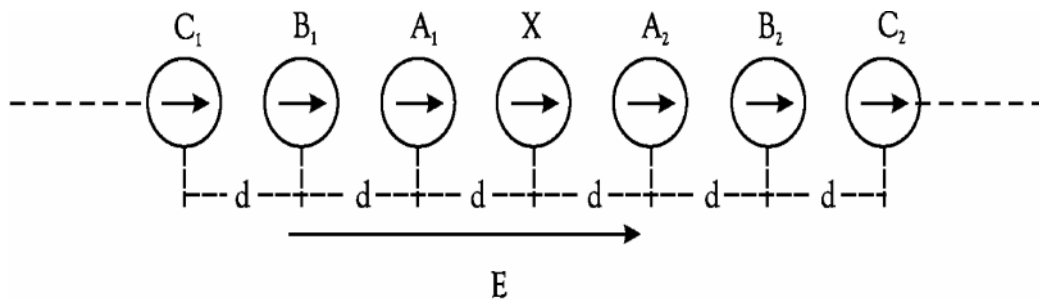


Figure 4.7 Alignment of electric dipoles due to applied field

Let d be the distance of separation between each dipole in a linear array or inter atomic distance as shown in Fig. 4.7.

Let μ be the atomic dipole moment of an individual dipole. The electric field component at a point P due to an electric dipole is expressed in polar form as

$$E_{\theta} = \frac{\mu \sin \theta}{4\pi\epsilon_0 r^3} \text{ and } E_r = \frac{\mu \cos \theta}{2\pi\epsilon_0 r^3} \quad \dots(4.6)$$

Where E_{θ} and E_r are the tangential and radial component of the field respectively at P , μ is the dipole moment, r is the distance of separation between the dipoles.

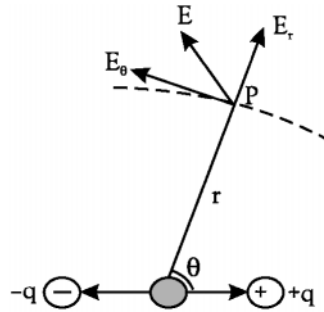


Figure 4.8 *Dipoles separated by a distance d*

Now, let us estimate the electric field at X due to all the dipoles as follows.

The electric field at X due to the dipole A_1 is given by

$$E_{XA_1} = E_r + E_q$$

$$E_{XA_1} = \frac{\mu}{2\pi\epsilon_0 d^3} \text{ since } E_q = 0 \text{ and } \theta = -180^\circ \text{ and } r = -d.$$

Similarly, the electric field at X due to the dipole A_2 is given by

$$E_{XA_2} = \frac{\mu}{2\pi\epsilon_0 d^3}$$

The field E_1 at X due to both the dipoles A_1 and A_2 is given by

$$E_1 = E_{XA_1} + E_{XA_2}$$

$$E_1 = \frac{\mu}{2\pi\epsilon_0 d^3} + \frac{\mu}{2\pi\epsilon_0 d^3} = \frac{\mu}{\pi\epsilon_0 d^3}$$

Similarly, the field E_2 at X due to both B_1 and B_2 dipole which are located at a distance of $2d$ from X is given by

$$E_2 = \frac{\mu}{2\pi\epsilon_0 (2d)^3} + \frac{\mu}{2\pi\epsilon_0 (2d)^3} = \frac{\mu}{\pi\epsilon_0 (2d)^3}$$

Similarly, the field at X due to both C_1 and C_2 is given by

$$E_3 = \frac{\mu}{2\pi\epsilon_0 (3d)^3} + \frac{\mu}{2\pi\epsilon_0 (3d)^3} = \frac{\mu}{\pi\epsilon_0 (3d)^3}$$

Therefore, the total field at X due to all the dipoles in the linear array is given by

$$E_T = E_1 + E_2 + E_3 + \dots$$

$$E_T = \frac{\mu}{\pi\epsilon_0 d^3} + \frac{\mu}{\pi\epsilon_0 (2d)^3} + \frac{\mu}{\pi\epsilon_0 (3d)^3} + \dots$$

$$E_T = \frac{\mu}{\pi\epsilon_0 d^3} \left[1 + \frac{1}{2^3} + \frac{1}{3^3} + \dots \right]$$

$$E_T = \frac{\mu}{\pi\epsilon_0 d^3} \sum_{n=1}^{\infty} \frac{1}{n^3} \quad \text{where } n=1,2,3,\dots,\infty$$

But,

$$\sum_{n=1}^{\infty} \frac{1}{n^3} = 1.2$$

Therefore,

$$E_T = \frac{1.2\mu}{\pi\epsilon_0 d^3}$$

Therefore the total internal field at X is given by

$$E_i = E + E_T$$

i.e

$$E_i = E + \frac{1.2\mu}{\pi\epsilon_0 d^3}$$

If α_e is the electronic Polarizability for the dipole, then

$$\mu = \alpha_e E_i$$

Therefore,

$$E_i = E + \frac{1.2\alpha_e E_i}{\pi\epsilon_0 d^3}$$

or

$$E_i = \frac{E}{1 - \frac{1.2\alpha_e}{\pi\epsilon_0 d^3}} \quad \dots(4.7)$$

The above equation is the expression for the internal field.

4.5 CLAUSSIUS–MOSSOTI EQUATION

Claussius–Mossoti Equation gives the relationship between dielectric constant of a material and the polarizability of its atoms.

Consider an elemental solid dielectric material of dielectric constant ϵ_r . Let N is the number of atoms/unit volume of the material and μ is the atomic dipole moment. Therefore the Dipole moment/unit volume = $N\mu$

Let E_i be the internal field, α_e is the electronic Polarizability of the atom

$$\mu = \alpha_e E_i$$

$$\text{Dipole moment/unit volume} = N\alpha_e E_i$$

$$P = N\alpha_e E_i$$

Therefore,

$$E_i = \frac{P}{N\alpha_e}$$

But,

$$P = \epsilon_0(\epsilon_r - 1)E \quad \text{where } E \text{ is the applied field}$$

Rearranging we get

$$E = \frac{P}{\epsilon_0(\epsilon_r - 1)} \quad \dots(4.8)$$

The Expression for the internal field in the case of three dimensional array of atoms is given by

$$E_i = E + \left(\frac{\gamma}{\epsilon_0} \right) P \quad \dots(4.9)$$

where γ is the proportionality constant known as internal field constant.

Substitute for E_i and E we get,

$$\frac{P}{N\alpha_e} = \frac{P}{\epsilon_0(\epsilon_r - 1)} + \left(\frac{\gamma}{\epsilon_0} \right) P$$

$$\frac{1}{N\alpha_e} = \frac{1}{\epsilon_0} \left[\frac{1}{(\epsilon_r - 1)} + \gamma \right]$$

Consider the internal field in the material to be Lorentz field

i.e $\gamma = 1/3$

$$\frac{1}{N\alpha_e} = \frac{1}{\epsilon_0} \left[\frac{1}{(\epsilon_r - 1)} + \frac{1}{3} \right] = \frac{1}{\epsilon_0} \left[\frac{3 + \epsilon_r - 1}{3(\epsilon_r - 1)} \right]$$

$$\frac{\epsilon_0}{N\alpha_e} = \left[\frac{(\epsilon_r + 2)}{3(\epsilon_r - 1)} \right]$$

Rearranging we get

$$\frac{(\epsilon_r - 1)}{(\epsilon_r + 2)} = \frac{N\alpha_e}{3\epsilon_0} \quad \dots(4.10)$$

The above equation is known as Claussius-Mossotti equation

4.6 FREQUENCY DEPENDENCE OF DIELECTRIC CONSTANT

When dielectrics are subjected to influence of alternating external field, the dielectric constant also vary according to frequency of the alternating field. Therefore ϵ_r becomes complex quantity and is given by

$$\epsilon_r = \epsilon_r' - j\epsilon_r'' \quad \dots(4.11)$$

Where ϵ_r' is real part of the dielectric constant and responsible for increase of capacitance and ϵ_r'' is imaginary part of the dielectric constant and represents the dielectric loss.

Most capacitors are used in alternating electric circuits to store energy. This requires the dipoles to reorient quickly under a rapidly changing electric field. Depending on the frequency of the external field different polarization mechanisms respond with different time scale. The space charge polarization magnitude is larger at lower frequency due to the absorption of energy by the dielectric material. Therefore, space charge polarization response time is large. Many molecules are relatively sluggish in reorientation. Thus, molecular polarization breaks down at relatively higher frequency compared to space charge polarization. The magnitude of molecular polarization is less compared to magnitude of space charge polarization. In contrast, electronic polarization responds quite rapidly to an alternating electric field even at frequencies up to 10^{16} Hz. At very high frequency all the polarization mechanism fails, will fade off, which means that there will not be any kind of response to extremely high frequency fields. Relaxation frequency for different polarization mechanism is different

$$\tau_e < \tau_i < \tau_o \quad \dots(4.12)$$

where τ_e , τ_i and τ_o are electronic, ionic and molecular relaxation frequencies, respectively. If the relaxation frequency of the given polarization mechanism is matches with the applied field frequency then the energy absorption is maximum. At certain frequencies a substantial amount of the excitation energy is absorbed and transferred into heat. This process is called dielectric loss. The dielectric loss is more at low frequency and decreases as the frequency increases. It is imperative to know the frequency for dielectric losses for a given material so that the respective device is not operated in this range.

4.7 FERRO AND PIEZO-ELECTRICITY

4.7.1 Ferroelectric Materials

Ferroelectric materials exhibit spontaneous polarization even in the absence of an external electric field.

Examples: BaTiO_3 , KH_2PO_4 , Triglycine sulphate (TGS), Rochelle salt etc. The dielectric constants of ferroelectrics may be orders of magnitude larger than those of dielectrics. Thus, they are quite suitable for the manufacturing of small-sized, highly efficient capacitors. Most of all, however, ferroelectric materials retain their polarization even after an external electric field has been removed. The ferroelectric materials have high dielectric constant compared to dielectrics. The spontaneous polarization vanishes at phase transition temperature which varies from material to material. It should be noted that ferroelectrics do not contain iron, as the name might suggest. Instead, the name is derived from the similarity of some properties of ferroelectric substances to those of ferromagnetic materials such as iron.

4.7.2 Properties of Ferroelectric materials

Ferroelectric hysteresis:

When a ferroelectric material is exposed to a strong electric field, E , its permanent dipoles become increasingly aligned with the external field direction until eventually all dipoles are parallel to E and saturation of the polarization, P_s , has been achieved, as depicted in Fig. 4.9. Once the external field has been withdrawn, a remanent polarization, P_r , remains which can only be removed by inverting the electric field until a coercive field, E_c , is reached (Fig. 4.9). By further increasing the reverse electric field, parallel orientation of the dipoles in the opposite direction is achieved. Finally, when reversing the field once more, a complete hysteresis loop is obtained, as depicted in Fig. 4.9. Therefore, ferroelectrics can be utilized for memory devices in computers, etc. The area within a hysteresis loop is proportional to the energy per unit volume that is dissipated once a full field cycle has been completed.

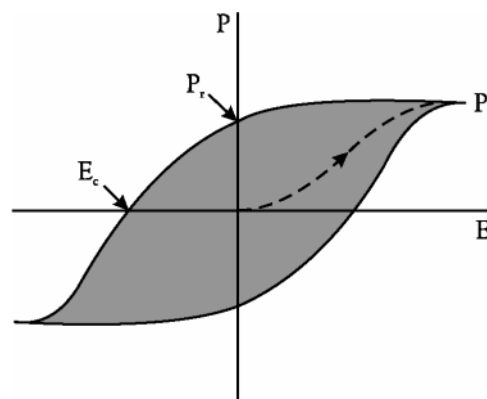


Figure 4.9 Schematic representation of a hysteresis loop for a ferroelectric material in an electric field

4.7.3 Piezoelectric Materials

If pressure is applied to a ferroelectric material, such as BaTiO_3 , a change in the polarization may occur, which results in a small voltage across the sample. Specifically, the slight change in dimensions causes a variation in bond lengths between cations and anions. This effect is called piezoelectricity. It is found in a number of materials, such as quartz (however, much weaker than in BaTiO_3), ZnO , and complicated ceramic

compounds such as PbZrTiO_6 . Piezoelectricity is utilized in devices that are designed to convert mechanical strain into electricity. Such devices are called transducers. Piezoelectrics are used in many applications that include strain gauges, microphones, sonar detectors, and phonograph pickups. The inverse mechanism, in which an electric field produces a change in dimensions in a ferroelectric material, is called electrostriction.

4.8 IMPORTANT APPLICATIONS OF DIELECTRIC MATERIALS

The dielectric materials find many applications in industry and day today life. Some of the important applications of dielectric materials are :

- **Information Storage:** Some of the dielectric show ferroelectric behavior. It means that the information can be stored in the materials and hence such materials can be used for fabricating memory devices.
- **As Capacitors:** Dielectric materials are used in capacitor to enhance the operating voltage and storage capacity.
- **As Transducers:** The dielectric which show piezoelectric properties are used as transducers which convert the mechanical energy in to electrical energy.
- **Production of Ultrasonic Waves:** Dielectric materials are used to produce ultrasonic waves.
- **Security Applications:** All ferroelectric materials are pyrrro-electric and these pyrrroelectric materials find applications in night vision camera and high security applications.
- **Piezoelectric Applications:** Piezoelectric crystals are used to fabricate strain gauges, microphones, phonograph reproducers and sonar detectors.
- **Stable Frequency Signal Generators:** The most important application of piezoelectric materials is the crystal resonator, which is used in electronic devices as a *frequency selective element*. Specifically, a periodic strain is applied to a quartz crystal by an alternating electric field, which excites this crystal to vibrations. These vibrations are monitored, in turn, by piezoelectricity. The amplification occurs only when the applied frequency coincides with the natural resonance frequency of the molecules. Using this method very distinct frequencies are being produced to utilize them for clocks or radio frequency signals.

SOLVED PROBLEMS

1. The electronic Polarizability of a solid is given by $4.32 \times 10^{-36} \text{ F-cm}^2$. If the solid material has $1.45 \times 10^{22} \text{ atoms/cm}^3$, calculate the dielectric constant of the material. (assume that the internal field is Lorentz field)

Given data:

$$\text{Electronic Polarizability, } \alpha_e = 4.32 \times 10^{-36} \text{ F-cm}^2 = 4.32 \times 10^{-40} \text{ F-m}^2$$

$$\begin{aligned} \text{Number of atoms per unit volume } N &= 1.45 \times 10^{22} \text{ atoms/cm}^3 \\ &= 1.45 \times 10^{22} \times 10^6 \text{ atoms/m}^3 \\ &= 1.45 \times 10^{28} \text{ atoms/m}^3 \end{aligned}$$

To calculate:

Dielectric constant, $\epsilon_r = ?$

The dielectric constant can be calculated using Clausius-Mossotti equation given by

$$\left[\frac{(\epsilon_r - 1)}{(\epsilon_r + 2)} \right] = \frac{N\alpha_e}{3\epsilon_0}$$

$$\left[\frac{(\epsilon_r - 1)}{(\epsilon_r + 2)} \right] = \frac{1.45 \times 10^{28} \times 4.32 \times 10^{-40}}{3 \times 8.854 \times 10^{-12}} = 0.236$$

$$(\epsilon_r - 1) = (\epsilon_r + 2)0.236$$

$$\epsilon_r - 1 = 0.236\epsilon_r + 0.472$$

$$\epsilon_r - 0.236\epsilon_r = 1 + 0.472$$

i.e $\epsilon_r(1 - 0.236) = 1.472$

$$0.764\epsilon_r = 1.472$$

$$\epsilon_r = \frac{1.472}{0.764} = 1.93$$

The dielectric constant of given material is $\epsilon_r = 1.93$

2. Calculate the polarization induced in the material due to application of electric field of 350 Volt per meter. Given that the dielectric constant of the material is 4.2.

Given that:

Dielectric constant $\epsilon_r = 4.2$

Electric field strength, $E = 350 \text{ V/m}$

To calculate:

Polarization, $P = ?$

Relation between the dielectric constant and polarization is given by

$$P = \epsilon_0(\epsilon_r - 1)E$$

$$P = 8.854 \times 10^{-12} \times (4.2 - 1) \times 350 = 9.92 \times 10^{-9} \text{ Cm}^2$$

Therefore the polarization induced in the material is $9.92 \times 10^{-9} \text{ Cm}^2$.

3. The induced polarization in a solid due to the application of electric field of strength 2kV/m is $7.35 \times 10^{-9} \text{ Cm}^{-2}$. Calculate the dielectric constant of the material.

Given that:

Field strength $E = 2 \text{ kV/m} = 2000 \text{ V/m}$

$$\text{Polarization } P = 7.35 \times 10^{-9} \text{ Cm}^{-2}$$

To calculate:

$$\text{Dielectric constant of material } \epsilon_r = ?$$

The expression for polarization is given by

$$P = \epsilon_0(\epsilon_r - 1)E$$

$$\text{or } \frac{P}{\epsilon_0 E} = (\epsilon_r - 1)$$

$$\text{or } 1 - \frac{P}{\epsilon_0 E} = \epsilon_r$$

$$\epsilon_r = 1 - \frac{P}{\epsilon_0 E} = 1 - \frac{7.35 \times 10^{-9}}{8.854 \times 10^{-12} \times 2000} = 1 - 0.415 = 0.585$$

The dielectric constant of material is 0.585.

4.9 CLASSIFICATION OF MAGNETIC MATERIALS

The phenomenon of magnetism was known from ancient time. Turkey is the place well known for iron ore which was available in plenty. The word magnetism is said to be derived from a region in Turkey which was known by the name of Magnesia. One should note here that a piece of magnetic material such as iron ore does not immediately attract other pieces of the same material. In order a piece of iron has to attract the other, first, one of the pieces has to be magnetized. That means, its internal “elementary magnets” need alignment in order for it to become a permanent magnet. A piece of iron can be magnetized by placing it into an electric coil through which a direct current passes for a short duration (discovered by Oersted at the beginning of the 19th century). But the question obviously arises to anyone is that how the ancient people managed to magnetize the material? Possibly several methods may be used to produce permanent magnet. Among which one of the methods of magnetizing is the natural way i.e., due to the lightening. The large magnetic field in the lightening has a capacity to magnetize a piece of iron. Once after identifying the magnet produced due to the lightning, the other magnet can be produced by rubbing the magnetized piece to un-magnetized one. Another possible way to produce the magnet is that by hitting very hard. Magnetic materials made an important contribution to the development of the consciousness of mankind, because they paved the way to discoveries of new continents once the compass had been invented. Around 1500, the British coined the word lodestone for the iron ore Fe_3O_4 , which is derived from the old English word lode and which means to lead or to guide. Our modern technology would be unthinkable without magnetic materials and magnetic properties. Applications of magnetic materials are magnetic tapes or disks (computers), television, motors, generators, telephones, and transformers etc.

Depending on the magnitude and the sign of the susceptibility, the magnetic materials can be broadly classified as diamagnetic, paramagnetic and ferromagnetic materials. Further, solids possessing magnetic properties can be classified in to two major categories depending on whether the materials

have permanent magnetic dipole moment or not. The first category of materials is diamagnetic where the magnetic dipole moment in them is zero. The remaining class of materials can be accommodated due to the presence of permanent magnetic dipole moment.

4.9.1 Diamagnetic Materials

According to Ampere, the molecular currents are responsible for the magnetism in a solid. He compared the molecular currents to an electric current in a loop-shaped piece of wire, which is known to cause a magnetic moment. In order to understand the diamagnetism, electronic current has to be considered rather than molecular current. It was found by Lenz that a current is induced in a wire loop whenever a bar magnet is moved toward (or from) this loop. The current thus induced causes a magnetic moment which is opposite to the applied magnetic field direction.

Diamagnetism may be explained by stating that the external magnetic field induces a change in the magnitude of inner-atomic currents which means that the external field accelerates or decelerates the orbiting electrons, in order that their magnetic moment is in the opposite direction from the external magnetic field. Thus the responses of the orbiting electrons counteract the external field whereas the outermost electrons provide the largest contribution.

In the above discussion we considered only electrons that are bound to their respective nuclei. Now, let us consider free electron (referred to metals). These free electrons are forced to move in a magnetic field in a circular path. This leads to a second contribution to the diamagnetic moment; specifically, the circulating free electrons cause a magnetic moment, similarly as described above. It has been observed that superconducting materials expel the magnetic flux lines when in the superconducting state (Meissner effect). In other words, a superconductor behaves in an external magnetic field as if B is zero inside the superconductor. Thus, for superconductors we obtain

$$H = -M \quad \dots(4.13)$$

which means that the magnetization is equal and opposite to the external magnetic field strength. The result is a perfect diamagnet. The magnetic susceptibility of a material is a measure of the ease with which the material can be magnetized. It is defined as magnetization produced in the material per unit applied magnetic field. The susceptibility of diamagnetic material is given by

$$\chi = \frac{M}{H} \quad \dots (4.14)$$

where, M is the magnetization, which is equal to the magnetic moment per unit volume developed inside the solid, and H is the strength of magnetic field.

The susceptibility in superconductors is 1 compared to 10^{-6} (susceptibility for gold is $\sim 23 \times 10^{-6}$) in the non-superconductors. Owing to the strong diamagnetism, superconductors can be used for frictionless bearings, i.e., for support of loads by a repelling magnetic field. The levitation effect of superconducting material can be explained with the strong diamagnetic properties of superconductors.

The main properties of diamagnetic materials are as follows :

1. A diamagnetic material exhibit negative magnetic susceptibility and is of the order of 10^{-6} .

2. Since the diamagnetic susceptibility is negative, the relative permeability (μ_r) is slightly less than unity ($\mu_r < 1$). Permeability is a measure of the degree of magnetic field lines penetration in the material.
3. A diamagnetic material tends to repel by magnetic field. It tends to move from strong field to weak field region.
4. The magnetic susceptibility of diamagnetic material is practically independent of temperature.
5. Diamagnetism occurs in materials whose atoms consist of an even number of electrons so that the magnetic moment cancel each other resulting zero magnetic moment of the atom.
6. Diamagnetism is universal property of matter and all materials have a diamagnetic contribution to their susceptibility. However, in majority of materials, the diamagnetism is overshadowed by other magnetic properties.

4.9.2 Paramagnetic Materials

Paramagnetism in solids is attributed to a magnetic moment that results from electrons which spin around their own axes. According to Pauli principle, no two electrons having the same energy can have the same value and sign for the spin moment. This means that each electron state can be occupied by two electrons only i.e. one with up spin and one with down spin. An external magnetic field tries to turn the unfavorably oriented spin moments in the direction of the external field.

The Spin paramagnetism is slightly temperature dependent. It is in general very weak and is observed in some metals, salts of the transition elements, dilute gases as well as rare earth elements and their salts and oxides. In the absence of external magnetic field the magnetic moment of the orbiting electrons are oriented in random fashion. Therefore, the net magnetic moment in the materials will be zero due to random alignment of magnetic moment. However, when an external field is applied, the individual magnetic vectors tend to turn into the field direction. This direction alignment may be get disturbed due to the thermal agitation. Thus, paramagnetism is temperature-dependent.

The temperature dependence of many paramagnetic materials could be explained by Curie law, which states that the susceptibility, χ , is inversely proportional to the absolute temperature T,

$$\chi = \frac{C}{T} \quad \dots(4.15)$$

where C is called the Curie constant.

For many magnetic materials a more general relationship is observed which is referred as the Curie-Weiss law,

$$\chi = \frac{C}{T - \theta} \quad \dots(4.16)$$

where θ is a constant that has the same unit as the temperature and may possibly have positive as well as negative values. Metals, with a few exceptions, do not obey the Curie-Weiss law.

In most solids only paramagnetism due to electron spin is observed. This is due to the fact that in crystals the electron orbits are essentially coupled to the lattice, which prevents the orbital magnetic moments from turning into the field direction (except rare earth elements and their derivatives, which have 4f- electrons). The fraction of the total magnetic moment contributed by orbital motion versus by spin is defined as the “g-factor.”

The main properties of paramagnetic materials are as follows :

1. Paramagnetic materials, when placed in a magnetic field acquire feeble magnetism in the direction of the applied magnetic field.
2. Paramagnetic materials exhibit positive magnetic susceptibility of the order of 10^{-6} .
3. For paramagnetic materials, the relative permeability (μ_r) is slightly more than unity ($\mu_r > 1$) and hence the magnetic fields of lines are pulled towards the centre of the materials.
4. In non-uniform magnetic field, the paramagnetic materials are attracted towards the stronger region of magnetic field.
5. The paramagnetic susceptibility are strongly dependent on temperature. According to Curie’s Law,

$$\chi_{\text{para}} = \frac{C}{T} \text{ where } C \text{ is Curie constant.}$$

Thus one can clearly distinguish paramagnetic and diamagnetic materials. For paramagnetic materials, the magnetic moment of the electrons is thought to point in the direction of the external field, i.e., the magnetic moment enhances the external field. In diamagnetic materials the magnetic moment opposes the external field. Solids that have both orbital as well as spin moment are clearly paramagnetic since the sum of both paramagnetic components is commonly larger than the diamagnetism. Rare earth metals with unfilled 4f-electron bands are example of this kind.

4.9.3 Ferromagnetic Materials

The ferromagnetic materials are characterized by a spontaneous magnetization. It is well known that many paramagnetic materials, below a critical temperature, present *magnetic dipole moment ordering* even in the absence of applied magnetic fields and those materials which exhibit such a magnetic dipole moment ordering is known as ferromagnetic materials. In ferromagnetic materials the localized magnetic dipole moments lined up in the same direction so that a spontaneous magnetization is not zero. In general the ferromagnetic materials are the one when placed in a magnetic field they get strongly magnetized and retains the magnetization in them even after the removal of magnetic field. Examples of materials which exhibit ferromagnetic property or elements that show spontaneous magnetism are (1) transition or iron group elements (e.g. Fe, Ni, Co), (2) rare earth group elements (e.g. Gd or Dy), and (3) many compounds and alloys.

The main properties of ferromagnetic materials are as follows :

1. Ferromagnetic materials exhibit very high value of magnetic susceptibility which is as large as 10^{+6} .
2. The relative permeability is also positive and is of the order of a few thousands.
3. When a ferromagnetic material is placed in magnetic field, the magnetic field lines crowd in to the material.
4. Ferromagnetic materials are available only in crystalline state and the ferromagnetic property depends on the direction of magnetization.
5. The ferromagnetic materials are characterized by a definite temperature T_C , called Curie temperature, above which ferromagnetic behavior of material disappears.

4.10 HYSTERESIS IN FERROMAGNETIC MATERIALS

4.10.1 Definition

The word 'hysteresis' means lagging behind. The magnetization of a ferromagnetic substance depends on the history of the substance as well as on the magnitude of the applied field. A ferromagnetic substance has a "memory" because it remains magnetized even after the external magnetic field is removed. The closed loop shown in Fig. 4.10 is referred as a hysteresis loop. Its shape and size depend on the properties and type of the ferromagnetic substance and on the strength of the maximum applied field.

The magnetic hysteresis may be defined as "the lagging of intensity of magnetization behind the cyclic variation in magnetizing field".

4.10.2 Explanation of Hysteresis Curve

A typical magnetic hysteresis curve is shown in Fig. 4.10. When the external magnetic field strength is increased the magnetization slowly rises initially and then more rapidly. Finally the intensity of magnetization M reaches a maximum level and beyond which even if one increase the magnetizing field strength, magnetization remains constant and is referred as saturation magnetization, M_s . Saturation magnetization can be defined as the maximum point up to which the material can be magnetized by applying the external magnetic field. Once the intensity of magnetization reached saturation in the materials the magnetizing field, H , is slowly reduced to zero. When H is reduced to zero, the magnetization retains a positive value, called the remanent magnetization, or remanence, M_r . This retained magnetization that is usually utilized in permanent magnets. Therefore remanent magnetization is defined as the ability of the materials to retain the intensity of magnetization in them even after the removal of external magnetic field. The remanent magnetization can be removed by reversing the magnetic field strength to a value H_c , called the coercive field. The minimum magnetic field which should be applied in the reverse direction so that the intensity of magnetization in the materials becomes zero is known as coercive field.

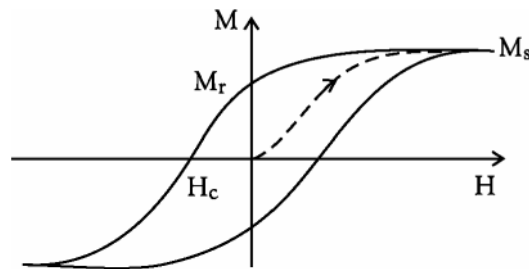


Figure 4.10 Schematic representation of a hysteresis loop of a ferromagnetic material

The saturation magnetization is temperature-dependent. Above the Curie temperature, T_c , ferromagnetics become paramagnetic. For ferromagnetics the Curie temperature, T_c , and the constant θ in the Curie-Weiss law are nearly identical. A small difference exists, however, because the transition from ferromagnetism to paramagnetism is gradual.

4.10.3 Hysteresis Loss

Hysteresis losses are encountered when the ferromagnetic material is subjected to a complete hysteresis cycle. The work thus dissipated into heat is proportional to the area enclosed by a B/H loop. The area enclosed by the magnetization curve represents the work required to take the material through the hysteresis cycle. The energy acquired by the material in the magnetization process comes from the external field. When the magnetization cycle is repeated, due to realignment of the domains, dissipative processes occur within the material as a result of transformation of magnetic energy into heat energy. Due to this process the magnetic material temperature increases. Proper materials selection and rolling of the materials with subsequent heat treatment greatly reduces the area of a hysteresis loop. The energy put in during magnetization is larger than the energy released in demagnetization and the difference between these energies is called **Hysteresis loss**. The energy difference is released as heat. The area enclosed by the hysteresis curve is a measure of the energy loss per magnetization cycle.

4.11 SOFT AND HARD MAGNETIC MATERIALS

The ferromagnetic materials can be classified in to two classes depending on the hysteresis size and shape as soft and hard magnetic materials.

4.11.1 Hard Magnetic (H.M.) Materials

Magnetic materials having a large combination of M_r and H_c are called hard magnetic materials. In the case of hard magnetic materials the resistance to the movement of the domain walls is very large hence require large magnetic field to demagnetize the substance. The hysteresis loop for “hard” ferromagnetic materials is characteristically wide like the one shown in Fig. 4.11, corresponding to a large remanant magnetization. Such materials cannot be easily demagnetized by an external field. In hard magnetic materials the free movement of domain wall is restricted due to presence of lattice defects, imperfections

and presence of precipitated nonmagnetic materials in them. The presence of defects and imperfection in hard magnetic materials lead to high hysteresis loss and increase the mechanical hardness and electrical resistivity.

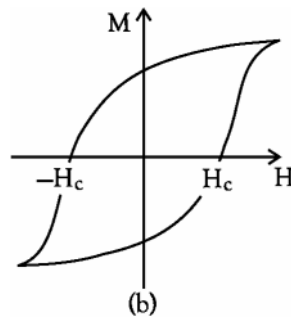


Figure 4.11 Hysteresis loop for “hard” ferromagnetic materials

4.11.2 Properties H.M. Materials

The fundamental properties of hard magnetic materials are high saturation magnetization, high coercive field, high remanant magnetization, large hysteresis loss and wider hysteresis loop (area of hysteresis loop is large), low eddy current, high mechanical hardness and resistivity, low permeability.

4.11.3 Applications of H.M. Materials

1. Due to the high coercivity and high retentivity (remnant magnetization) these materials are used for the fabrication of permanent magnet. These materials have the capability to retain the magnetization in the adverse condition (withstand the environmental changes) and therefore suitable for producing permanent magnet. Example: Alnico alloys (Alnico alloys contain various amounts of aluminum, nickel, cobalt, and iron, along with some minor constituents such as copper and titanium).
2. Permanent magnets are used to fabricate magnetic detectors, microphones, magnetic flux meters, magnetic separators and electronic devices.
3. The Most important use of hard magnetic materials is in storage devices (e.g., for recorder tapes, video tapes, hard disks).
4. Permanent magnets are also used in electric motors, speakers for audio systems, wiggler magnets in synchrotrons etc.

4.11.4 Soft Magnetic (S.M.) Materials

Magnetic materials having a small M_r and H_c are called soft magnetic materials. Soft ferromagnetic materials, such as iron, have a very narrow hysteresis loop and a small remanant magnetization

(Fig. 4.12). Such materials are easily magnetized and demagnetized. An ideal soft ferromagnet would exhibit no hysteresis and hence would have no remanent magnetization. In soft magnetic materials the resistance to the movement of the domain walls is very small and hence require a very small magnetic field to magnetize and demagnetize the substance. The hysteresis loop for “soft” ferromagnetic materials is characteristically narrow (Fig. 4.12), corresponding to a small remanant magnetization. Due to narrow hysteresis loop the energy dissipated is very small compared to hard magnetic materials.

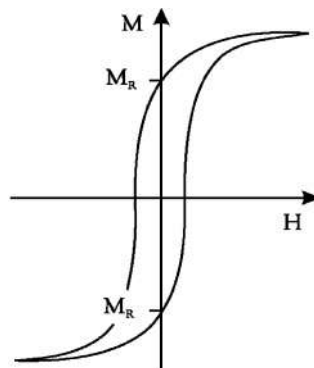


Figure 4.12 Hysteresis loop for “soft” ferromagnetic materials

4.11.5 Properties S.M. Materials

The basic properties of soft magnetic materials are low coercive field, low remanent magnetization, low hysteresis loss and narrow hysteresis loop (area of hysteresis loop is small due to low coercive field), high permeability and susceptibility. Examples: iron-silicon alloy (Fe-Si), Iron-Nickel alloy (Fe-Ni), ferrites (nickel Zinc ferrite, magnesium-manganese ferrite etc.) and garnets.

4.11.6 Applications of S.M. Materials

1. These materials are used as Transformer Core materials, in magnetic switching circuits and as magnetic amplifiers and in current machinery.
2. These materials also find application in electronic communication, motors, generators etc. Permalloys form a very common class of soft magnets. These are Ni-Fe alloys with sometimes small additions of other elements.
3. Soft magnetic materials are used in microwave isolators, electromechanical transducers and to produce ultrasonic waves.
4. Magnetic materials with characteristic rectangular hysteresis loop are used for memory cores in computers.

EXERCISES

I. Descriptive Type Questions

1. What is dielectric polarization? Derive an expression relating dielectric constant and polarization.
2. Write a note on ferroelectric and ferromagnetic materials.
3. Derive the equation for internal field in case of solid or liquid dielectric for one dimensional array of dipoles. *(VTU June 2009)*
4. Derive Clausius Mossuti equation for 3-dimensional cubic solid dielectric. *(VTU June 2009)*
5. Derive an expression for internal field in case of one dimensional array of atoms in dielectric solids. *(VTU Jan 2009)*
6. Describe Ferroelectrics. *(VTU Jan 2009)*
7. Explain the term internal field. Derive an expression for internal field in the case of one dimensional array of atoms in dielectric solids. *(VTU Jan 2008)*
8. Describe the nature of hard and soft magnetic materials. Discuss their applications. *(VTU Jan 2008)*
9. What are dielectrics? Derive the equation for internal field in liquids and solids for one dimensional array of atoms. *(VTU June 2008)*
10. What are hard and soft magnetic materials? Give their characteristic properties and applications. *(VTU June 2008)*
11. Derive the equation for internal field in liquid and solids *(VTU June 2007)*
12. Distinguish between hard and soft magnetic materials *(VTU June 2007)*
13. What is internal field? Derive an expression for the internal field incase of one- dimensional array of atoms in solids or liquids. *(VTU June 2010)*
14. What are soft magnetic materials? Discuss their properties. *(VTU June 2010)*
15. Explain briefly the various types of polarization. *(VTU Jan 2007)*
16. Derive an expression for internal field in case of liquids and solids. *(VTU Jan 2007)*
17. What is meant by polarization mechanism in dielectrics? Discuss any three different polarization mechanisms in dielectrics and their frequency dependence. *(VTU Jan 2010)*
18. Describe hard and soft magnetic materials. *(VTU Jan 2010)*

II. Multiple Choice Questions

1. The Polarization that occur in the frequency range 10^{12} Hz is

| | |
|-----------------|------------------|
| (a) Ionic | (b) Electronic |
| (c) Orientation | (d) Space charge |

2. If two electric charges are q , separated by a distance L . The dipole moment of the system is
 - (a) q/L
 - (b) L/q
 - (c) qL
 - (d) q/L^2
3. Choose the correct relation
 - (a) $E = E_0(\epsilon_r - 1)P$
 - (b) $P = \epsilon_0(\epsilon_r - 1)E$
 - (c) $\epsilon_r = K - 1$
 - (d) $E = \epsilon_0(\epsilon_r - 1)E$
4. If the distance between the plates of capacitor is increased double, the capacitance is
 - (a) Doubled
 - (b) Increased to four times
 - (c) Halved
 - (d) Constant
5. The unit of dipole moment/unit volume is
 - (a) Coulomb/metre
 - (b) Coulomb/metre²
 - (c) Coulomb/metre³
 - (d) Coulomb
6. The flux density is related to the electric field as
 - (a) $D = \epsilon + E$
 - (b) $D = \epsilon - E$
 - (c) $D = \epsilon/E$
 - (d) $D = \epsilon E$
7. In a solid or liquid dielectric with external applied electrical field, as the electronic polarizability α_e increases the internal field E_i
 - (a) Increases
 - (b) Reduces
 - (c) Remains constant
 - (d) None of these.
8. In a dielectric, the polarization is
 - (a) Linear function of applied field
 - (b) Square function of applied field
 - (c) Exponential functions of applied field
 - (d) Logarithmic function of applied field.
9. For a given dielectric, the electron polarizability, α_e
 - (a) Increases with temperature
 - (b) Decreases with temperature
 - (c) Independent of temperature
 - (d) May increase or decrease with temperature.
10. If two point charges of opposite sign $+q$ and $-q$ are separated by a distance l . The electric dipole moment is
 - (a) q/l
 - (b) q/l^2
 - (c) $[(+q)(-q)]l^2$
 - (d) ql
11. The polarization that occurs in the frequency range 10^3 to 10^{16} Hz is
 - (a) Electronic
 - (b) Orientational
 - (c) Ionic
 - (d) Space charge

12. For ferromagnetic substance, the Curie-Weiss law is given by
- (a) $\chi = C/T$ (b) $\chi = \frac{C}{(T-\theta)}$
- (c) $\chi = \frac{(T-\theta)}{C}$ (d) $\chi = \frac{C}{(T+\theta)}$
13. What changes in the capacitance of a capacitor occurs if the dielectric material is removed?
- (a) Increases (b) Decreases
- (c) Remains same (d) None of these
14. The relation between B, M and H is
- (a) $H = \mu_0(M + B)$ (b) $\mu_0 M = (H + B)$
- (c) $B = \mu_0(H + M)$ (d) None of these
15. Sulphur is an elemental solid dielectric of atomic weight 32.07 and density $2.07 \times 10^3 \text{ kg/m}^3$. The number of atoms per unit volume for sulphur is
- (a) $3.89 \times 10^{28}/\text{m}^3$ (b) $3.89 \times 10^{25}/\text{m}^3$
- (c) $9.3 \times 10^{24}/\text{m}^3$ (d) None of these
16. Which one of the following is necessarily the piezoelectric material?
- (a) Lead (b) Mica
- (c) Iron (d) Quartz.
17. The piezoelectric effect is observed only in _____ crystals
- (a) non-centrosymmetric (b) centrosymmetric
- (c) ionic (d) none of these
18. Above Curie temperature the ferroelectric phase of the materials changes to
- (a) para electric phase (b) paramagnetic phase
- (c) anti-ferro electric phase (d) none of these
19. The electronic polarization is also referred as
- (a) Orientational polarization (b) Migrational polarization
- (c) Optical polarization (d) ionic polarization
20. At lower frequencies of the applied field _____ polarization has the maximum magnitude
- (a) Electronic (b) ionic
- (c) space charge (d) Orientational
21. Which of the following polarization mechanism sets faster in the dielectric material due to the application of external electric field
- (a) Ionic polarization (b) Orientational polarization
- (c) Electronic polarization (d) Space charge

22. The net magnetic moment in the paramagnetic substance in the absence of the external magnetic field is
 (a) Infinite (b) Zero
 (c) One (d) None of these
23. Spontaneous magnetization is the characteristic of
 (a) Diamagnetic materials (b) paramagnetic materials
 (c) Both (a) and (b) (d) ferromagnetic materials
24. The Magnetic materials characterized by high coercivity, high remanent magnetization and high hysteresis loss are known as
 (a) Soft magnetic materials (b) Hard magnetic materials
 (c) Demagnetized materials (d) None of these
25. The magnetic materials with high remanent magnetizations are used to fabricate
 (a) Memory devices (b) Permanent magnets
 (c) Transformer cores (d) None of these

III. Numerical Problems

- Sulphur is elemental solid dielectric whose dielectric constant is 3.4. Calculate electronic polarizability if its density is $2.07 \times 10^3 \text{ kg/m}^3$ and atomic wt. is 32.07. (VTU Jan 2009, Jan 2008)
- A parallel plate capacitor has an area of $6.45 \times 10^{-4} \text{ m}^2$ and plates are separated by a distance of $2 \times 10^{-3} \text{ m}$ across which a potential of 10 V is applied. If a material with dielectric constant 6 is introduced between the plates, determine the capacitance, the charge stored on each plate and the polarization. (VTU June 2008)
- The atomic weight and density of sulphur are 32 and $2.08 \times 10^3 \text{ kg/m}^3$ respectively. The electronic polarizability of the atom is $3.28 \times 10^{-40} \text{ F-m}^2$. If sulphur solid has cubic structure, calculate its dielectric constant. (VTU June 2007)
- A solid dielectric material has electronic polarizability $7 \times 10^{-40} \text{ Fm}^2$. If it is a cubic structure, calculate the relative permittivity of the material It has $3 \times 10^{28} \text{ atoms/m}^3$. (VTU June 2010)
- What is the polarization produced in sodium chloride by an electric field of 600 V/mm if it has a dielectric constant of 6? (VTU Jan 2007)
- An elemental solid dielectric material has polarizability $7 \times 10^{-40} \text{ Fm}^2$. Assuming the internal field to be Lorentz field, calculate the dielectric constant for the material, if it has $3 \times 10^{28} \text{ atoms/m}^3$. (VTU Jan 2010)

Answers to Multiple Choice Questions

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

LASERS

OBJECTIVES

This chapter introduces the fundamental aspects, mainly construction, working and applications of lasers. The invention of LASER in 1960 by Maiman had created plenty of opportunities and development in various disciplines. Today the LASER are being used for surgery, photo dynamic therapy of skin related diseases, material cutting and welding, photonics etc. The main goal of this chapter is to study the

- Characteristics, construction and working principle of He-Ne, and semiconductor laser
- Definition of stimulated and spontaneous emission
- Einstein coefficients, Requisites for laser system and conditions for laser action
- Applications of Laser in welding, cutting, drilling and measurement of atmospheric pollutants
- Holography—recording and reconstruction of 3-D images and applications

5.1 INTRODUCTION

Laser is an acronym for Light Amplification by Stimulated Emission of Radiation. In 1917, based on thermodynamic equilibrium between atoms and radiation, **Albert Einstein** predicted that there are two kinds of light emission from matter, namely spontaneous and stimulated emissions. He further proved that both spontaneous emission and stimulated emission are necessary to derive Planck's Quantum theory of radiation, which is the basis for theoretical prediction of Laser. In 1960, **Charles Townner** demonstrated experimentally stimulated emission for first time at Microwave frequencies as MASER and received Noble prize in 1964. In the same year, **Theodore Maiman** demonstrated stimulated emission based LASER in optical frequencies using Ruby rod as lasing medium, and Ali Javan and his co-workers constructed laser device using He-Ne gas as lasing medium. In 1962, lasing action using semiconductor medium was invented. Since then a variety of materials were used to demonstrate lasing action using liquids, ionized gases, dyes etc.

5.1.1 Characteristics of Laser

Some of the unique characteristics of lasers which are different from ordinary incoherent light are:

- (1) Directionality
- (2) High intensity
- (3) Monochromaticity and
- (4) High degree of coherence

Directionality

Any conventional light source like incandescent light emits radiations in all direction whereas a laser source emits radiation only in one direction. The directionality of the laser beam is generally expressed in terms of full angle beam divergence which is twice the angle that the outer edge of the beam makes with the axis of the beam. The outer edge is defined as a point at which the intensity (I) of the beam drops to $1/e$ times its value at the centre.

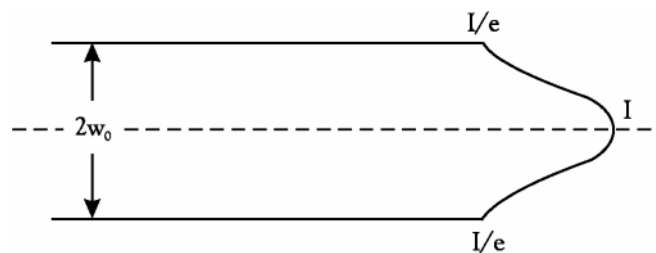


Figure 5.1 Gaussian beam

A Gaussian shape of laser beam is shown in Fig. 5.1 and the full angle divergence in terms of minimum spot size of radius w_0 is given by

$$\phi = 1.27 \lambda / 2w_0 \quad \dots(5.1)$$

where λ is the wavelength of the beam. For a typical planar wavefront emerging from an aperture of diameter d , it propagates as a parallel beam for a distance of d^2/λ called the Rayleigh's range, beyond which the beam due to diffraction diverges with an angular spread of $\Delta\phi = \lambda/d$. For a typical laser the beam divergence is less than 0.01 milliradian, i.e. a laser beam spreads less than 0.01 millimeter for every metre. However, on the other hand, for ordinary light the spread is 1m for every 1 m of travel.

If a_1 and a_2 are the diameters of laser radiation at distances d_1 and d_2 from a laser source respectively, then the angle of beam divergence in degrees is given by

$$\phi = (a_2 - a_1) / 2(d_2 - d_1) \quad \dots(5.2)$$

Intensity

A laser emits light radiation into a narrow beam, and its energy is concentrated in a small region. This concentration of energy both spatially and spectrally accounts for the great intensity of lasers. It can be

shown that even a one-watt laser would appear many thousand times more intense than a 100 watt ordinary lamp. If we compare the number of photons emitted in one second from a square centimetre of a surface of a laser source with those from an ordinary source, the ratio is of the order of 10^{28} to 10^{12} .

Monochromaticity

The light from a laser source is highly monochromatic compared to light from a conventional incoherent monochromatic source. The monochromaticity is related to the wavelength spread of radiation given by

$$\Delta\lambda = (-c/f^2) \Delta f \quad \dots(5.3 (a))$$

The value of $\Delta\lambda$ is in the order of 300 nm for white light, 0.01 nm for gas discharge lamp, while it is 0.0001 nm for laser.

Coherence

Laser radiation is characterized by a high degree of ordering of the light field compared to radiation from other sources. In other words, laser light has a high degree of coherence, both spatial and temporal. Spatial coherence, also called transverse coherence, describes how far apart two sources or two portions of the same source can be located in a direction transverse to the direction of observation and still exhibit coherent properties over a range of observation points. The high degree of coherence of laser radiation makes it possible to realise a tremendous spatial concentration of light power such as 10^{13} watt in a space with linear dimensions of only 1 μm .

The temporal coherence on the other hand, normally refers to the relative phase or the coherence of two waves at two separate locations along the propagation direction of the two beams. It is sometimes referred to as longitudinal coherence. If we assume that two waves are exactly in phase at the first location, then they will maintain the same phase at the second location up to a distance l_c where l_c is defined as the coherence length. For white light the coherence length is of the order of hundred nm while for monochromatic incoherent light its value is of hundred microns. For lasers the value of coherence length is of the order of several metres.

The relationship between coherence length, wavelength and wavelength spread is given by:

$$l_{\text{coh}} = \frac{\lambda^2}{\Delta\lambda} \quad \dots(5.3 (b))$$

The above characteristics of lasers supported their unprecedented scientific and technological application. Thus lasers have been used in telecommunications, meteorology, metrology, biology, cybernetics, optical computations etc.

5.2 PRINCIPLE AND PRODUCTION OF LASER

5.2.1 Induced Absorption

In 1917, Albert Einstein showed that an atom can absorb a photon of energy, hf , from an external radiation field and make a transition from a lower energy state, E_1 , to a higher state, E_2 , where $E_2 - E_1 = hf$.

This process is called induced absorption or stimulated absorption (Fig. 5.2 (a)). The probability of absorption of radiation P_{12} from state 1 (ground state) to state 2 (excited state) is proportional to the energy density of external radiation $u(f)$ and the number of electrons N_1 in the ground state.

$$\text{Thus} \quad P_{12} \propto N_1 u(f) = B_{12} N_1 u(f) \quad \dots(5.4)$$

where B_{12} is proportionality constant called Einstein's coefficient for absorption of radiation.



where a^* represents an excited atom.

5.2.2 Spontaneous Emission

When an atom is in excited state (higher energy state 2 of energy E_2), it can make a transition to lower energy state 1 of energy E_1 spontaneously, without any external radiation field. During such transition from higher energy state to lower energy state the atom emits radiation and such process is called spontaneous emission. The probable rate of spontaneous emission is proportional to number of electrons in excited state.

$$\text{Thus} \quad P_{21} \propto N_2 = A_{21} N_2 \quad \dots(5.5)$$

Where A_{21} is proportionality constant called Einstein's coefficient for spontaneous emission.

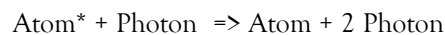


Thus in spontaneous emission

- (i) The emitted photon has energy hf and can move in any random direction.
- (ii) The photons emitted from various atoms in the assembly have no phase relationship between them and hence are incoherent.
- (iii) The rate at which electrons fall from excited level E_2 to lower level E_1 is at every instant proportional to the number of electrons remaining in E_2 .
- (iv) The transition probability depends only on number of electrons in excited state.

5.2.3 Stimulated Emission

In addition to spontaneous emission, which is independent of the radiation density, another kind of emission can occur that is dependent on the external radiation density. If a photon of energy hf interacts with an atom when it is in higher energy level 2, the electric field associated with this photon can stimulate or induce atomic emission such that the emitted electromagnetic wave (photon) vibrates in-phase with the stimulating wave (photon) and travels in the same direction. This phenomenon is called stimulated emission. Two such photons are said to be **coherent**.



The probable rate of stimulated emission depends on radiation density of external radiation and the number of atoms in higher energy level 2.

$$\text{Thus } P_{21} \propto N_2 u(f) = B_{21} N_2 u(f) \quad \dots(5.6)$$

where B_{21} is Einstein's coefficient of stimulated emission. Fig. 5.2 summarizes the three processes of absorption, spontaneous emission, and stimulated emission.

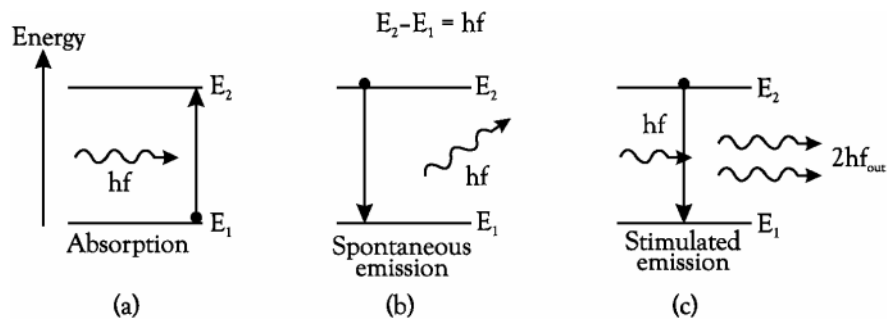


Figure 5.2 The processes of (a) induced absorption and (b) spontaneous emission. The lifetime of the upper state is t_s , and the photon is emitted in a random direction (c) stimulated emission

Hence in stimulated (or induced) emission:

- (i) For every incident photon, two photons will be emitted moving in the same direction.
- (ii) The emitted photons travel in the direction of the incident photon.

Thus the emitted photons have the same frequency and are in phase with the incident photon.

The rate of stimulated emission is proportional to:

- (i) The instantaneous number of atoms in the excited state E_2 .
- (ii) The energy density of the incident radiation.

5.2.4 Einstein's Coefficients (expression for energy density)

Consider a mixture of atoms and radiation in thermal equilibrium at temperature T . Let N_1 and N_2 are the number of atoms of the energy levels E_1 and E_2 respectively and using Eqns. (5.4), (5.5), and (5.6), we write:

$$\text{Number of atoms going from 1 to 2 per unit time} = N_1 u(f) B_{12}$$

$$\text{Number of atoms going from 2 to 1 per unit time spontaneously} = N_2 A_{21}$$

$$\text{Number of atoms going from 2 to 1 per unit time by stimulated emission} = N_2 u(f) B_{21}$$

At thermal equilibrium, the number of upward transitions per unit time must equal to the number of downward transitions per unit time, we have

$$N_1 u(f) B_{12} = N_2 A_{21} + N_2 u(f) B_{21}$$

$$u(f) [N_1 B_{12} - N_2 B_{21}] = N_2 A_{21}$$

$$u(f) = N_2 A_{21} / [N_1 B_{12} - N_2 B_{21}] \quad \dots(5.7)$$

Dividing throughout by $N_2 B_{21}$, Eq. (5.7) becomes

$$u(f) = [A_{21} / B_{21}] / [(N_1 B_{12} / N_2 B_{21}) - 1] \quad \dots(5.8)$$

According to Boltzmann distribution law, the number of atoms N_1 and N_2 in energy states E_1 and E_2 in thermal equilibrium at temperature T are given by

$$N_1 = N_0 e^{-E_1/kT} \text{ and } N_2 = N_0 e^{-E_2/kT}$$

Where N_0 is the total number of atoms present in the ground state and k is Boltzmann's constant.

or

$$\frac{N_1}{N_2} = e^{hf/kT} \quad \dots(5.9)$$

where $hf = E_2 - E_1$
Using Eqn. (5.9) in Eqn. (5.8) we get,

$$u(f) = [A_{21}/B_{21}] / \left[\frac{B_{12}}{B_{21}} [e^{hf/kT}] - 1 \right] \quad \dots(5.10)$$

which is the expression for energy density in terms of Einstein's coefficients.

Comparing Eqn. (5.10) with the Planck's radiation formula given by

$$u(f) = \left[\frac{8\pi hf^3}{c^3} \right] / \left[[e^{hf/kT}] - 1 \right] \quad \dots(5.11)$$

which is the expression for energy density.

Comparing Eqns. (5.9) and (5.10), we find the interesting results

$$B_{12}/B_{21} = 1 \quad \text{or} \quad B_{21} = B_{12} \quad \dots(5.12)$$

and

$$\frac{A_{21}}{B_{21}} = \frac{8\pi hf^3}{c^3} \quad \dots(5.13)$$

Eqn. 5.12 states that any atom that has a finite probability per unit time of absorption has an *equal* probability of stimulated emission. Eqns (5.12) and (5.13) are called **Einstein's relations**.

From Eqn. (5.13), the ratio of spontaneous emission to stimulated emission is proportional to f^3 . It means that the probability of spontaneous emission dominates over the spontaneous emission more and more as the energy difference between two energy states increases.

Also, Using Eqns. (5.5) and (5.6), we can write the ratio of spontaneous emission to stimulated emission as:

$$R = N_2 A_{21} / N_2 B_{21} u(f) = A_{21} / B_{21} u(f) \quad \dots(a)$$

Using the Eqns. (5.10) and (5.13) we can write that

$$R = A_{21}/B_{21} u(f) = \left[\frac{hf}{e^{kT}} - 1 \right] \quad \dots(b)$$

Case 1: When $f \ll \frac{kT}{h}$, i.e., at low frequency, stimulated emission exceeds the spontaneous emission.

Case 2: When $f \gg \frac{kT}{h}$, i.e., at high frequency, spontaneous emission exceeds stimulated emission.

5.2.5 Requisites of a Laser System

(1) Population Inversion and Laser Action

Since $B_{12} = B_{21}$, there is an equal probability that a photon will cause an upward (absorption) or downward (stimulated emission) atomic transition.

When light is incident on a system of atoms in thermal equilibrium, there is usually a net absorption of energy since, according to the Boltzmann distribution, there are more atoms in the ground state than in excited states. However, if one can invert the situation so that there are more atoms in an excited state than in a lower state—a condition called **population inversion**—amplification of photons can result. Under the proper conditions, a single input photon can result in a cascade of stimulated photons, all of which are in-phase, traveling in the same direction and of the same frequency as the input photon. Since the device that does this is a light amplifier, it is called a laser, an acronym for light amplification by stimulated emission of radiation.

Consider an energy state E containing N atoms per unit volume. This number N is called population and is given by Boltzmann's equation

$$N = N_0 e^{-E/kT} \quad \dots(5.14)$$

where N_0 is the population of the ground state with $E = 0$, k is the Boltzmann's constant and T is the absolute temperature.

From Eqn. (5.14), it is clear that the population is maximum in the ground state and decrease exponentially as we go to a higher energy state.

If N_1 is the population in energy state E_1 , N_2 in E_2 then

$$N_1 = N_0 e^{-E_1/kT} \quad \text{and} \quad N_2 = N_0 e^{-E_2/kT}$$

$$\frac{N_2}{N_1} = \frac{e^{-E_2/kT}}{e^{-E_1/kT}} \quad \dots(5.15)$$

$$N_2 = N_1 e^{-(E_2-E_1)/kT} \quad \dots(5.16)$$

where $E_2 > E_1$, $N_2 < N_1$

As $N_1 > N_2$, therefore, if an electromagnetic radiation is incident on the substance at the thermal equilibrium condition, then there is net absorption of radiation.

Usually the population of atoms decreases with the increase in energy of the state.

If N_1, N_2, N_3 are the populations in energy states E_1, E_2, E_3 respectively such that $E_1 < E_2 < E_3$, then $N_1 > N_2 > N_3$. This situation is shown in Fig. 5.3(a).

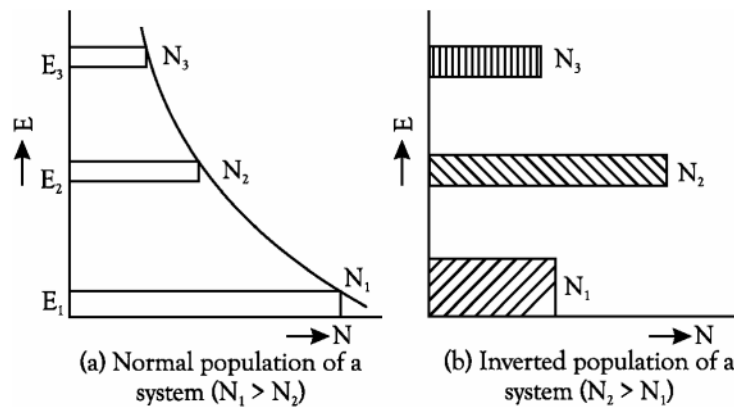


Figure 5.3 Population of atoms

If the process of stimulated emission predominates over the process of spontaneous emission, it may then be possible that $N_2 > N_1$. If this happens then the state is called the *population inversion*. In the state of populated inversion the upper levels are more populated than the lower levels. Fig. 5.3(b) represents a state in which $N_2 > N_1$, i.e. the state of population inversion. To achieve population inversion the external energy is supplied to excite the atoms of the substance. In some substances which contain metastable states, population inversion condition is achieved practically.

(2) Pumping

The population inversion can be achieved by exciting the laser medium with a suitable form of energy. This process is called **pumping**. There are several methods of pumping a laser medium and producing population inversion necessary for the occurrence of stimulated emission. Some of the commonly used methods are:

- (i) Optical pumping
- (ii) Electrical discharge
- (iii) Inelastic atom-atom collision
- (iv) Direct conversion
- (v) Chemical reactions

Optical pumping

If luminous energy is supplied to a medium for causing population inversion, then the pumping is called

the optical pumping. In optical pumping the luminous energy usually comes from a light source in the form of short flashes of light. The optical pumping mechanism is used for lasing material having broadband higher energy levels as in Ruby laser or in Nd:YAG laser.

Electrical discharge

The pumping by electric discharge is preferred in lasing materials whose higher energy levels have a narrow bandwidth, e.g. Argon-ion laser. When a potential difference is applied between cathode and anode in a discharge tube, the electrons emitted from cathode are accelerated towards anode. Some of these electrons collide with atoms of the active medium, ionize the medium and raise it to the higher level. This produces the required population inversion. This is also called direct-electron excitation.

Inelastic atom-atom collision

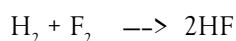
In electric discharge one type of atoms are raised to their excited state. These atoms collide inelastically with another type of atoms. The latter atoms provide the population inversion needed for laser emission. The example is He-Ne laser.

Direct conversion

A direct conversion of electrical energy into radiant energy occurs in light emitting diodes (LEDs). The example of population inversion by direct collision occurs in semiconductor lasers.

Chemical conversion

In a chemical laser, energy comes from a chemical reaction without any need for other energy sources. For example, hydrogen can combine with fluorine to form hydrogen-fluoride :



This reaction is used to pump a CO₂ laser to achieve population inversion.

5.2.6 Components and Condition for Laser action

- (i) The pumping source
- (ii) The active medium
- (iii) The optical resonator

Although there are many different types of lasers, most lasers have certain essential features:

(i) The pumping source:

An energy source capable of producing either pulsed or continuous population inversions. In the case of the Helium-Neon gas laser, the energy source is an electrical discharge that imparts energy by electron-atom collisions.

In the case of the ruby crystal laser, the population inversion is produced by intense flashes of broadband illumination from flash lamps. The process of excitation with intense illumination is called optical pumping.

(ii) The active medium:

A lasing medium with at least *three* energy levels: a ground state; an intermediate (metastable) state with a relatively long lifetime, t_s ; and a high energy pump state (Fig. 5.4). To obtain population inversion, t_s must be greater than t_2 , the lifetime of the pump state E_2 . It should be noted that amplification cannot be obtained with only two levels, because such a system cannot support a population inversion. At most, with extremely intense optical pumping we can increase the population of the upper state in a two-level system until it equals the population of the lower state.

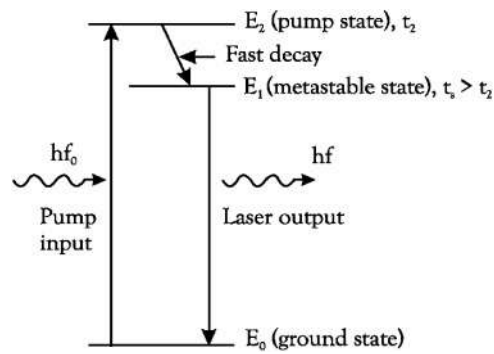


Figure 5.4 A three-level laser system. t_2 is the lifetime of the state E_2 , and t_s is the lifetime of the state E_1 .

Further pumping serves only to excite as many downward transitions as upward transitions, since the probability of absorption is equal to the probability of stimulated emission for a *given* transition. For a population inversion to be produced, energy absorption must occur for a transition *different* from the transition undergoing stimulated emission—thus the need for at least a three-level system.

(iii) The optical resonator:

A method for holding the initially emitted photons within the laser so that they can stimulate further emission from other excited atoms. In practice this is usually achieved by placing mirrors at the ends of the lasing medium so that photons make multiple passes through the laser. Thus the laser may be thought of as an optical resonator or oscillator with two opposing reflectors at right angles to the laser beam. The oscillation consists of a plane wave bouncing back and forth between the reflectors in either longitudinal or transverse mode as shown in Fig. 5.5 (a) and (b). The oppositely traveling plane waves, in turn, generate a highly monochromatic standing wave, which is strongest at resonance when an integral number of half-wavelengths just fits between the reflectors (Fig. 5.5). To extract a highly collimated beam from the laser, one of the parallel mirrors is made slightly transmitting so that a small amount of energy leaks out of the cavity.

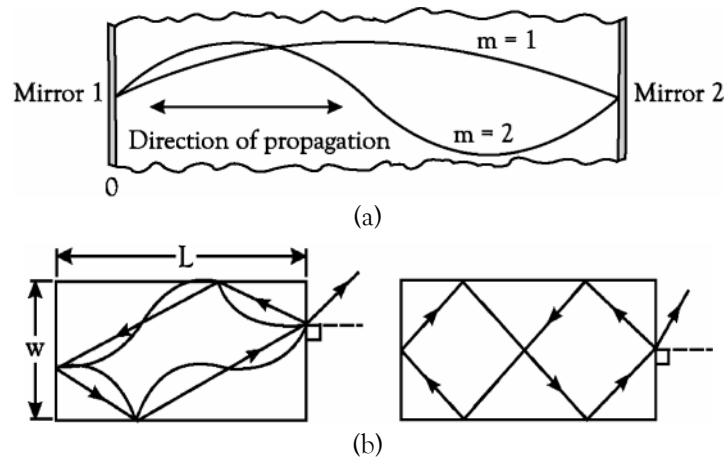


Figure 5.5 Cavity modes in a laser (a) Longitudinal modes have $L = m\lambda/2$, where m is an integer, λ is the laser wavelength in the laser material, and L is the distance between the two mirrors (b) Modes with transverse components can exist if both ends and sides of the laser are made reflective. Arrows show the direction of propagation of light rays

These three features of lasers lead to the unique characteristics of laser light that make it a much more powerful technological tool than light from ordinary sources.

What is metastable state ?

The existence of metastable levels follows from quantum mechanical considerations and can be explained the term “forbidden transition.” The mechanism by which energy exchange takes place between an atom and the electromagnetic fields is the dipole radiation. As a consequence of quantummechanical considerations and the ensuing selection rules, transfer between certain states cannot occur due to forbidden transitions. The term “forbidden” means that a transition among the states concerned does not take place as a result of the interaction of the electric dipole moment of the atom with the radiation field. As a result of the selection rules, an atom may get into an excited state from which it will have difficulty returning to the ground state. A state from which all dipole transitions to lower energy states are forbidden is **metastable state**. An atom entering such a state will generally remain in that state much longer time (upto 10^{-3} sec) than it would in an ordinary excited state (up to 10^{-8} sec) from which escape is comparatively easy.

In the absence of a metastable level, the ions which become excited by pump radiation and are transferred to a higher energy level will return either directly to the ground state by spontaneous radiation or by cascading down on intermediate levels, or they may release energy by phonon interaction with the lattice.

5.2.7 Types of Lasers

Lasers are divided into different types based on the lasing materials used. Accordingly the important types of lasers are Solid state lasers, gas lasers, and semiconductor lasers. Most of the lasers emit light in

IR or visible region, work in Continuous wave (CW) mode or in pulsed mode. Table 5.1 gives some important types of Lasers with examples.

Table 5.1 Types of Lasers with Examples

| S. No. | Type of lasers | Examples with Wavelength of emission |
|--------|----------------------|--|
| 1 | Solid state lasers | Ruby laser ($\lambda = 0.6928 \mu\text{m}$) CaF ₂ laser ($\lambda = 2.49 \mu\text{m}$) Nd:YAG laser ($\lambda = 1.064 \mu\text{m}$) Nd:Glass laser ($\lambda = 1.6928 \mu\text{m}$) |
| 2 | Gas lasers | He-Ne laser ($\lambda \approx 0.633 \mu\text{m}$) Cu-vapour laser ($\lambda = 0.5106 \mu\text{m}$) |
| 3 | Ion lasers | Argon ion laser ($\lambda = 0.4881 \mu\text{m}$ and $\lambda = 0.5145 \mu\text{m}$. Power up to 100 W) |
| 4 | Metal vapour laser | He-Cd laser ($\lambda = 0.4416 \mu\text{m}$. Power up to 300 mW) |
| 5 | Molecular gas laser | CO ₂ laser—invented by C.K.N. Patel in 1963. ($\lambda = 10.6 \mu\text{m}$, Power = 1 kW) Nitrogen laser ($\lambda = 0.3371 \mu\text{m}$) Hydrogen laser ($\lambda = 0.116 \mu\text{m}$) |
| 6 | Excimer laser | Xenon excimer laser ($\lambda = 0.172 \mu\text{m}$), power = 15 MW Argon excimer laser ($\lambda = 0.126 \mu\text{m}$) power = several MW |
| 7 | Semiconductor lasers | GaAs laser ($\lambda = \text{visible and IR region}$) |

5.3 He-Ne LASER

The Helium-Neon laser was the first continuous wave (CW) laser. It was invented by **Ali Javan** and his co-workers in 1961 at the Bell Telephone Laboratory, New Jersey. The most common and inexpensive gas laser, the helium-neon laser is a four level laser and usually constructed to operate in the red at 632.8 nm. It can also be constructed to produce laser action in the green at 543.5 nm and in the infrared at 1523 nm. The collimation of the beam is accomplished by mirrors on each end of the evacuated glass tube which contains about 85% helium and 15% neon gas at 1/300 atmospheres pressure.

5.3.1 Principle

The Helium-Neon laser is a four level laser. The energy level diagram is shown in Fig. 5.6. The left side of the representation shows the lower levels of the helium atoms. A characteristic of helium is that its first states to be excited, 2^1S_1 and 2^1S_0 are metastable, i.e. optical transitions to the ground state 1^1S_0 are not allowed. The atoms can be excited to metastable state by means of electron collision provided by electric discharge. Apart from the electron collision, the electric discharge pumping also supports the

atomic collision in which, an excited helium atom reaches back to the ground state by transferring its energy to excite Ne atom and creates population inversion in the Ne system. The population inversion in Ne leads to laser transition.

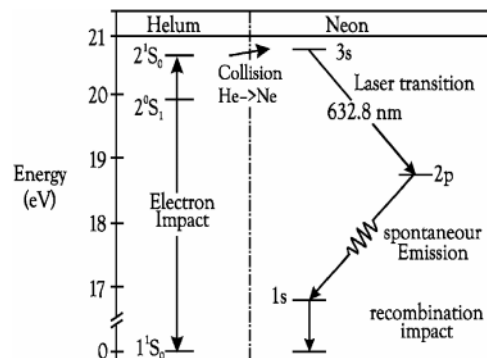


Figure 5.6 Excitation and laser process for the visible laser emission

5.3.2 Construction

The setup consists of a discharge tube of length 50 cm and bore diameter of 0.5 cm (Fig. 5.7). The gain medium of the laser, as suggested by its name, is a mixture of helium and neon gases, in a ratio 5:1, contained at low pressure (an average of 1 torr) in a glass envelope. The energy or pump source of the laser is provided by an electrical discharge of around 1000 volts through an anode and cathode at each end of the glass tube. A current of 5 to 100 mA is typical for CW operation. The optical cavity of the laser typically consists of a plane, high-reflecting mirror at one end of the laser tube, and a concave output coupler mirror of approximately 1% transmission at the other end. He-Ne lasers are normally small, with cavity lengths of around 15 cm up to 0.5 m, and optical output powers ranging from 1 mW to 100 mW.

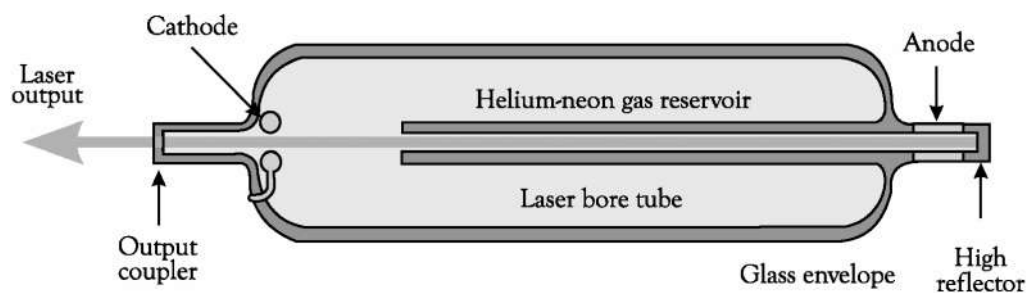


Figure 5.7 Diagrammatic representation of He-Ne laser

5.3.3 Working

He-Ne excitation process can be explained in terms of the following four steps:

- (a) When the power is switched on, an energetic electron of electric discharge collisionally excites a He atom to the state labeled 2^1S_0 . This excited state is often written as $He^*(2^1S_0)$, where the asterisk means that the He atom is in an excited state.
- (b) The excited $He^*(2^1S_0)$ atom collides with an unexcited Ne atom and transfers internal energy to it, resulting an excited Ne atom written as $Ne^*(3S_2)$. This energy exchange process occurs with high probability only because of the accidental near equality of the two excitation energy levels of these two atoms. The excited Ne atom $Ne^*(3S_2)$ is metastable and no spontaneous transition directly to the ground state is allowed. Thus, population inversion is created.
- (c) When the excited Ne atom passes from metastable state (3s) to lower level (2p), it emits photon of wavelength 632.8nm. This photon travels through the gas mixture parallel to the axis of the tube, reflected back and forth by the mirror ends until it stimulates an excited Ne atom and causes it to emit a photon of 632.8 nm with the stimulating photon.
- (d) The stimulated transition from (3s) level to (2p) level is laser transition.

This process is continued and when a beam of coherent radiation becomes sufficiently strong, a portion of it escape through partially silvered end. The Ne atom passes to lower level (1s) by spontaneous emission and finally the Ne atom comes to ground state through collision with tube wall and undergoes radiationless transition.

5.3.4 Applications

- (1) The Narrow red beam of He-Ne laser is used in supermarkets to read bar codes.
- (2) The He-Ne Laser is used in Holography in producing the 3D images of objects.
- (3) He-Ne lasers have many industrial and scientific uses, and are often used in laboratory demonstrations of optics.

5.4 SEMICONDUCTOR LASER

5.4.1 Principle

Stimulated emission is a phenomenon falling into the same category as generation and recombination, but in which an incident photon with an energy triggers the recombination of an excited electron in the conduction band. During the recombination event a new photon is emitted. This photon has the same wavelength as the incident photon and is in phase with it. This is why laser light is monochromatic (all photons have the same wavelength, fixed by the energy bandgap) and coherent (all photons have the same phase). This photon generation can be repeated, and the original photon can be amplified by 2, 4, 8, etc. as shown in Fig. 5.8, resulting in a light amplification effect. If two parallel mirrors (which can reflect light) are placed at both sides of the semiconductor crystal, light can travel back and forth inside the crystal and undergo significant amplification. Such a structure constitutes a Fabry-Pérot cavity. In

practice, one of the mirrors is semitransparent, such that some of the laser light can escape from the crystal. Emitted photons which do not travel perpendicular to the mirrors exit the semiconductor and are lost (Fig. 5.8).

A photon with energy can not only stimulate the emission of another photon, but it can be absorbed by the semiconductor material and generate an electron-hole pair. This effect is highly undesirable in a laser diode since we do not want to see photons absorbed. Unfortunately, photon absorption is unavoidable. It is, however, possible to favor stimulated emission with respect to absorption. This can be achieved if the number of electrons in the excited state (*i.e.*, in the conduction band) is larger than the number of electrons in the ground state (*i.e.*, in the valence band). This condition is called “population inversion”. It can be realized if an external source of energy “pumps” a large quantity of electrons from the fundamental state into the excited state. In a laser diode population inversion is obtained by injecting a large amount of electrons into a Pn-junction.

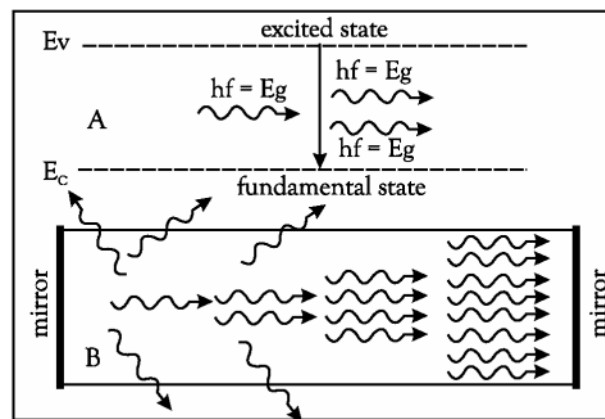


Figure 5.8 A. Principle of stimulated emission. B. Light amplification by stimulated emission

5.4.2 Construction

Fig. 5.9 shows a laser Pn homojunction. The N⁺ and P⁺ type regions are degenerately doped and the Fermi level in the N⁺ and P⁺ type material is above the conduction band minimum and below the valence band maximum, respectively. When a forward bias is applied to the junction a thin region is formed which, instead of being depleted, is in population inversion. In that region there is a strong electron population in the conduction band and a high density of empty states (or holes) in the valence band. Under these conditions laser light is emitted through stimulated emission within the transition region.

A complete laser diode is presented in Fig. 5.10. Two semi-transparent, parallel mirrors are obtained by cleaving the semiconductor along a natural crystal direction (*e.g.* (100)). Since the refractive index of the semiconductor material is larger than that of the surrounding air, the cleaved surfaces act as mirrors which reflect the light back into the crystal. These mirrors do not have a 100% reflectivity, however, which allows some of the laser light to be emitted from the device.

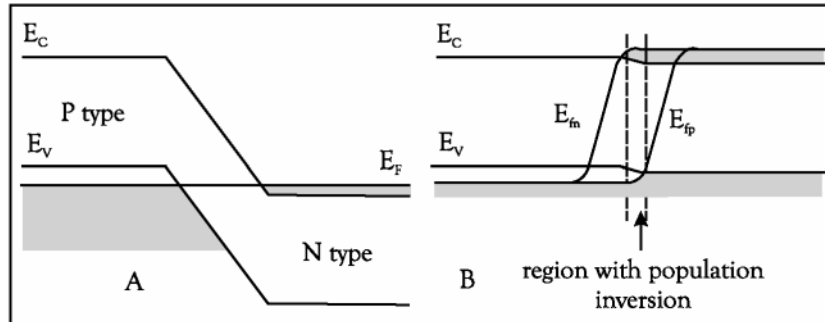


Figure 5.9 Laser PN junction. (a) At equilibrium, (b) Under forward bias

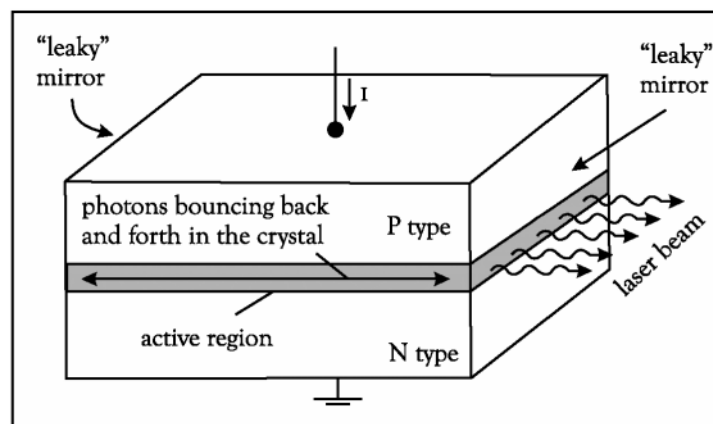


Figure 5.10 Laser diode in forward bias

5.4.3 Working

The output light power of a laser diode is presented in Fig. 5.11 as a function of the current injected into the diode. Below a given threshold, population inversion is not reached, however light is emitted because of radiative recombination. This light is incoherent and is similar to the light emitted by a LED. Above this threshold, population inversion takes place, and laser light is emitted. The light intensity then increases sharply as a function of the current in the diode. Because of the Fabry-Pérot cavity the spectrum of emitted light is compressed into one single spectral line. The emitted laser light is, therefore, monochromatic. Beside the “useful recombination” of electrons by stimulated emission in the population inversion region, a large quantity of electrons are injected into the P-type semiconductor where they can also recombine and emit either photons which do not take part in the lasing process, or phonons (heat). This renders homojunction laser diodes quite inefficient, and only a fraction of the electrical power supplied to the device is converted into laser light.

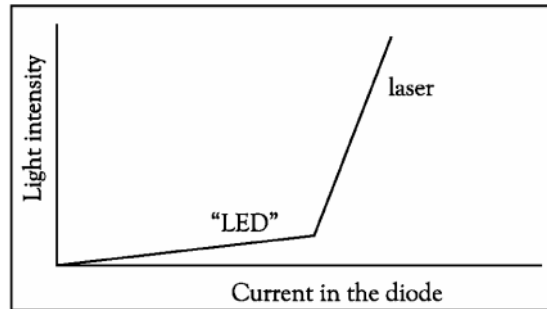


Figure 5.11 Emission of incoherent light (LED) and coherent light (laser) intensity as a function of current (I)

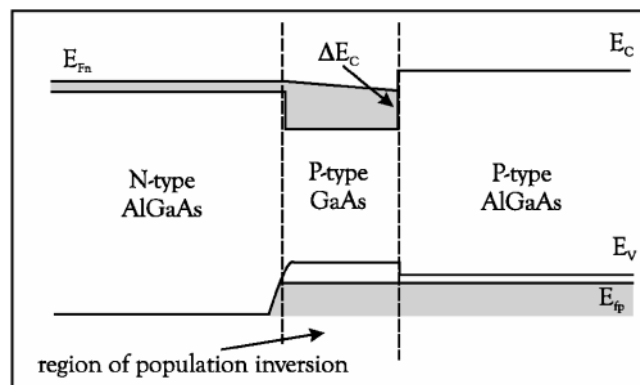


Figure 5.12 AlGaAs/GaAs/AlGaAs heterojunction laser diode

This problem can be solved by the use of a heterojunction structure. Let us take the example of the AlGaAs/GaAs/AlGaAs heterojunction laser diode shown in Fig. 5.12, the electrons in the conduction band which are injected from a forward bias from the N-type AlGaAs into the P-type GaAs cannot spill over the potential barrier ΔE_c created by the P-type GaAs / P-type AlGaAs junction. These electrons are thus confined in the GaAs layer where the inversion population, and thus laser light emission, is produced. In addition, the refractive index of AlGaAs is lower than that of GaAs, which causes the junctions to act as mirrors. This helps confine the photons in the GaAs layer and limits the leakage of light into the AlGaAs layers. As a result the laser light emission efficiency is greatly enhanced and the current threshold for laser light emission is reduced. In 2000, Zhores I. Alferov and Herbert Kroemer got Nobel Prize for developing semiconductor heterostructures used in optoelectronics and Jack St.Clair Kilby for participating in the invention of the integrated circuits.

5.4.4 Applications

Semiconductor laser is eminently suited to fiber-optic communication because of its small size (maximum dimension is several tenths of a millimeter), high efficiency (25 to 30%), simplicity, long lifetime (P-N

junctions have estimated working lifetimes of about 100 years), ease of modulation (through control of the junction current), and fast response (extending well into the GHz range).

Research scope and challenges in Lasers:

1. **New wavelengths:** towards development of Visible, UV, VUV, soft X-ray; towards far infrared regions of electro-magnetic radiation.
2. **Shorter pulses:** of the order of pico, femto, sub-femto seconds.
3. **High powers:** High CW powers, high pulse peak powers, & high efficiency.
4. **Other Parameters:** Compactness, ruggedness, higher life, lower cost, light weight etc.

5.5 APPLICATIONS OF LASER

5.5.1 Laser welding

High-power lasers such as CO₂, Ruby laser, Nd:YAG lasers are important lasers used for accurate welding of materials. For example, a weld of 1/4 inch thick stainless steel can be made using a CO₂ laser with a power output of 3 KW. Laser welding finds an important place in the fields of electronics and microelectronics which require precise and accurate spot welding of very thin wires of 10⁻¹¹m thickness or welding of two thin films together. Use of laser welding in electronics industries offers some unique advantages like: (a) shorter duration for welding, (b) welding can be done in regions adjacent to heat sensitive areas without affecting those elements. (c) welding in inaccessible areas like inside a glass envelope can be done. In laser welding of two wires, we can achieve an effective welding joint even without the removal of the insulation.

Laser welding can be done easily between the two dissimilar metals. Thus a thermocouple may be easily welded to a substrate without much damage to the adjacent material. One can make a junction and attach the junction simultaneously to the substrate. This method has been used in attaching the measuring probes to transistors, turbine blades, etc. In laser welding, material is added to join the two components. Thus the laser power used must not be very high which would evaporate the material. Hence the lasers used in welding processes must possess a high average power rather than a high peak power. Photos of laser welded samples are shown in Fig. 5.13.

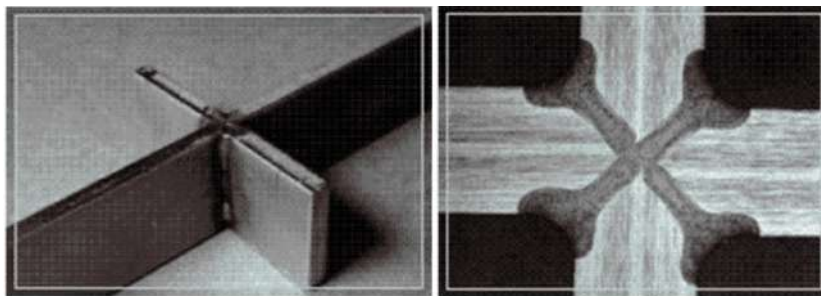


Figure 5.13 Photos of laser welded samples

Advantages of the Laser welding:

- High aspect ratios (Penetration depth and melted width ratio)
- Very low thermal input energy
- Job flexibility
- Easy access to parts to join or weld
- High mechanical characteristics of the laser weld

Some of the Materials commonly used for laser welding are:

- Carbon and stainless steels
- Aluminium and its alloys
- Nickel and its alloys
- Titanium and its alloys
- Copper and its alloys

5.5.2 Laser Cutting

For high precision cutting, high power lasers such as a carbon dioxide laser or Nd:YAG laser are used. In the cutting process it is required that the materials along the cut must be removed. When pulsed lasers are used for the cutting process, the repetition frequency of the pulse and the motion of the laser across the material is adjusted so that a series of partially overlapping holes are produced. It must be taken care of that the width of the cut should be as small as possible and any re-welding must be avoided. The efficiency of laser cutting may be improved by using a gas jet co-axial with the laser as shown in Fig. 5.14 (a). A cross-sectional view is shown in Fig. 5.14 (b).

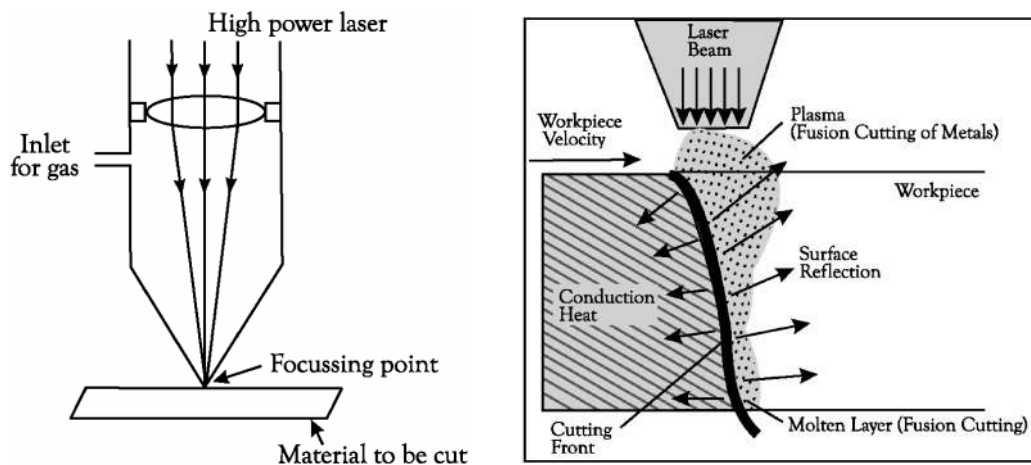


Figure 5.14 (a) Laser cutting scheme with a gas-jet assisted for removing the molten material from the cutting point. (b) Fusion cutting of metals

If a gas is projected at a very high velocity with the laser beam on the material, the gas will then remove the molten material away from the cutting point. This type of gas-jet assisted laser cutting process is used to cut materials like low-carbon steel, stainless steel, titanium, etc. Using a 190 W CO₂ laser with oxygen jet, it is possible to cut a stainless steel sheet of 0.13 cm thickness at a rate of 0.8 m/min. Nitrogen or argon may also be used as jet gases in the laser cutting process. Wood, paper, plastic, etc. are also cut using such a method. When wood is cut with CO₂ lasers, carbonization occurs at the cut edges but it is usually limited to a small depth (about 10-20 μm) of the material. This causes a discolouration only and can be decreased by increasing the cutting speed. Cutting of nickel alloys, stainless steel and other materials by laser finds application in aircraft and automobile manufacturing units. It is estimated that laser cutting can save 60-70% power compared to conventional methods in aerospace industries. Laser cutting also finds a place in textile industries for cutting the cloth.

Advantages of Laser cutting

- Cutting edges are tight and parallel
- Reduced Heat Affected Zone
- Possibility to operate on complex profiles and reduced curving radius
- Absence of mechanical distortion of the laser worked piece
- No influence of the hardness of the material
- No problems to cut materials previously coated

5.5.3 Laser Drilling

Drilling of holes in different substances such as metals, ceramics, plastics, cloth, paper, glass etc., is another important application of the laser. A laser beam with power of 0.05 J can produce a hole of 0.1 mm radius in a 1 mm thick steel plate. In conventional methods for drilling holes, less than 250 μm diameter is very difficult and some times it leads to the breakage of materials. However, using laser, even in the hardest materials holes of 10 μm diameter may be drilled easily and precisely. The pulsed Nd:YAG lasers, Ruby lasers and CO₂ CW lasers are normally used for this purpose. The drilling is achieved without the usual problem of breakage or wear of drill-bits. Hard and brittle materials (like diamond, ceramics, stainless steel, ferrites), and softer materials (like rubber, glass, plastics) have been processed alike with lasers. Photos of laser drilled samples are shown in Fig. 5.15.

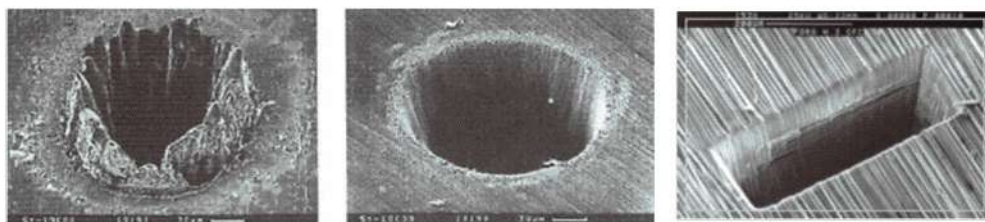


Figure 5.15 *Photos of Holes drilled in steel using laser*

5.5.4 Measurement of Atmospheric Pollutants

Laser is a very useful tool for the measurement of the concentrations of various atmospheric pollutants such as (1) Hydrocarbons like Alkanes, olefins (emitted during non-complete combustion of oil-derivative products), (2) CO (carbon monoxide, constituting around 2/3 of all volatile poisons originating from motor exhaust fumes), (3) NO₂ and SO₂ (emitted during combustion of fossil fuels mainly coal), and (4) Particulate matter (any solid or liquid matter dispersed in the atmosphere) such as dust and smoke. Conventional pollution measurement methods require the samples of pollutants in hand for chemical processing and therefore, these methods cannot give real-time data. In contrast, laser methods permit measurements by remotely sensing the pollutants in atmosphere without the need of sample collection or chemical processing. Most of the techniques used for this purpose of studying pollutants are based on the principle of light absorption or scattering.

Principle:

The primary influence of the atmosphere on laser beam is through scattering and absorption. Both processes cause an attenuation of the beam according to Beer's law:

$$I = I_0 e^{-\alpha R} \quad \dots(5.17)$$

where I is the intensity of the optical beam after transmission over a distance R, α is the atmospheric extinction coefficient, and I₀ is the initial intensity of the beam. It is possible to express α as a sum of terms:

$$\alpha = \alpha_{\text{Ray}} + \alpha_{\text{Mie}} + \alpha_{\text{Raman}} + \alpha_{\text{abs}} \quad \dots(5.18)$$

where α_{Ray} , α_{Mie} , and α_{Raman} are the extinction coefficients related to Rayleigh, Mie and Raman Scattering, respectively, and α_{abs} is the molecular absorption coefficient.

Rayleigh scattering is due to particles in the atmosphere, such as molecules or fine dust, that are much smaller than the optical wavelength λ , of the laser. Mie scattering is associated with larger particles such as aerosols whose size is on the order of λ . Rayleigh and Mie processes are elastic scattering, i.e., the scattered light is the same wavelength as the incident laser beam. Raman scattering is an inelastic interaction of the optical beam involving excitation of energy levels of a molecule and re-radiation at a different wavelength. Absorption of the laser beam is a resonant interaction (direct absorption) leading to excitation of the molecule, followed possibly by fluorescence.

Measurement Techniques:

In one of the laser techniques, which uses the principle of light scattering by pollutants is called Light Detection and Ranging (LIDAR). In this technique, a pulsed laser beam is used as the source of light and the light scattered back by the atmospheric sample is detected by means of a photodetector. The distance to particulate matter (sample) and the concentrations of particulate matter is obtained in this method. The distance is inferred from the time that light takes to travel up to the pollutant region and to return back. The principle of LIDAR is very much similar to that of RADAR except that microwave radiation

is replaced by laser radiation. The method helps in determining the concentration of particulate matter as a function of distance. However, this method cannot provide any information regarding the nature of the scattering particles. It is mainly useful in knowing the distribution of atmospheric pollutants in different vertical sections and in monitoring their variations. This technique allows environmental agencies to measure concentrations of harmful gases such as SO_2 and NO_2 . LIDAR technique is also used to measure Ozone concentrations in the lower troposphere and for climate monitoring.

The second technique uses the principle of absorption of laser beam by pollutants. The presence of specific gases/pollutants in the atmosphere can be detected using absorption spectroscopy techniques. A laser beam is transmitted through polluted sample and the attenuation of intensity of light due to absorption in the sample is detected and recorded. Each pollutant absorbs light of characteristic wavelengths and from the absorption spectrum, its existence can be determined.

A third technique uses Raman scattering to detect the pollutants. The Raman scattering involves scattering of laser light by gas molecules accompanied by a shift in the wavelength of scattered light. Raman shifts are characteristic of each molecular species present in the atmosphere. Hence, analysis of back scattered laser light reveals the constituents of the pollutant.

5.6 HOLOGRAPHY

5.6.1 Introduction to Holography

Holography is a technique for recording and reproducing an image of an object without the use of lenses. This technique is discovered by **Dennis Gabor**, a Hungarian scientist during 1948, uses the principle of interference to record both the amplitude and phase of a wave/particle. In ordinary photography, we record the intensity of light reaching the film at every point from an object. Each point of the object sends out waves and the waves from all the points of the object together constitute the object wave. The object wave is converted into an image of the object by a lens. Since amplitude and intensity of a wave are related, an ordinary photograph is a two-dimensional record of amplitude of the light wave. On the other hand, in holography what we record the object wave itself on a recording medium in the form of interference pattern instead of optically formed image of the object. When this record is illuminated during the reproduction, a three-dimensional image of the object is seen. The permanent record of the interference pattern on the recording medium is called a hologram. A hologram can be viewed from different directions to reveal different sides, and from various distances to reveal changing perspective. Thus, holography is two-step process by which images of objects can be formed without the help of lenses. When Gabor coined the idea of hologram, laser was yet to be discovered. Later after the discovery of lasers in 1960, some of the first laser holograms were prepared in 1964 by Leith and Upatniek of University of Michigan. Dennis Gabor won the Nobel prize in 1971.

5.6.2 Principle of Holography

The process of generating holograms consists of two stages:

- (i) Recording of the hologram, and
- (ii) Reconstructing the image

5.6.3 Recording of 3-D Images using hologram

During the recording process, we superimpose a coherent wave called the reference wave, as shown in Fig. 5.16 on the wave emerging from the object.

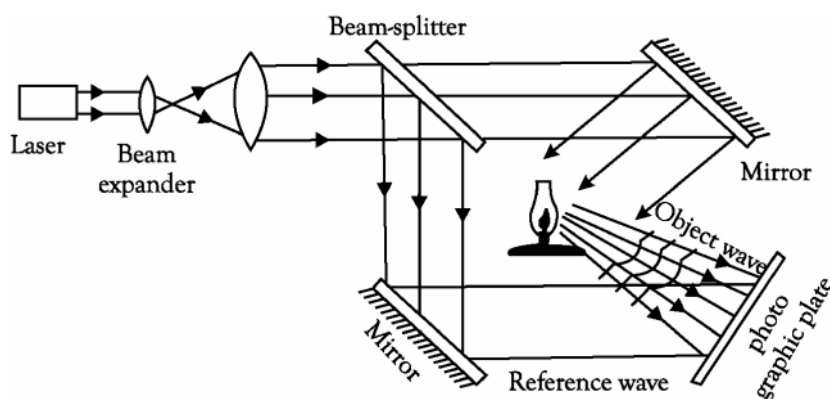


Figure 5.16 Recording of hologram

A beam of monochromatic light from a coherent source is split into two beams with the help of a beam splitter. One of the beams is sent towards the object to be holographed and the other is directed towards a photographic emulsion plate (Fig. 5.16). The photographic plate is placed such that it receives light scattered from the object and also the direct light from the source reflected by a mirror. The wave that is directed to the photographic plate is called the reference wave. The light beam that is directed to the object gets scattered by the object is called object wave. The object wave and the reference wave interfere each other and produce interference pattern on the photographic plate. This interference pattern carries a record of both the intensity and relative phase of light at each point of the object. Gabor called the recording pattern as hologram.

5.6.4 Reconstruction of 3-D Images

For reconstructing the image, the hologram is illuminated by a beam of light similar to the reference wave used for recording the hologram. Light is transmitted through the clear portions of the hologram. The transmitted wave is a complex wave consisting of three components. One is the duplicate of the object wave, the second is complex conjugate of the object wave and the third is the reconstruction wave itself. By viewing at the duplicate of the object wave, an exact replica of the original object is seen, which is in fact the virtual image of the object. In addition to the virtual image, we can also see a real image if we view in the direction of the complex conjugate of the object wave. Thus, two images are formed, a virtual image on the side of the plate nearer to the source and a real image on the opposite side (Fig. 5.17). The virtual image has all the characteristics of the object as far as the viewing is concerned. We can change the viewing position and obtain a different view of the object. The real image can be photographed by keeping the photographic plate at the position of the real image.

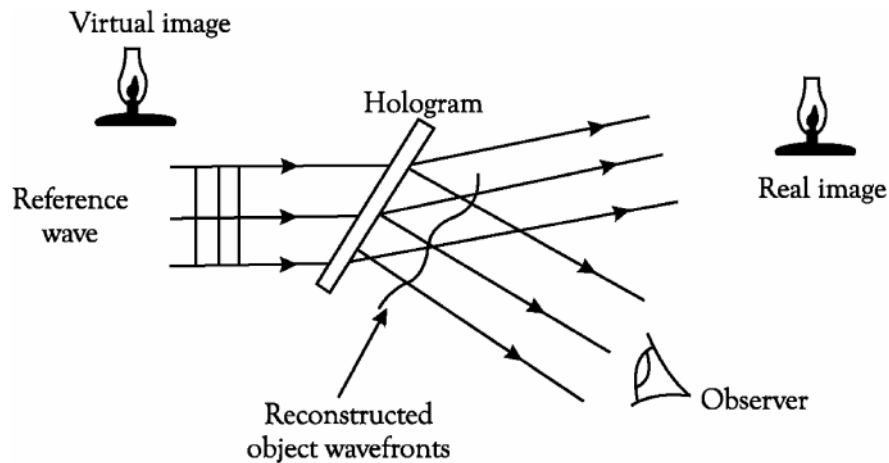


Figure 5.17 Reconstruction of the image

5.6.5 Selected Applications of Holography

Holographic principle is used a wide variety of applications in different fields of Science and technology. Some of them are:

1. Holographic interferometry: One of the most important applications of holography is in interferometry. The technique called double exposure holographic interferometry and is proved to be highly useful in nondestructive testing of objects. In this technique, the undisturbed object is first recorded on the photographic plate with an exposure to a reference wave. Then, the object is stressed and is recorded on the same photographic plate through a second exposure along with the same reference wave. After this double exposure, the hologram is developed. If the hologram is now illuminated by a reconstruction wave, there would emerge from the hologram two object waves - one corresponding to the unstressed object and the other corresponding to the stressed object. These two object waves interfere to produce interference pattern. Thus, on viewing through the hologram, one finds a reconstruction of the object superposed with the fringes. The fringe pattern is indicative of the distribution of strain in the object.

Another technique known as the time-average holographic interferometry is used in studying vibrating objects. In this technique, a hologram of the vibrating object is prepared by exposing the photographic plate to a reference wave, for a relatively long period of time such that the vibrating object has undergone a number of oscillations during that time. The resulting hologram consists of a standing wave pattern caused by a superposition of the number of images corresponding to the successive states of vibration of the object. The bright areas in the hologram correspond to undeflected regions whereas the contour lines indicate the regions of constant amplitude of vibration. This technique is very much useful in the vibrational analysis of any vibrating system or vibrating component of a machine. Nowadays, the above techniques are widely used in nondestructive testing.

2. Acoustical holography: Light waves cannot propagate to considerable distances in dense liquids and solids where as sound waves can propagate through them. Therefore a three dimensional

acoustical hologram can be recorded using ultrasonic waves initially and then visible light can be used for reconstruction of the visual image of an opaque object. By viewing such hologram in visible light the internal structure of the object can be observed. Such techniques will be highly useful in the fields of medicine and technology. As sound waves can propagate through dense liquids and solids, acoustical holography has an advantage in locating underwater submarines etc., and study of internal body organs.

3. Data storage: Holograms can be used for data storage devices in computer. A large amount of information such as 10^{12} bits can be stored in a cubic cm of a volume hologram. These memories have long lifetime because a small mechanical damage to the portion of a hologram will not erase the stored information.

4. Three-dimensional photography: Holographic technique is used in the production of a three-dimensional photograph, with the distance and orientation of each point of the object recorded in the image.

5. Microscopy: Holography can be used in microscopy to obtain a magnified image of an object. In such cases the recording is done with light of smaller wavelength and reconstruction of the image is done with light of longer wavelength. Smaller areas in an object can be examined in greater detail. This has great potential in observing micro-objects such as blood cells, amoebas, cancer affected tissues etc.

6. Holographic optical elements: Holography can be used to make diffraction gratings known as holographic optical elements (HOEs). They function like a lens. They are less efficient than ruled gratings. HOEs are compact, lightweight and inexpensive. The scanners used for reading the bar code on the items in super market are made by HOEs.

7. Character recognition: Holography can be used for character recognition. A complicated wave front from an object can be generated from a hologram by the simple wave front of the reference beam. The process is reversible so that reference wave can be generated by the object wave. This principle forms the basis of holographic pattern recognition. This could be used to identify fingerprints.

8. Photolithography: Holography is used in the production of photographic masks used to fabricate microelectronic integrated circuits.

SOLVED PROBLEMS

1. For the He-Ne laser at 2 m and 4 m distances from the laser, the output beam spot diameters are 2 mm and 3 mm. Calculate the angle of divergence ?

Given: $a_1 = 2$ mm, $a_2 = 3$ mm, $d_2 = 4$ m, $d_1 = 2$ m

Required: $\phi = ?$

Formula: $\phi = \frac{a_2 - a_1}{2(d_2 - d_1)}$

$$\phi = \frac{(3 - 2) \times 10^{-3}}{2(4 - 2)} = \frac{10^{-3}}{4} = 0.25 \times 10^{-3}$$

Result: Angle of divergence = 0.25×10^{-3} rad

2. A ruby laser emits pulse of 20 ns duration with average power per pulse being 100 KW. If the number of photons in each pulse is 6.981×10^{15} , calculate the wavelength of photons.

[VTU Jan 2010]

Given : Time = 20×10^{-9} s, Average Power $P = 100$ KW, $n = 6.981 \times 10^{15}$

Required: λ

$$\text{Formula: } P = nhf = \frac{nhc}{\lambda}$$

$$\text{or } \lambda = \frac{nhc}{P} = \frac{6.981 \times 10^{15} \times 3 \times 10^8 \times 6.62 \times 10^{-34}}{[100 \times 10^3 / 20 \times 10^{-9}]} = 2.77 \times 10^{-12} \text{ m}$$

$$\therefore \lambda = 2.77 \times 10^{-12} \text{ m}$$

3. A pulsed laser emits photons of wavelength 780 nm with 20 mW average power/pulse. Calculate the number of photons contained in each pulse if the pulse duration is 10 ns.

Given : $\lambda = 780$ nm , $P = 20$ mW, Pulse duration = 10×10^{-9} s

$$\text{Formula : power } P = nhf = \frac{nhc}{\lambda} \quad \text{or } n = \frac{P \lambda}{hc} = \frac{20 \times 10^{-3} \times 780 \times 10^{-9}}{3 \times 10^8 \times 6.62 \times 10^{-34}}$$

$$n = 7.9 \times 10^{19} \text{ photons/sec}$$

For 10×10^{-9} sec,

$$n = 7.9 \times 10^{19} \times 10 \times 10^{-9} \text{ photons} = 7.9 \times 10^{11} \text{ photons}$$

EXERCISES

I. Descriptive Type Questions

1. With the help of energy level diagram, describe the construction and working of He-Ne Laser. [VTU June 2009]
2. Write a note on measurement of Pollutants in a atmosphere using laser. [VTU June 2009]
3. Obtain an expression for energy density of radiation under equilibrium condition in terms of Einstein co-efficient. [VTU Jan 2009]
4. Describe the construction and working of Semiconductor laser. [VTU Jan 2009]
5. Describe the construction and working of He-Ne laser with the help of energy level diagram. [VTU Jan 2008]
6. Describe the recording and reconstruction processes in Holography with the help of suitable diagrams. [VTU Jan 2008]
7. Derive the expression for energy density of radiation using Einstein's Coefficients. Compare the expression with Planck's equation. [VTU June 2008]
8. Explain the construction and working of He - Ne Laser. [VTU June 2008]
9. What are semiconductor diode lasers? Describe with energy band diagram the construction and working of semiconductor diode laser. Mention the uses of diode lasers. [VTU June 2007]
10. Describe briefly the application of lasers in welding, cutting and drilling. Mention the nature and property of the lasers used. [VTU June 2007]
11. Discuss the possible ways through which radiation and matter interaction takes place. [VTU June 2010]
12. Describe the construction and working of semi conductor laser. [VTU June 2010]
13. Explain with sketches the basic principle of operation of lasers. [VTU Jan 2007]
14. Describe the construction and working of He-Ne laser, with energy level diagram. [VTU Jan 2007]
15. Obtain an expression for energy density of radiation under equilibrium condition in terms of Einstein coefficient. [VTU Jan 2010]
16. Describe the recording and reconstruction processes in holography, with the help of suitable diagrams. [VTU Jan 2010]

II. Multiple Choice Questions

1. Pumping process used in diode laser is

| | |
|------------------------|-------------------|
| (a) Optical pumping | (b) Forward bias |
| (c) Electric discharge | (d) None of these |

2. The life time of an atom on a metastable state is of the order
 - (a) a few seconds
 - (b) unlimited
 - (c) a nano second
 - (d) few milli second
3. The purpose of the optical resonator in a laser is
 - (a) to provide cover to the active medium
 - (b) to provide path for atoms
 - (c) to provide selectivity of photons
 - (d) to send laser in specified direction
4. In He-Ne lasers, the ratio of He-Ne is in the order
 - (a) 1:10
 - (b) 1:1
 - (c) 10:1
 - (d) 100:1
5. The emission of photon without being aided by any external agency is called
 - (a) Light amplification
 - (b) Induced absorption
 - (c) Stimulated emission
 - (d) Spontaneous emission
6. n_1 be the number density of lower energy E_1 , and n_2 be the number density of higher energy E_2 , if $n_2 > n_1$ is called
 - (a) Thick population.
 - (b) Inverted population
 - (c) Normal population
 - (d) No population.
7. Supply of energy to atoms for excitation is called
 - (a) Glowing
 - (b) Bombarding
 - (c) incidenting
 - (d) Pumping
8. Important characteristic of Laser beam is
 - (a) Interference
 - (b) Diffraction
 - (c) Dispersion
 - (d) Coherence
9. Which of the following is not a laser property?
 - (a) Highly monochromatic
 - (b) High directionality
 - (c) Very narrow band width
 - (d) Highly divergent
10. The life time of an atom in the excited state is of the order of
 - (a) Millisecond
 - (b) Few seconds
 - (c) Nano seconds
 - (d) Unlimited.
11. Pumping technique used in He - Ne gas laser is
 - (a) Forward bias
 - (b) Optical pumping
 - (c) Electrical discharge
 - (d) High injection current.

12. 3D image of an object constructed by hologram is the process of
 (a) Intensity recording (b) Phase information recording
 (c) Both phase and intensity information recording
 (d) Transmission and reflection recording
13. The life time of an atom at the ordinary excited state is of the order of
 (a) few mili second (b) few nano second
 (c) few micro second (d) Unlimited.
14. The relation between Einstein's coefficients A and B is
 (a) $\frac{8\pi h\nu^2}{c^2}$ (b) $\frac{8\pi h^2\lambda^2}{c^2}$
 (c) $\frac{8\pi hf^3}{c^3}$ (d) $\frac{8\pi hf^3}{c^2}$
15. The number of modes of standing waves in the resonant cavity of length 1m, if He-Ne laser operating at wavelength of 6328\AA is
 (a) 3.14×10^6 (b) 1.58×10^6
 (c) 3.16×10^8 (d) None of these
16. For a broken hologram which is 10% of the original, if reconstruction of image is being done, then
 (a) Only 10%of information of the object can be obtained
 (b) Complete information of the object is obtained
 (c) No information of the object can be obtained
 (d) None of these.
17. In case of lasers _____
 (a) At low frequency, stimulated emission exceeds the spontaneous emission
 (b) At low frequency, spontaneous emission exceeds the stimulated emission
 (c) At low frequency, stimulated emission and the spontaneous emission are equal in amount
 (d) None of these are correct
18. For laser, the coherence length is of the order of _____
 (a) several micrometers (b) several meters
 (c) several kilometers (d) several nanometers
19. Which of the following method is not used in optical pumping
 (a) Electrical discharge (b) Direct heating
 (c) Chemical reactions (d) Direct conversion

20. An active medium is a substance which has ____
- (a) Two energy levels (b) Metastable state
(c) High energy state (d) Three energy state
21. Laser transition occurs when atoms Transferring from _____
- (a) excited state to metastable state (b) metastable state to lower state
(c) ground state to metastable state (d) metastable state to excited state
22. Useful recombination of electrons by stimulated emission in the population inversion region is achieved in _____
- (a) He-Ne laser (b) Carbon Dioxide Laser
(c) Semiconductor laser (d) Ruby laser
23. The idea of hologram is proposed by a Nobel Laureate _____
- (a) Leith and Upatniek (b) Dennis Gabor
(c) Einstein (d) Kumar Patel
24. Any atom that has a finite probability per unit time of absorption has an *equal* probability of stimulated emission. This is called _____
- (a) Einstein's relation (b) Laser relation
(c) Active medium (c) None of these
25. In spontaneous emission the emitted photon can move
- (a) in the directions of the field (b) in straight direction
(c) in any random direction (d) not moving
26. Two photons are coherent when
- (a) they travel at the same speed (b) their wavelengths are the same
(c) their phases are the same (d) they obey Planck's equation

III. Numerical Problems

1. A laser beam with Power per pulse is 1 mW lasts 10 ns, if the number of photons emitted per pulse is 3.941×10^7 , calculate the wavelength of laser. [VTU June 2009]
2. A He-Ne laser is emitting a beam with an average power of 4.5 mW. Find the number of photons emitted per second by the laser. The wavelength of the emitted radiation is 6328\AA . [VTU Jan 2008]
3. Find the ratio of population of two energy levels in a Laser if the transition between them produces light of wavelength 694.3 nm. Assume the ambient temperature to be 27°C . [VTU June 2008]

[Hint : $N_2 = N_1 e^{\frac{(E_2 - E_1)}{kT}}$]

4. Find the number of modes of the standing waves and their frequency separation in the resonant cavity of length 1m of He-Ne laser operating at wavelength 632.8 nm. [VTU June 2007]
5. Calculate on the basis of Einstein's theory the number of photons emitted per second by He- Ne laser source light of wavelength 6328 Å with an optical power 10 mW. [VTU June 2010]
6. A laser medium at thermal equilibrium temperature 300 K has two energy levels with a wavelength separation of 1 μm. Find the ratio of population densities of the upper and lower levels. [VTU Jan 2007]

[Hint: $N_2 = N_1 e^{-\frac{(E_2 - E_1)}{kT}}$]

Answers to Multiple Choice Questions

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

OPTICAL FIBERS AND SUPERCONDUCTIVITY

OBJECTIVES

This chapter describes the break through achieved in noiseless communication system using optical fibers which led to Nobel prize in Physics recently during last year 2009. Superconductivity is another phenomenon where materials show zero resistance to the flow of current. Until recently only materials exhibiting superconductivity at very low temperatures have been reported and the practical application of this phenomenon is possible only when the room temperature superconductors with desired properties are available. Optical fibers are today's communication tools which gives high speed, low loss, high bit rate data transfer compared to conventional communication system. The objectives of this chapter are to study

- Fundamentals of Optical Fiber, construction, principle, mechanism of light propagation, acceptance angle, and numerical aperture of optical fibers
- Types of optical fibers and attenuation in fibers
- Applications of optical fibers
- Introduction to Superconductivity, temperature dependence of resistivity
- Effect of magnetic field, Meissner effect, Type I and Type II superconductors, and Temperature dependence of critical field
- BCS theory and High temperature superconductors
- Applications of superconductors- superconducting magnet and Maglev vehicles

6.1 INTRODUCTION TO OPTICAL FIBER

Optical fibers are cylindrical waveguides used to guide light beams over long distances in optical communication system. An optical fiber consists of two concentric cylinders, an inner cylinder called core surrounded by the outer cylinder called cladding as shown in Fig. 6.1. Both the core and the cladding are made of transparent plastic or glass or polymer material that transmits signals in the form of light. Optical fiber use reflections to guide light through a channel. The density of core and cladding must differ sufficiently to reflect the beam of light instead of refracting.

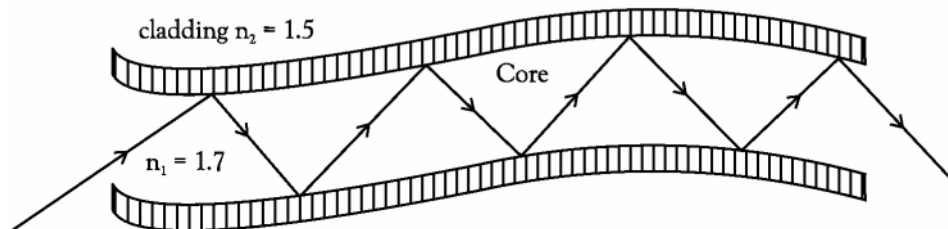


Figure 6.1 Basic structure of an optical fiber

The core is used for guiding a light beam, whereas the cladding (which has a different refractive index) acts as a reflector to prevent the light escaping from the core. Optical fiber uses a light signal instead of electrons, and hence it does not suffer from the various noise problems associated with electronic signals. The signal is usually generated by a laser or Light Emitting Diode (LED). Optical fibers can provide bandwidth to distance ratios in order of 100s of MHz per kilometer. Like other cables, hundreds of optical fibers are usually housed within one cable. They are being increasingly used by telecommunication carriers for long distance digital trunk lines and in backbone networks for internet. Current trends promise that they will replace twisted pair residential loops in the near future. Cable TV companies use a combination of optical fiber and coaxial cable.

Advantages:

1. Higher band width—Optical fibers can support higher bandwidth and hence can transfer data at a higher rate.
2. Less signal attenuation—In optical fibers, the signal transmission distance is greater than the other transmission mediums and signal can travel 60 km without regeneration.
3. Optical fibers are immune to electromagnetic interference.
4. Optical fiber cables are much lighter than the copper cables
5. Optical fiber cables are more immune to tapping than the copper cables.

Disadvantages:

1. Installation or maintenance—Since the technology is new and hence needs expertise to installation and maintenance.
2. Unidirectional - Propagation of light in optical fiber is unidirectional and hence need two fibers for bidirectional communication.
3. Costly—the optical fiber cables and interconnectors used are relatively expensive.

6.1.1 Structure of Optical Fiber

Optical fibers are long, thin strands about the diameter of a human hair. They are arranged in bundles called optical cables.

A single optical fiber has the following parts (Fig. 6.2):

- **Core**—Central thin part of the fiber with higher refractive index where the light travels
- **Cladding**—Outer optical material surrounding the core that reflects the light back into the core.
- **Buffer coating**—Plastic coating that protects the fiber from damage and moisture.
- **Jacket**—Hundreds or thousands of these optical fibers are arranged in bundles in optical cables. The bundles are protected by the cable's outer covering, called a jacket. The jacket is sometimes also formed on buffer coating of single fiber for specific applications.

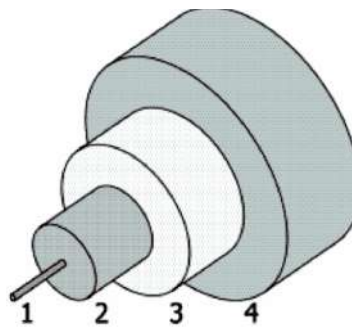


Figure 6.2 *The structure of a typical single-mode fiber*

1. Core: 8 μm diameter
2. Cladding: 125 μm dia.
3. Buffer: 250 μm dia.
4. Jacket: 400 μm dia.

The working of an optical fiber is dependent on the principle of total internal reflection. Light reflects or refracts based on the angle at which it strikes the surface. Restricting the angle at which the light waves are delivered makes it possible to control how efficiently light waves reach their destination. The light waves are directed to the other end of the fiber by being reflected within the core.

The composition of the cladding glass relative to the core glass determines the fiber's ability to reflect light. This reflection is usually caused by creating a higher refractive index in the core of the glass than in the surrounding cladding glass, creating a "waveguide." The refractive index of the core is increased by slightly modifying the composition of the core glass, generally by adding small amounts of a dopant. Alternatively, the waveguide can be created by reducing the refractive index of the cladding using different dopants.

An optical fiber consists of two different types of highly pure, solid glass or polymer, composed to form the core and cladding. A protective acrylate coating called buffer (Fig. 6.2) then surrounds the cladding. In most cases, the protective coating is a dual layer composition.

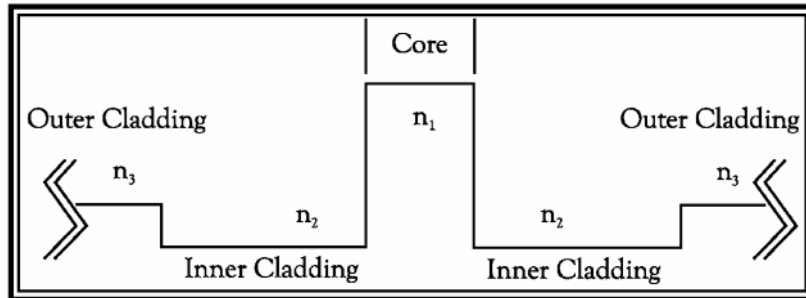


Figure 6.3 Index profile of a depressed-clad fiber design

A class of optical fibers called depressed-clad fibers are made with two different cladding glasses that form an inner and an outer cladding region (Figs. 6.3 and 6.4). The inner cladding region adjacent to the fiber core has an index of refraction that is lower than that of pure-silica, while the outer cladding has an index equal to that of pure silica. Hence, the index of the glass adjacent to the core is depressed.

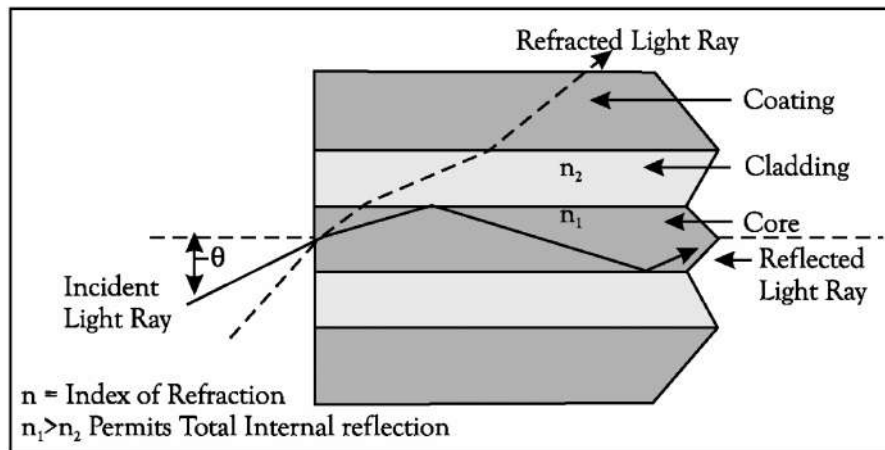


Figure 6.4 Core, cladding and coating

A protective coating is applied to the glass fiber as the final step in the manufacturing process. This coating protects the glass from dust and scratches that can affect fiber strength. This protective coating can be comprised of two layers: a soft inner layer called *buffer* that cushions the fiber and allows the coating to be stripped from the glass mechanically and a harder outer layer called *jacket* that protects the fiber during handling, particularly the cabling, installation, and termination processes (Fig. 6.2).

6.1.2 Principle of Optical fiber

The operation of an optical fiber is based on the principle of total internal reflection. Light reflects (bounces back) or refracts (alters its direction while penetrating a different medium), depending on the angle at which it strikes a surface. The light entered in an optical fiber cable undergoes repeated total internal reflections along the fiber. This is because the angle of incidence is greater than the Critical angle of the fiber material core with respect to the cladding. Critical angle is the angle of incidence in denser medium corresponding to angle of refraction is 90° .

Conditions for total internal reflection:

1. The ray of light must travel from denser medium towards rarer medium.
2. The angle of incidence in the denser medium must be greater than the critical angle for the pair of the media in contact.

Relation between refractive index and critical angle:

Let a ray of light travels from denser medium of refractive index n_1 towards rarer medium of refractive index n_2 with an angle of incidence i_c and angle of refraction 90° as shown in Fig. 6.5. Applying Snell's

law to the interface, $n_1 \sin i_c = n_2 \sin 90^\circ$ or $\frac{n_2}{n_1} = \frac{\sin i_c}{\sin 90^\circ} = \frac{\sin i_c}{1}$

or $\sin i_c = n_2 / n_1$

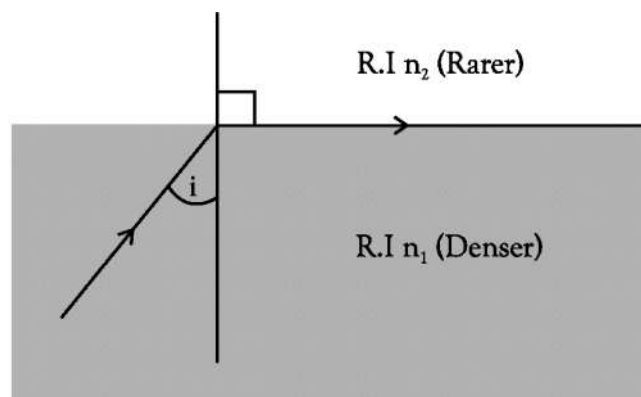


Figure 6.5 Representation of critical angle

Thus $\text{Critical angle, } i_c = \sin^{-1}(n_2/n_1)$... (6.1)

To confine the optical signal in the core, the refractive index of the core must be greater than that of the cladding to support total internal reflection.

6.1.3 Manufacturing of Optical Fibers

Outside Vapor Deposition (OVD) Process is commonly used method of manufacturing optical fibers. Basic OVD optical fiber manufacturing consists of three steps: laydown, consolidation, and draw.

(1) Laydown

In the laydown step, a soot preform is made from ultra pure vapors as they travel through a traversing burner and react in the flame to form fine soot particles of silica or Germania as shown in Fig. 6.6. The OVD process is distinguished by the method of depositing the soot. These particles are deposited on the surface of a rotating target rod. The core material is deposited first, followed by the pure silica cladding. As both core and cladding raw materials are vapor-deposited, the entire preform becomes totally synthetic and extremely pure.

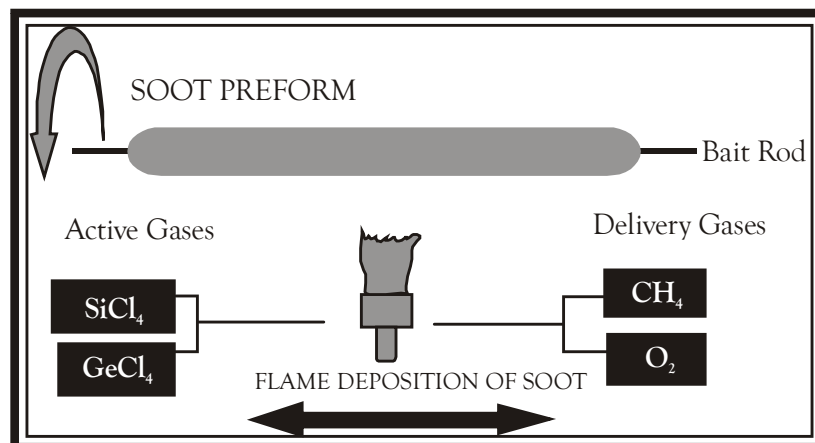


Figure 6.6 OVD laydown process

(2) Consolidation

When deposition is complete, the bait rod is removed from the center of the porous preform, and the preform is placed into a consolidation furnace. During the consolidation process, the water vapor is removed from the preform. This high-temperature consolidation step sinters the preform into a solid, dense, and transparent glass.

(3) The Draw

The finished glass preform is then placed on a draw tower and drawn into one continuous strand of glass fiber (see Fig. 6.7).

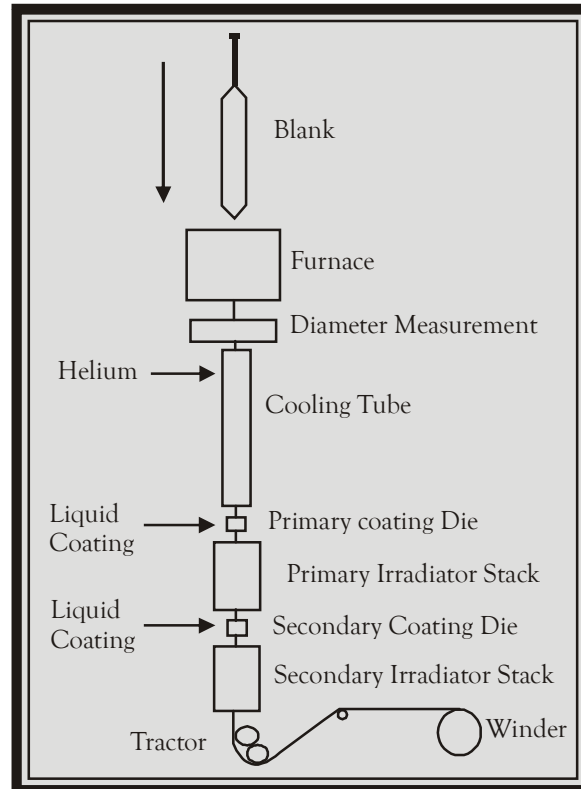


Figure 6.7 *Optical fiber drawing process*

First, the glass blank is lowered into the top of the draw furnace. The tip of the blank is heated until a piece of molten glass, called a gob, begins to fall from the blank like hot taffy. As the gob falls it pulls behind it a thin strand of glass, the beginning of an optical fiber. The gob is cut off, and the fine fiber strand is threaded into a computer controlled tractor assembly and drawn. The assembly speeds up or slows down to precisely control and monitor the size of the fiber's diameter.

The fiber progresses through a diameter sensor that measures the diameter hundreds of times per second to ensure specified outside diameter. Next, the inner and outer primary coatings are applied and cured, using ultraviolet lamps. At the bottom of the draw, the fiber is wound on spools for further processing.

Fiber from these spools is proof-tested and then measured for performance of relevant optical and geometrical parameters. Each fiber has a unique identification number that can be traced to all relevant manufacturing data (including raw materials and manufacturing equipment). Each fiber reel is then placed into protective shipping containers and prepared for shipment to customers worldwide.

6.2 TYPES OF OPTICAL FIBERS

6.2.1 Based on Index

Based on change in refractive index between core and cladding, optical fibers come in two types as Step-index fiber and Graded-index fiber. The boundary between the core and cladding of an optical fiber may either be abrupt, in case *step-index fiber*, or gradual, in case *graded-index fiber*.

1. Step-Index Multimode Fiber:

It has a large core, up to 100 microns in diameter. As a result, some of the light rays that make up the digital pulse may travel a direct route, whereas others zigzag as they bounce off the cladding. These alternative pathways cause the different groupings of light rays, referred to as modes, to arrive separately at a receiving point. The pulse, an aggregate of different modes, begins to spread out, losing its well-defined shape. The need to leave spacing between pulses to prevent overlapping limits bandwidth that is, the amount of information that can be sent. Consequently, this type of fiber is best suited for transmission over short distances, in an endoscope, for instance.

2. Graded-Index Multimode Fiber:

It contains a core in which the refractive index diminishes gradually from the center axis out toward the cladding. The higher refractive index at the center makes the light rays moving down the axis advance more slowly than those near the cladding. Also, rather than zigzagging off the cladding, light in the core curves helically because of the graded index, reducing its travel distance. The shortened path and the higher speed allow light at the periphery to arrive at a receiver at about the same time as the slow but straight rays in the core axis. The result is a digital pulse suffers less dispersion.

6.2.2 Based on Modes of Propagation

Single-Mode and Multi-mode Fibers

There are two general categories of optical fibers based on modes of propagation of optical signal through the fiber. They are single-mode fibers and multimode fibers as shown in Fig. 6.8.

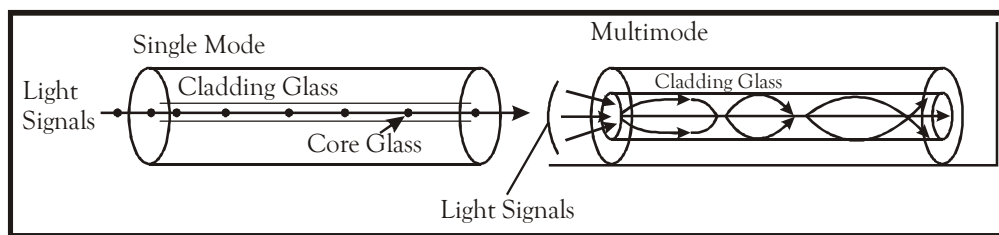


Figure 6.8 Single-mode and multimode fibers

Multimode fiber was the first type of fiber to be commercialized. It has a much larger core than

single-mode fiber, allowing hundreds of modes of light to propagate through the fiber simultaneously. Additionally, the larger core diameter of multimode fiber facilitates the use of lower-cost optical transmitters (such as light emitting diodes [LEDs] or vertical cavity surface emitting lasers [VCSELs]) and connectors.

Single-mode fiber, on the other hand, has a much smaller core that allows only one mode of light at a time to propagate through the core. While it might appear that multimode fibers have higher capacity, in fact the opposite is true. Single mode fibers are designed to maintain spatial and spectral integrity of each optical signal over longer distances, allowing more information to be transmitted.

Its tremendous information-carrying capacity and low intrinsic loss have made single-mode fiber the ideal transmission medium for a multitude of applications. Single-mode fiber is typically used for longer-distance and higher-bandwidth applications. Multimode fiber is used primarily in systems with short transmission distances (under 2 km), such as premises communications, private data networks, and parallel optic applications.

Optical Fiber Sizes

The international standard for outer cladding diameter of most single-mode optical fibers is 125 μm for the glass and 245 μm for the coating. This standard is important because it ensures compatibility among connectors, splices, and tools used throughout the industry.

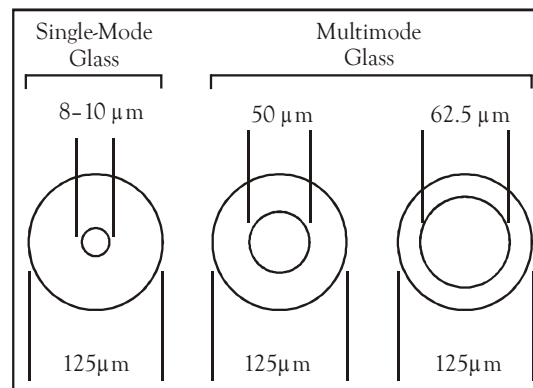


Figure 6.9 Dimension of fibres

Standard single-mode fibers are manufactured with a small core size, approximately 8 to 10 μm in diameter. Multimode fibers have core sizes of 50 to 62.5 μm in diameter as shown in Fig. 6.9.

6.3 PROPAGATION MECHANISM IN OPTICAL FIBERS

Fig. 6.10 shows the mechanism of optical pulse propagation in step-index, graded-index, and single mode optical fiber. Compared to step-index and graded-index fibers, the single-mode fiber provides output pulse with less attenuation and broadening.

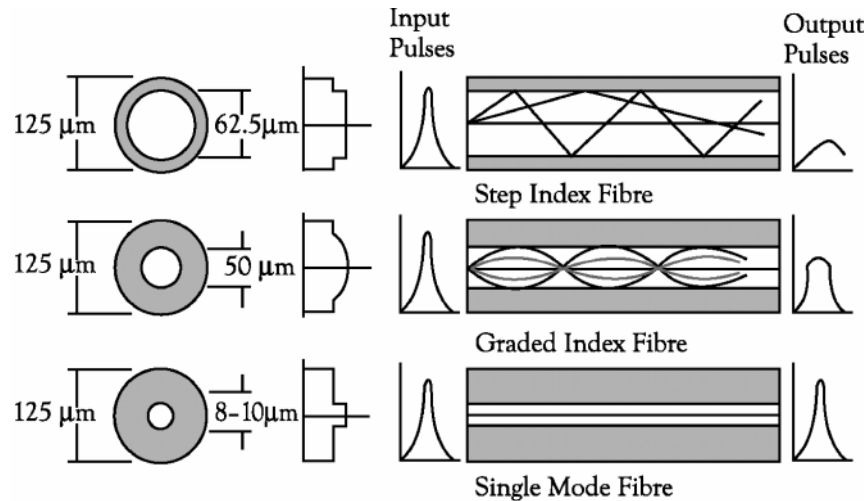


Figure 6.10 Optical fiber types & propagation mechanisms

6.3.1 Angle of Acceptance

When light traveling in a dense medium hits a boundary at a steep angle (larger than the “critical angle” for the boundary), the light will be completely reflected. This effect is used in optical fibers to confine light in the core. Light travels along the fiber bouncing back and forth off of the boundary. Because the light must strike the boundary with an angle greater than the critical angle, only light that enters the fiber within a certain range of angles can travel down the fiber without leaking out. This range of angles is called the acceptance cone of the fiber. The size of this acceptance cone is a function of the refractive index difference between the fiber’s core and cladding. The half-angle of this acceptance cone is called the acceptance angle, θ_{\max} as shown in Fig. 6.11.

6.3.2 Numerical Aperture

The angle of acceptance is the maximum angle from the fiber axis at which light may enter the fiber so that it will propagate in the core of the fiber without any refraction to the cladding. The sine of the angle of acceptance is called the numerical aperture (NA) of the fiber. Fiber with a larger NA requires less precision to splice and work with than fiber with a smaller NA. Single-mode fiber has a small NA. Numerical Aperture of a fiber in air = $\sin \theta_{\max}$.

For step-index multimode fiber, the acceptance angle is determined only by the indices of refraction :

$$n \sin \theta_{\max} = \sqrt{n_1^2 - n_2^2} \quad \dots(6.2)$$

where n_1 is the refractive index of the fiber core, and n_2 is the refractive index of the cladding, and n is the refractive index of outer medium (air) and is usually equal to 1.

Proof:

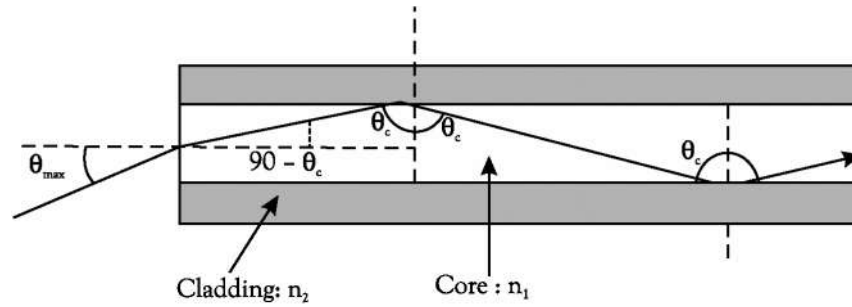


Figure 6.11 Propagation of light in a fiber

When a light ray is incident from a medium of refractive index n to the core of index n_1 as shown in Fig. 6.11, Snell's law at medium-core interface gives

$$n \sin \theta_i = n_1 \sin \theta_r \quad \dots(6.3)$$

From the above Fig. 6.11 and using trigonometry, we get:

$$\sin \theta_r = \sin (90^\circ - \theta_c) = \cos \theta_c$$

where $\theta_c = \sin^{-1} \frac{n_2}{n_1}$ is the critical angle for total internal reflection.

Substituting for $\sin \theta_r$ in Snell's law (Eqn. 6.3), we get:

$$\frac{n}{n_1} \sin \theta_i = \cos \theta_c. \quad \dots(6.4)$$

By squaring both sides

$$\frac{n^2}{n_1^2} \sin^2 \theta_i = \cos^2 \theta_c = 1 - \sin^2 \theta_c = 1 - \frac{n_2^2}{n_1^2}$$

$$n^2 \sin^2 \theta_i = n_1^2 \left(1 - \frac{n_2^2}{n_1^2} \right) = (n_1^2 - n_2^2)$$

Taking square root on both sides, we get,

$$n \sin \theta_i = \sqrt{n_1^2 - n_2^2}, \quad \dots(6.5)$$

This has the same form as the numerical aperture in other optical systems, so it has become common to define the NA of any type of fiber to be

$$NA = \sqrt{n_1^2 - n_2^2} \quad \dots(6.6)$$

where n_1 is the refractive index along the central axis of the fiber. Note that when this definition is used, the connection between the NA and the acceptance angle of the fiber becomes only an approximation. In particular, manufacturers often quote “NA” for single-mode fiber based on this formula, even though the acceptance angle for single-mode fiber is quite different and cannot be determined from the indices of refraction alone. The fractional index change when the signal propagates in the

fiber is given by, $\Delta = \frac{n_1 - n_2}{n_1}$.

The number of bound modes (or the mode volume) is related to the normalized frequency and thus to the NA.

In multimode fibers, the term *equilibrium numerical aperture* is sometimes used. This refers to the numerical aperture with respect to the extreme exit angle of a ray emerging from a fiber in which equilibrium mode distribution has been established.

6.3.3 Fibre Parameter or Normalised Frequency - “V”

One often quoted and very useful measure of an optical fiber is usually called the “V” number. In some texts it is called the “normalised frequency” and in others just the “dimensionless fiber parameter”. V summarizes all of the important characteristics of a fiber in a single number. It can be used directly to determine whether the fiber is single-moded or not at a particular wavelength and also to calculate the number of possible bound modes. In addition, it can be used to calculate the spot size, the cutoff wavelength, and even chromatic dispersion. However, it is important to note that V incorporates the wavelength that we are using on the fiber and so to some extent it is a measure of a fiber within the context of a system rather than the fiber alone.

$$V = \frac{\pi d}{\lambda} \sqrt{n_{\text{core}}^2 - n_{\text{cladding}}^2} = \frac{\pi d}{\lambda} NA \quad \dots(6.7)$$

Where, d = core diameter, λ = wavelength, n = refractive index, and NA = numerical aperture. If $V \leq 2.405$ the fibre will be single-moded at the wavelength used to calculate V.

For the multimode situation the number of modes (N) may be calculated as follows:

$$N = \frac{V^2}{2} \text{ for Step Index Fiber}$$

$$N = \frac{V^2}{4} \text{ for Graded Index Fiber}$$

6.4 ATTENUATION IN FIBERS

Attenuation in optical fibers, also known as transmission loss, is the reduction in intensity of the light beam (or signal) with respect to distance traveled through a transmission medium. Attenuation coefficients in fiber optics usually use units of dB/km through the medium due to the relatively high quality of transparency of modern optical transmission media. Attenuation is an important factor limiting the transmission of a digital signal in the form of light rays across large distances. Thus, much research has gone into both limiting the attenuation and maximizing the amplification of the optical signal through the fiber. Empirical research has shown that attenuation in optical fiber is caused primarily by both scattering and absorption.

Light Scattering

The propagation of light through the core of an optical fiber is based on total internal reflection of the light wave. Rough and irregular surfaces, even at the molecular level, can cause light rays to be reflected in random directions. This is called diffuse reflection or scattering, and it is typically characterized by wide variety of reflection angles (Fig. 6.12).

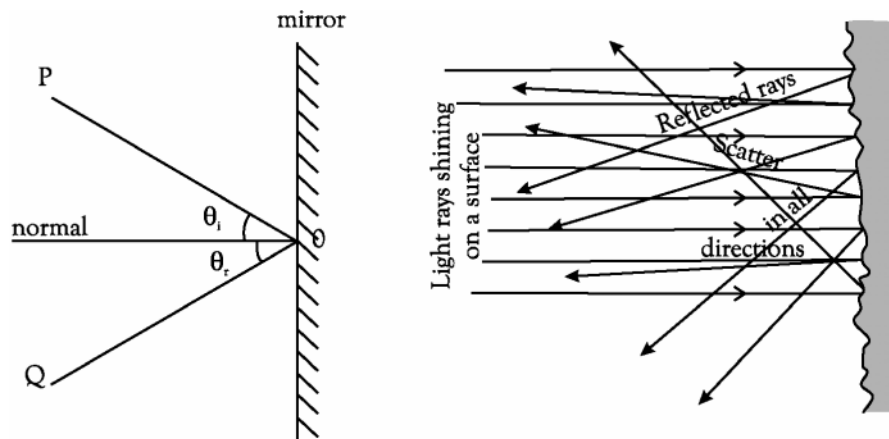


Figure 6.12 (a) *Specular reflection*, (b) *Diffuse reflection*

Light scattering depends on the wavelength of the light being scattered. Thus, limits to spatial scales of visibility arise, depending on the frequency of the incident light-wave and the physical dimension (or spatial scale) of the scattering center, which is typically in the form of some specific micro-structural feature. Since visible light has a wavelength of the order of one micron (one millionth of a meter) scattering centers will have dimensions on a similar spatial scale.

Thus, attenuation results from the incoherent scattering of light at internal surfaces and interfaces. In (poly)crystalline materials such as metals and ceramics, in addition to pores, most of the internal

surfaces or interfaces are in the form of grain boundaries that separate tiny regions of crystalline order. It has recently been shown that when the size of the scattering center (or grain boundary) is reduced below the size of the wavelength of the light being scattered, the scattering no longer occurs to any significant extent. This phenomenon has given rise to the production of transparent ceramic materials.

Similarly, the scattering of light in optical quality glass fiber is caused by molecular level irregularities (compositional fluctuations) in the glass structure. Indeed, one emerging school of thought is that a glass is simply the limiting case of a polycrystalline solid. Within this framework, “domains” exhibiting various degrees of short-range order become the building blocks of both metals and alloys, as well as glasses and ceramics. Distributed both between and within these domains are micro-structural defects which will provide the most ideal locations for the occurrence of light scattering. This same phenomenon is seen as one of the limiting factors in the transparency of IR missile domes.

At high optical powers, scattering can also be caused by nonlinear optical processes in the fiber.

UV-Vis-IR absorption

In addition to light scattering, attenuation or signal loss can also occur due to selective absorption of specific wavelengths, in a manner similar to that responsible for the appearance of color. Primary material considerations include both electrons and molecules as follows:

- (1) At the electronic level, it depends on whether the electron orbitals are spaced (or “quantized”) such that they can absorb a quantum of light (or photon) of a specific wavelength or frequency in the ultraviolet (UV) or visible ranges. This is what gives rise to color.
- (2) At the atomic or molecular level, it depends on the frequencies of atomic or molecular vibrations or chemical bonds, how close-packed its atoms or molecules are, and whether or not the atoms or molecules exhibit long-range order. These factors will determine the capacity of the material transmitting longer wavelengths in the infrared (IR), far IR, radio and microwave ranges.

The design of any optically transparent device requires the selection of materials based upon knowledge of its properties and limitations. The lattice absorption characteristics observed at the lower frequency regions (mid IR to far-infrared wavelength range) define the long-wavelength transparency limit of the material. They are the result of the interactive coupling between the motions of thermally induced vibrations of the constituent atoms and molecules of the solid lattice and the incident light wave radiation. Hence, all materials are bounded by limiting regions of absorption caused by atomic and molecular vibrations (bond-stretching) in the far-infrared ($>10\ \mu\text{m}$).

Thus, multi-phonon absorption occurs when two or more phonons simultaneously interact to produce electric dipole moments with which the incident radiation may couple. These dipoles can absorb energy from the incident radiation, reaching a maximum coupling with the radiation when the frequency is equal to the fundamental vibrational mode of the molecular dipole (e.g. Si-O bond) in the far-infrared, or one of its harmonics.

The selective absorption of infrared (IR) light by a particular material occurs because the selected frequency of the light wave matches the frequency (or an integral multiple of the frequency) at which the

particles of that material vibrate. Since different atoms and molecules have different natural frequencies of vibration, they will selectively absorb different frequencies (or portions of the spectrum) of infrared (IR) light.

Reflection and transmission of light waves occur because the frequencies of the light waves do not match the natural resonant frequencies of vibration of the objects. When IR light of these frequencies strikes an object, the energy is either reflected or transmitted.

The groundbreaking event happened in around 1965, Charles K. Kao and George A. Hockham of the British company Standard Telephones and Cables (STC) were the first to promote the idea that the attenuation in optical fibers could be reduced below 20 decibels per kilometer (dB/km), allowing fibers to be a practical medium for communication. They proposed that the attenuation in fibers available at the time was caused by impurities, which could be removed, rather than fundamental physical effects such as scattering. They correctly and systematically theorized the light-loss properties for optical fiber, and pointed out the right material to manufacture such fibers - silica glass with high purity. This discovery led to Kao being awarded the Nobel Prize in Physics in 2009.

Attenuations in modern optical cables are far less than those in electrical copper cables, leading to long-haul fiber connections with repeater distances of 70–150 kilometers (43–93 miles). The **erbium-doped** fiber amplifier, which reduced the cost of long-distance fiber systems by reducing or even in many cases eliminating the need for optical-electrical-optical repeaters, was co-developed by teams led by David N. Payne of the University of Southampton, and Emmanuel Desurvire at Bell Labs in 1986.

6.5 APPLICATIONS OF OPTICAL FIBERS

6.5.1 Fiber Optic Communications

Optical fiber is the basic building block for a fiber optic based network. A model of this simple link is shown in Fig. 6.13.

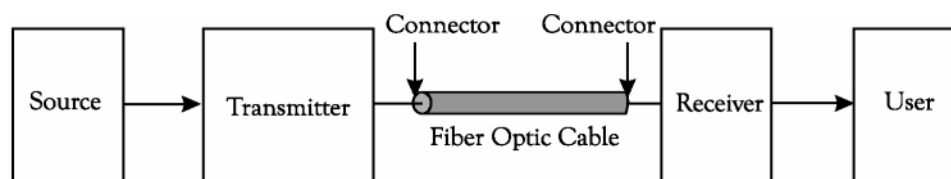


Figure 6.13 Block diagram of point to point fiber optic communication

The above illustration (Fig. 6.13) indicates the Source-User pair, Transmitter and Receiver. It also clearly shows the fiber optic cable constituting the Transmission Medium as well as the connectors that provide the interface of the Transmitter to the Transmission Medium and the Transmission Medium to the Receiver. All of these are components of the simple fiber optic data link.

Optical fiber can be used as a medium for telecommunication and networking because it is flexible and can be bundled as cables. It is especially advantageous for long-distance communications, because

light propagates through the fiber with little attenuation compared to electrical cables. This allows long distances to be spanned with few repeaters. Additionally, the per-channel light signals propagating in the fiber have been modulated at rates as high as 111 gigabits per second. Each fiber can carry many independent channels, each using a different wavelength of light using a technique called wavelength-division multiplexing (WDM)).

Advantages of Optical Fibers:

Optical fibers are used in information and data transmission for short & long distance communication due to following advantages :

1. Large bandwidth so that several thousand voice & data channels can be simultaneously transmitted in a single fiber.
2. Light in weight and small in size, particularly in underwater cables.
3. No possibility of internal noise and cross-talk generation.
4. Lower cost of cables per unit length and no hazards of short circuits as in metal wires.
5. Better signal security & immunity to adverse temperature and moisture conditions.

Limitations of Optical Fibers:

1. The optic connectors used to connect (splicing) two fibers are highly expensive. Splicing is a skilful task, which if not done precisely, the signal loss will be so much that it is virtually a break in the communication line.
2. While system modification is made, or because of accidents, a fiber may suffer line break. Operations required to re-establish the connections are highly skilful and time consuming. This results in escalation of maintenance costs.
3. Though fibers could be bent to circles of few centimeters radius, they may break when bent to still smaller curvatures. Also for small curvature bends, the loss becomes considerable.
4. Fibers undergo expansion and contraction with temperature that upset some critical alignments which lead to loss in signal power.

6.5.2 Fiber Optic Sensors

Fibers have many uses in remote sensing. In some applications, the sensor is itself an optical fiber. In other cases, fiber is used to connect a non-fiberoptic sensor to a measurement system. Depending on the application, fiber may be used because of its small size, or the fact that no electrical power is needed at the remote location, or because many sensors can be multiplexed along the length of a fiber by using different wavelengths of light for each sensor, or by sensing the time delay as light passes along the fiber through each sensor. Time delay can be determined using a device such as an optical time-domain reflectometer.

Optical fibers can be used as sensors to measure strain, temperature, pressure and other quantities by modifying a fiber so that the quantity to be measured modulates the intensity, phase, polarization, wavelength or transit time of light in the fiber. Sensors that vary the intensity of light are the simplest, since only a simple source and detector are required. A particularly useful feature of such fiber optic sensors is that they can, if required, provide distributed sensing over distances of up to one meter.

Extrinsic fiber optic sensors use an optical fiber cable, normally a multi-mode one, to transmit modulated light from either a non-fiber optical sensor, or an electronic sensor connected to an optical transmitter. A major benefit of extrinsic sensors is their ability to reach places which are otherwise inaccessible. An example is the measurement of temperature inside aircraft jet engines by using a fiber to transmit radiation into a radiation pyrometer located outside the engine. Extrinsic sensors can also be used in the same way to measure the internal temperature of electrical transformers, where the extreme electromagnetic fields present make other measurement techniques impossible. Extrinsic sensors are used to measure vibration, rotation, displacement, velocity, acceleration, torque, and twisting.

6.5.3 Other Applications of Optical Fibers

1. **Illumination:** Fibers are widely used in illumination applications. They are used as light guides in medical and other applications where bright light needs to be shone on a target without a clear line-of-sight path. In some buildings, optical fibers are used to route sunlight from the roof to other parts of the building. Optical fiber illumination is also used for decorative applications, including signs, art, and artificial Christmas trees.
2. **Imaging Optics:** Optical fiber is also used in imaging optics. A coherent bundle of fibers is used, sometimes along with lenses, for a long, thin imaging device called an endoscope, which is used to view objects through a small hole. Medical endoscopes are used for minimally invasive exploratory or surgical procedures (endoscopy). Industrial endoscopes (like fiberscope or borescope) are used for inspecting anything hard to reach, such as jet engine interiors.
3. **Spectroscopy:** In spectroscopy, optical fiber bundles are used to transmit light from a spectrometer to a substance which cannot be placed inside the spectrometer itself, in order to analyze its composition. A spectrometer analyzes substances by bouncing light back and forth through them. By using fibers, a spectrometer can be used to study objects that are too large to fit inside, or gasses, or reactions which occur in pressure vessels.
4. **Laser Gain Medium:** An optical fiber doped with certain rare earth elements such as erbium can be used as the gain medium of a laser or optical amplifier. Rare-earth doped optical fibers can be used to provide signal amplification by splicing a short section of doped fiber into a regular (undoped) optical fiber line. The doped fiber is optically pumped with a second laser wavelength that is coupled into the line in addition to the signal wave. Both wavelengths of light are transmitted through the doped fiber, which transfers energy from the second pump wavelength to the signal wave. The process that causes the amplification is stimulated emission.

Table 6.1 Attenuation and Bandwidth characteristics of different fiber optic cable candidates

| Mode | Material | Index of Refraction Profile | λ microns | Size (microns) | Atten. dB/km | Bandwidth MHz/km |
|-------------|----------|-----------------------------|-------------------|----------------|--------------|------------------|
| Multi-mode | Glass | Step | 800 | 62.5/125 | 5.0 | 6 |
| Multi-mode | Glass | Step | 850 | 62.5/125 | 4.0 | 6 |
| Multi-mode | Glass | Graded | 850 | 62.5/125 | 3.3 | 200 |
| Multi-mode | Glass | Graded | 850 | 50/125 | 2.7 | 600 |
| Multi-mode | Glass | Graded | 1300 | 62.5/125 | 0.9 | 800 |
| Multi-mode | Glass | Graded | 1300 | 50/125 | 0.7 | 1500 |
| Multi-mode | Glass | Graded | 850 | 85/125 | 2.8 | 200 |
| Multi-mode | Glass | Graded | 1300 | 85/125 | 0.7 | 400 |
| Multi-mode | Glass | Graded | 1550 | 85/125 | 0.4 | 500 |
| Multi-mode | Glass | Graded | 850 | 100/140 | 3.5 | 300 |
| Multi-mode | Glass | Graded | 1300 | 100/140 | 1.5 | 500 |
| Multi-mode | Glass | Graded | 1550 | 100/140 | 0.9 | 500 |
| Multi-mode | Plastic | Step | 650 | 485/500 | 240 | 5 @ 680 |
| Multi-mode | Plastic | Step | 650 | 735/750 | 230 | 5 @ 680 |
| Multi-mode | Plastic | Step | 650 | 980/1000 | 220 | 5 @ 680 |
| Multi-mode | PCS | Step | 790 | 200/350 | 10 | 20 |
| Single-mode | Glass | Step | 650 | 3.7/80 or 125 | 10 | 600 |
| Single-mode | Glass | Step | 850 | 5/80 or 125 | 2.3 | 1000 |
| Single-mode | Glass | Step | 1300 | 9.3/125 | 0.5 | * |
| Single-mode | Glass | Step | 1550 | 8.1/125 | 0.2 | * |

* Too high to measure accurately. Effectively infinite.

6.5.4 Advantages of Optical Fibre Communication

The advantages of optical fiber communication system over the existing coaxial cable system are discussed in the following subsections.

Easy handling

Optical fibres are typically about a 100 μm in diameter and are basically made of silica or glass. This results in a heavy reduction in weight and in volume of space required, which is an important consideration

for laying cables in already crowded available conditions. This saving in weight and volume is also important for shipboard applications and data handling using optical fibres in aircraft.

Low transmission loss and wide bandwidth

Optical fibres have lower transmission losses and wider bandwidths than those of coaxial wires. This means that with optical fibre cable systems more data can be transmitted over long distances, thereby decreasing the number of wires and reducing the number of repeaters needed for these spans. The reduction in equipment and components decrease the system's cost and complexity.

Immunity to interference

Optical fibres are immune to electromagnetic interference such as inductive pick-ups from signal-carrying wires and lightning. Hence there will be no cross talk. This is an important consideration for secure communications in defence.

Electrical isolation

Optical fibres can be used in explosive as well as high-voltage environments due to the absence of any hazard caused by short-circuit etc. As optical fibres are constructed of glass, which is an insulator, use of fibres in an electrically-hazardous environment is not going to create any problem since the fibre creates no arcing or sparking.

Signal security

By using an optical fibre a high-degree of security is afforded since the optical signal is well confined within the waveguide. This makes optical fibre communication more attractive in applications where information security is important such as banking, computer networks and military applications.

Abundant raw material

The raw material silica used in fabrication of optical fiber is abundant and inexpensive since it is found in sand.

Noise-free transmission

The optical fiber communication is noise-free unlike electrical signal transmission.

Longer life span

Optical fibres have a life span of about 20-30 years while copper cables have a life span of 12-15years.

Easy maintenance

Optical fibres are more reliable and easier to maintain than copper cables.

6.6 INTRODUCTION TO SUPERCONDUCTIVITY

Electrical conductors show some extent of resistance to the flow of charge through them at ordinary temperatures. At very low temperatures, however, most metals, many alloys, and some chemical compounds

all allow current to pass freely through them. This phenomenon is called superconductivity. Superconductivity occurs when the resistance of a sample falls suddenly to zero at some critical temperature or transition temperature T_c (Fig. 6.14).

Superconductivity was discovered in 1911 by the Dutch physicist Heike Kamerlingh Onnes. He found that, down to 4.15 K, the resistance of a mercury sample decreased with temperature as other metals do. The critical temperature T_c for other superconducting elements varies from less than 0.1 K to nearly 10 K, and it is significant that the elements which are ordinarily good conductors, such as copper and silver, do not become superconducting when cooled. The highest critical temperatures, as much as 134 K, are found in certain ceramic materials.

To know whether, the superconductors actually have zero resistance or just very low resistance, an experiment has been done in which, a current carrying superconductor wire loop is observed for several years for its magnetic field. No decrease in such currents has ever been found and this shows that superconductors do not have resistance at all.

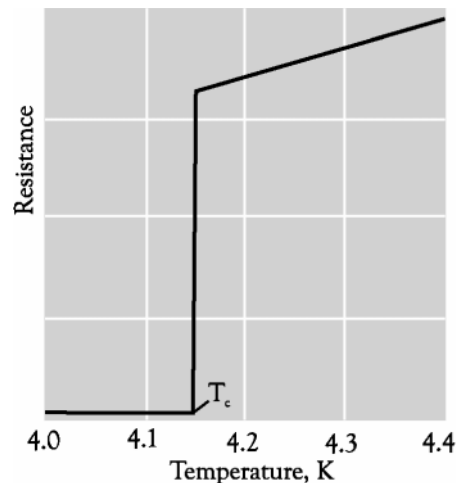


Figure 6.14 Resistance of Hg sample at low temperature. Below critical temperature $T_c = 4.14$ K, Hg shows zero electrical resistance

6.6.1 Temperature dependence of resistivity in superconducting materials

Experimental Observations:

- (1) **Effect of Impurity:** When impurities are added to superconducting material, the superconducting property is not lost but the transition temperature T_c is lowered.
- (2) **Isotope effect:** It has been observed that the critical temperature of superconductors varies with isotopic mass. In mercury, T_c varies from 4.185 K to 4.146 K as the average atomic mass

N varies from 199.5 to 203.4 atomic mass units. The experimental results within each series of isotopes may be fitted by a relation of the form $M^\alpha \cdot T_C = \text{constant}$. Here α is a number usually 0.5. From the dependence of T_C on the isotopic mass M , we learn that lattice vibrations and hence electron-lattice interactions are deeply involved in superconductivity.

- (3) **Effect on thermal properties:** The thermal properties such as the specific heat capacity and thermal conductivity of a substance change abruptly, when it passes over into the superconducting state.
- (4) **Persistent currents:** If a super conductor has the form of a ring, current can be induced in it by electromagnetic induction. The resistivity of a superconductor is usually measured by observing this current as a function of time. If the sample is in the normal state, the current damps out quickly because of the resistance of the ring. But if the ring has zero resistance, the current once set up, flows indefinitely without any decrease in value. In typical experiment, a lead ring could carry an induced current of several hundred amperes for over a year without any change. Such currents are called 'persistent currents'. Physicists found that the upper limit for the resistivity of a superconducting lead ring is about 10^{-25} ohm-m . Since this value is very low, it justifies taking $\rho = 0$ for the superconducting state.
- (5) **Destruction of superconductivity by Magnetic fields:** Superconductivity can be destroyed by the application of a magnetic field. If a strong enough magnetic field, called the *critical field*, is applied to a superconducting specimen, it becomes normal and recovers its normal resistivity even at $T < T_C$. The critical value of the applied magnetic field for the destruction of superconductivity is denoted by $H_C(T)$ and is a function of the temperature. For a given substance, value of H_C decreases as the temperature increases from $T = 0 \text{ K}$ to $T = T_C$. The variation can be represented by the formula $H_C(T) = H_C(0) [1 - (T/T_C)^2]$, where $H_C(0)$ is the critical field at 0 K. Thus the field has its maximum value $H_C(0)$ at $T = 0 \text{ K}$. At the critical temperature T_C , the critical field is zero i.e., $H_C(T_C) = 0$.
- (6) **Generation of Intense Magnetic field:** If the core of an electromagnet is wound with a coil of superconducting material, large current can be maintained in the coil without Joule heating. Thus very intense magnetic fields can be produced. Magnetic fields of the order of 10 T can be produced in this manner.

6.7 EFFECT OF MAGNETIC FIELD

6.7.1 Meissner Effect

At critical temperature T_C magnetic field lines are completely expelled from the interior to give $B = 0$ inside the superconductor, a phenomenon known as the Meissner effect.

Before 1933, it was assumed that superconductivity was a manifestation of perfect conductivity. If a perfect conductor is cooled below its critical temperature in the presence of an applied magnetic field, the field should be trapped in the interior of the conductor even after the external field is removed. In addition, the final state of the perfect conductor should depend on which occurs first, the application of the field or the cooling to below T_C . If the field is applied after the material has been cooled, the field

should be expelled from the superconductor. If the field is applied before the material is cooled, the field should not be expelled once the material has been cooled. In 1933, however, W. Hans Meissner and Robert Ochsenfeld discovered that when a metal becomes superconducting in the presence of a weak magnetic field, the field is expelled. Thus, the same final state $B = 0$ is achieved whether the field is applied before or after the material is cooled below its critical temperature.

Meissner and Ochsenfeld found that if a superconductor is cooled in a magnetic field to below the transition temperature (T_c), then at the transition, the lines of induction B are pushed out (Fig. 6.15).

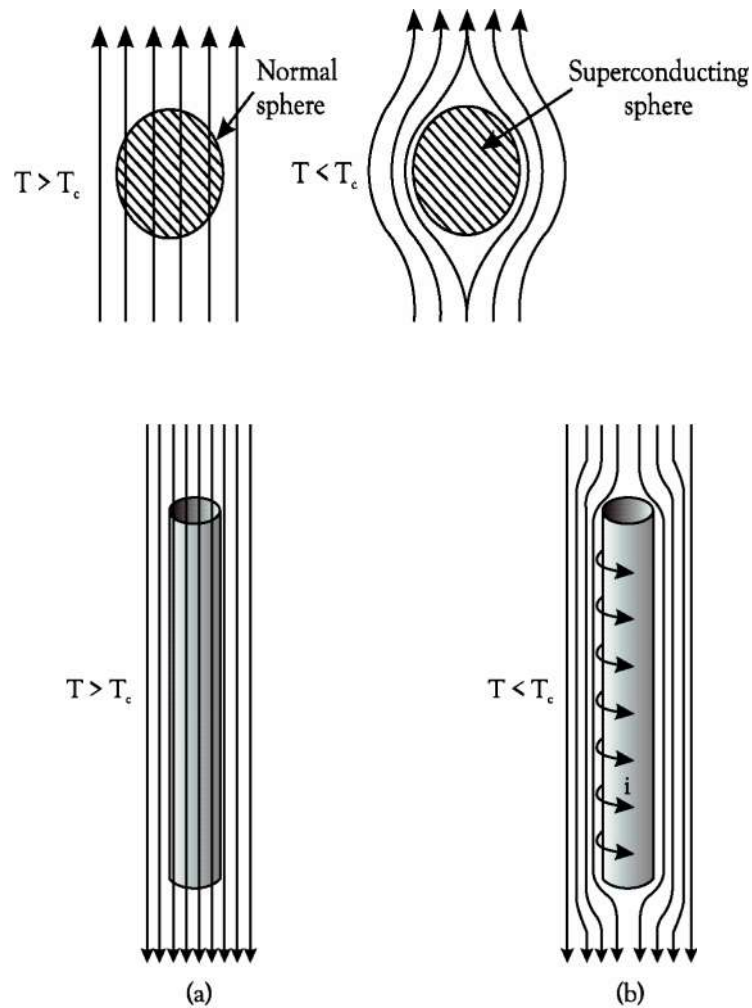


Figure 6.15 Demonstration of Meissner effect

The expulsion of magnetic *flux* from the interior of a piece of superconducting material as the material undergoes the transition to the superconducting phase is known as Meissner effect.

6.7.2 Type I and Type II Superconductors

Superconductors are classified into two types as Type I and Type II based on their behavior of magnetization with external applied magnetic field.

Type I (or Soft) Superconductors:

If we apply magnetic field across certain types of superconductors, at certain magnetic field, called critical magnetic field, H_C , the superconducting property of the material disappears abruptly and the applied magnetic field penetrates completely into the material. Such superconductors are called Type I superconductors. The magnetization curve for Type I superconductors is shown in Fig. 6.16. The magnetization curve shows that the transition at H_C is reversible. i.e., if the magnetic field is reduced below H_C , the material again gains the superconducting property and the magnetic field is expelled from the material. Most of the pure metals like lead, tin, mercury, aluminum etc. are the examples of Type I superconductors. It is found that the critical magnetic field H_C depends on the material of superconductor and its temperature. The critical field H_C would be maximum at 0 K.

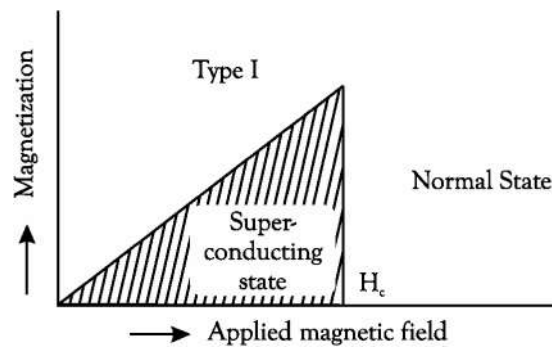


Figure 6.16 Magnetization curve for Type I superconductors

Type II (or Hard) Superconductors:

The superconducting materials which exhibit the magnetization curve as shown in Fig. 6.17 are called Type II or hard superconductors. Alloys of transition metals with high values of resistivity in the normal state fall under this type of superconductors. Such materials have two critical magnetic fields, H_{C1} and H_{C2} . For an applied magnetic field less than H_{C1} , a type II superconductor behaves just like its Type I counterpart when $H < H_{C1}$, and it is superconducting with no magnetic field in its interior. When $H > H_{C2}$, a type II superconductor exhibit normal behavior, again like Type I superconductor. However, in applied fields between H_{C1} and H_{C2} , a Type II superconductor is in a mixed state in which it contains some magnetic flux but is superconducting. The stronger the external field, the more flux penetrates the material, up to the higher critical field H_{C2} .

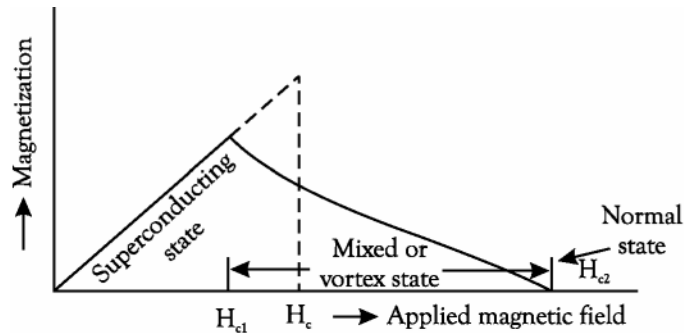


Figure 6.17 Magnetization curve of Type II or hard superconductors

A type II superconductor behaves as though it consists of filaments of normal and of superconducting matter mixed together. A magnetic field can exist in normal filaments, while the superconducting filaments are diamagnetic and resistance less like Type I superconductors. Since H_{C2} can be quite high (Table 6.2), Type II superconductors are used to make high field (up to 20 T) magnets for particle accelerators, fusion reactors, magnetic resonant imagery, experimental maglev (magnetic levitation) trains in which magnetic forces provide both propulsion and frictionless support.

Table 6.2 Critical temperatures and Upper critical magnetic fields (at $T=0$) of some Type II superconductors:

| Superconductor | T_c (K) | $H_{C2}(0)$ Tesla |
|----------------|-----------|-------------------|
| Nb_3Sn | 18.0 | 24.5 |
| Nb_3Ge | 23.2 | 38 |
| Nb_3Al | 18.7 | 32.4 |
| $Nb_3(AlGe)$ | 20.7 | 44 |
| V_3Ge | 14.8 | 2.08 |
| V_3Si | 16.9 | 2.35 |
| $PbMoS$ | 14.4 | 6.0 |

6.7.3 Temperature Dependence of Critical Field

In a series of experiments on superconducting cylinders, Meissner and Ochsenfeld demonstrated that, as the temperature is lowered to T_c , the flux is suddenly and completely expelled, as the specimen becomes superconducting, as shown in Fig. 6.15. The flux expulsion continues for all $T < T_c$. They established this by carefully measuring the magnetic field in the neighborhood of the specimen. Further, they demonstrated that the effect is *reversible*. When the temperature is raised from below T_c the flux suddenly penetrates the specimen after it reaches T_c and the substance is in the normal state.

A bulk super conductor behaves in an external magnetic field as if inside the specimen $B = \mu_0 (H+M) = \mu_0(1 + \chi) H=0$. (Here M = magnetization in the medium and χ its magnetic susceptibility). Hence $\chi = -1$ i.e., a super conductor exhibits *perfect diamagnetism*.

Table 6.3 Critical Temperatures for Various Superconductors

| Material | T_c (K) |
|--|-----------|
| Zn | 0.88 |
| Al | 1.19 |
| Sn | 3.72 |
| Hg | 4.15 |
| Pb | 7.18 |
| Nb | 9.46 |
| Nb ₃ Sn | 18.05 |
| Nb ₃ Ge | 23.2 |
| YBa ₂ Cu ₃ O ₇ | 92 |
| Bi–Sr–Ca–Cu–O | 105 |
| Tl–Ba–Ca–Cu–O | 125 |
| HgBa ₂ Ca ₂ Cu ₃ O ₈ | 134 |

6.8 BCS THEORY

The modern theory of superconductivity was promulgated by Bardeen, Cooper, and Schrieffer in 1957. Starting from first principles, and employing a completely quantum treatment, the BCS theory explains the various observable effects, such as zero resistance, the Meissner effect etc. This theory led to a Nobel Prize in Physics for the three scientists in 1972 (the second Nobel prize for Bardeen!, first Nobel prize for semiconductor transistor invention). In an ordinary metal, the electrical resistance is the result of the collisions of the conduction electrons with the vibrating ions in the crystal lattice. In the superconducting state, the forces of attraction between the conduction electrons exceed the force of electrostatic repulsion.

BCS theory explains superconductivity in terms of the formation of pairs of free electrons, called Cooper pairs. Cooper pairs can move unhindered through the lattice without scattering from lattice ions.

In this theory, two electrons can interact via distortions in the array of lattice ions so that there

is a net attractive force between the electrons. As a result, the two electrons are bound into an entity called a Cooper pair. The Cooper pair behaves like a particle with integral spin. Recall that particles with integral spin are *bosons*. (Particles with half-integer spins are *fermions*.) An important feature of bosons is that they *do not* obey the Pauli exclusion principle. Consequently, at very low temperatures, it is possible for all bosons in a collection of such particles to be in the lowest quantum state. As a result, the entire collection of Cooper pairs in the metal is described by a single wavefunction. Above the energy level associated with this wavefunction is an energy gap equal to the binding energy of a Cooper pair. Under the action of an applied electric field, the Cooper pairs experience an electric force that causes them to move through the metal. A random-scattering event of a Cooper pair from a lattice ion represents resistance to the electric current. Such a collision changes the energy of the Cooper pair because some energy is transferred to the lattice ion. But there are no available energy levels below that of the Cooper pair (it is already in the lowest energy level), and none available above, because of the energy gap. As a result, collisions are forbidden and there is no resistance to the movement of Cooper pairs.

Cooper pair: Normally two electrons repel each other, because of Coulomb interaction. Suppose if for some reason, the two electrons attract each other, then they would form a bound state. This is very important, because, in a bound state, electrons are paired to form a single system, and their motions are correlated. The pairing can be broken only if an amount of energy equal to the binding energy is applied to the system. This pair of electrons is called a *Cooper pair*. At temperature $T < T_c$, the lattice-electron interaction is stronger than electron-electron force. At this stage, the Cooper pairs of electrons will have a peculiar property of smoothly sailing over the lattice point without any energy exchange *i.e.*, the Cooper pairs are not scattered by the lattice points. Hence no transfer of energy takes place from the electron pair to the lattice ions. If an electric field is established inside the substance, the electrons gain additional kinetic energy and give rise to a current. But they do not transfer this energy to the lattice, that they do not get slowed down. As a consequence of this, the substance does not possess any electrical resistivity. So BCS theory explains the zero resistivity of a super conductor. Cooper pair of electrons can maintain the couple upto a certain distance among the lattice points in a superconductor called *Coherence length*. This is found to be of the order of 10^{-6} m.

In superconductive materials, electron-electron attraction results from the electron-lattice interaction (Fig. 6.18). Suppose that the two electrons, 1 and 2 pass each other. Because electron 1 is negatively charged, it attracts positive ions toward itself (electron-lattice interaction).

Thus electron 2 does not 'see' the bare electron 1. Electron 1 is screened by ions. The screening may greatly reduce the effective charge of this electron. In fact, the ions may over respond and produce a net positive charge. If this happens, then electron 2 will be attracted toward electron 1. This leads to a net attractive interaction, as required for the formation of Cooper pair. It is assumed that each electron is surrounded by "phonon cloud", and that the two electrons establish an attractive interaction by exchanging phonons; for example, electron 1 emits phonons which are very quickly absorbed by electron 2, as in Fig. 6.18.

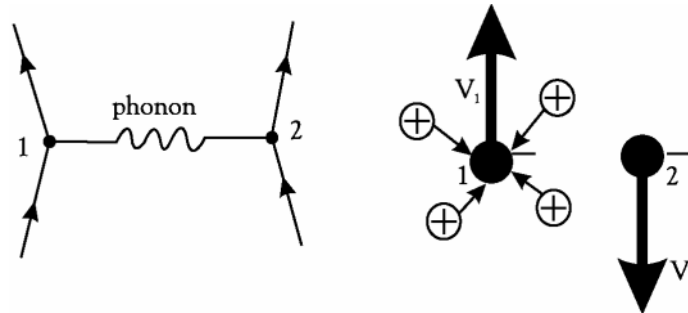


Figure 6.18 *Electron–electron interaction and electron-lattice interaction*

6.9 HIGH TEMPERATURE SUPERCONDUCTORS

An important development in physics that elicited much excitement in the scientific community was the discovery of high-temperature copper oxide-based superconductors. The excitement began with a 1986 publication by Georg Bednorz and K. Alex Müller, scientists at the IBM Zurich Research Laboratory in Switzerland. In their research paper, Bednorz and Müller reported strong evidence for superconductivity at 30 K in an oxide of barium, lanthanum, and copper. They were awarded the Nobel Prize for Physics in 1987 for their remarkable discovery. Shortly thereafter, a new family of compounds was open for investigation, and research activity in the field of superconductivity proceeded vigorously. In early 1987, groups at the University of Alabama at Huntsville and the University of Houston announced superconductivity at about 92 K in an oxide of yttrium, barium, and copper ($\text{YBa}_2\text{Cu}_3\text{O}_7$). Later that year, teams of scientists from Japan and the United States reported superconductivity at 105 K in an oxide of bismuth, strontium, calcium, and copper. More recently, scientists have reported superconductivity at temperatures as high as 150 K in an oxide containing mercury. Today, one cannot rule out the possibility of room-temperature superconductivity, and the mechanisms responsible for the behavior of high-temperature superconductors are still under investigation. The search for novel superconducting materials continues both for scientific reasons and because practical applications become more probable and widespread as the critical temperature is raised. In 2003, Alexei Abrikosov, Anthony Leggett, and Vitaly Ginzburg got Nobel Prize for their contributions to the study of superconductivity.

While BCS theory was very successful in explaining superconductivity in metals, there is currently no widely accepted theory for high-temperature superconductivity.

6.10 APPLICATIONS OF SUPERCONDUCTORS

Two important properties of the superconductors are used in practical application. (1) Their zero resistance and (2) Their wave mechanical behaviour. The wave mechanical behavior is important for a number of device applications. It arises because superconducting electrons have to be described as waves rather than as single particles. A wave of superconducting electrons circulating in a ring has to join its head to its tail exactly, otherwise it will interact destructively with itself on subsequent orbits. Just as the essential

wave nature of electrons leads to the quantization of energy levels in an atom, the current associated with superconducting electrons circulating in a ring can only assume specific values. This results in the quantization of magnetic flux passing through the ring.

Superconductors are mainly used in

- (1) Superconducting Magnets
- (2) Magnetic levitation and permanent magnets
- (3) Wires and cables for motors and power distribution systems
- (4) Microwave filters for cellular telephone networks
- (5) SQUIDS as sensors of foetal heart beats and brain signals, and
- (6) Single flux quantum logic in quantum computing system

6.10.1 Superconducting Magnets

In 1962, B.D. Josephson, a postgraduate student at Cambridge, predicted that a 'supercurrent' consisting of correlated pairs of electrons can be made to flow across a thin insulating layer between two superconductors. Such a junction is called Josephson junction.

6.10.2 Maglev Vehicles

The magnetic levitation of a superconductor above a magnet is one of the most significant features of superconductivity. The performance of bulk High Temperature Superconductor (HTS) materials for levitation continues to improve-in 1994, the Japanese succeeded in levitating a goldfish and in 1997, they levitated a sumo wrestler. In Japan, commercial MAGLEV trains are being developed using conventional superconducting magnets to levitate trains travelling faster than 300 mph (480 km/h) between Tokyo and Osaka. The first two carriage trains and 42 km of track have been already built and successfully operated. Each carriage carries four very large superconducting magnets cooled to liquid helium temperatures by an electrically powered refrigeration unit. As the train moves forward, the eddy currents set up by the magnets skimming over the aluminum track cause the train to be levitated 10 cm above it.

In addition to magnetic levitation, researchers at Houston have recently demonstrated a large grained HTS sample irradiated with very high energetic nuclei, which can trap field as high as 10 T at 23 K. Such fields are almost ten times more powerful than can currently be achieved with conventional magnets. Introducing such material into electrical machines would revolutionize the power-to-weight ratio of motors and magnetic transducers.

6.10.3 Superconducting Wires for Electrical Power Distribution and Motors

HTS tapes can now be fabricated in kilometre length for the field winding of magnets and electrical motors. The best HTS wires now support currents about 100 times larger than those that pass through a typical 15 A mains cable. The main technological challenge is to produce long lengths of such wires with uniform properties and no weak spots.

6.10.4 Superconducting Quantum Interference Device (SQUID)

SQUIDs are devices formed from two or more Josephson junctions, which are the most sensitive sensors known to man and are able to detect minute changes in magnetic field as small as 10^{-23} T. Such minute magnetic fields are produced from the tiny currents associated with mental processes in the brain. Helmets that contains over 100 helium-cooled SQUIDs which can precisely map the various regions of the brain associated with certain sensory and motor activities are developed to locate epileptic seizure, thus providing a valuable diagnostic tool to the brain surgeons.

6.10.5 Superconducting Microwave Filters for Cellular Telephone Networks

High temperature Superconducting microwave filter systems are used in cellular telephone base stations. These systems combine high-performance HTS RF filter with cryocooled semiconductor preamplifiers to offer enhanced sensitivity to improve signal reception and exceptional selectivity to reject interfering signals. There are now thousands of installed HTS systems and the prospects are good for widespread future deployment. In particular, superconducting filters utilizing HTS epitaxial films can provide better interference rejection, full use of the available frequency spectrum, decrease in the noise floor and size and weight reduction in receiver subsystems.

6.10.6 Single Flux Quantum Logic in Quantum Computing System

The qubits are superconducting circuits made with Josephson junctions and operating at millikelvin (mK) temperatures. The information is stored in either the charge on a nanoscale superconducting island, the flux or phase drop in a circulating current, or in the energy levels in a single junction. The qubits are prepared in their initial state by cooling the system to their ground state. Then radio frequency (rf) electromagnetic pulses are used to manipulate the qubits to perform quantum operations. The manipulation of the superconducting qubits can be controlled by on-chip, ultrafast superconducting circuitry. For example, simple single-flux quantum (SFQ) circuitry can operate at speeds up to 700 GHz with small power dissipation and hence can be used in quantum computing systems.

SOLVED PROBLEMS

1. Calculate the numerical aperture and angle of acceptance for an optical fiber having refractive indices 1.563 and 1.498 for the core and the cladding respectively. (V.T.U. Feb 03)

Given: Refractive index of the core, $n_1 = 1.563$, Refractive index of the cladding, $n_2 = 1.498$.

To calculate: (a) Numerical aperture, N.A. =? (b) Angle of acceptance, $\theta = ?$

Formula: $N.A. = \sqrt{n_1^2 - n_2^2}$, $\theta = \text{Sin}^{-1} (N.A.)$

$$(a) \quad N.A. = \sqrt{n_1^2 - n_2^2} = \sqrt{1.563^2 - 1.498^2} = 0.446$$

$$(b) \quad \text{The angle of acceptance } \theta = \text{Sin}^{-1} (N.A.) = \text{sin}^{-1} (0.446) = 26.49^\circ$$

Thus, the values of numerical aperture and angle of acceptance are 0.446 and 26.49° respectively.

2. An optical fiber has a core material with refractive index 1.55, and its cladding material has a refractive index of 1.50. The light is launched into it in air. Calculate its numerical aperture, the acceptance angle and also the fractional index change. (V.T.U., July 03)

Given: Refractive index of core, $n_1 = 1.55$; Refractive index of cladding, $n_2 = 1.50$; Surrounding medium is air, i.e., $n = 1$.

To calculate: Numerical aperture, N.A. = ?; Acceptance angle, $\theta = ?$; Fractional index change $\Delta = ?$

Formula: $N.A. = \sqrt{n_1^2 - n_2^2}$ NA = $n \sin \theta$ or $\theta = \sin^{-1} (N.A.)$; Fractional index $\Delta = \frac{n_1 - n_2}{n_1}$

Solution:

$$N.A. = \sqrt{1.55^2 - 1.50^2} = 0.39$$

$$\theta = \sin^{-1} \left(\sqrt{1.55^2 - 1.50^2} \right) = 22.98^\circ$$

$$\Delta = \frac{n_1 - n_2}{n_1} = \frac{0.05}{1.55} = 0.032$$

EXERCISES

I. Descriptive Type Questions

1. Explain how transmission of light takes place in optical fibers.
[V.T.U., July 05, Jan 04, (O.S.) July 03, March 2001]
2. Explain the principle and working of optical fiber. *[V.T.U., Aug 2001]*
3. Describe the principle on which optical fiber works. *[V.T.U. July 02, Aug. 99]*
4. Explain the principle and applications of optical fibers.
[Bangalore Univ. Sept. 97, Feb. 96, Aug. 94., Kuwempu Univ. Aug 94.]
6. Give a general description of an optical fiber. Explain how an optical fiber function as a waveguide.
[Bangalore Univ. April 98]
7. Explain the mechanism of light propagation in an optical fiber. *[V.T.U. July 07]*
8. Explain the terms: modes of propagation, cone of acceptance and numerical aperture.
[V.T.U., Feb. 02]
9. Define the following in optical fibers:
 - (i) Critical angle of propagation.
 - (ii) Half angle of acceptance.
 - (iii) Numerical aperture.
10. With neat diagrams explain (i) acceptance angle, and (ii) numerical aperture. *[V.T.U. Jan 06]*
11. Obtain an expression for the numerical aperture. *[V.T.U. July 03, July 02, Aug 01]*
12. Obtain an expression for numerical aperture in terms of refractive indices of core and cladding of an optical fiber. *[V.T.U.]an06]*
13. What is numerical aperture? Obtain an expression for numerical aperture in terms of refractive indices of core and cladding, and then arrive at the condition for propagation.
[V.T.U. July 05, (O.S.), Feb 03]
14. With a neat diagram derive an expression for 'numerical aperture, and arrive at the condition for propagation of a signal in an optical fiber. *[V.T.U., Jan 09, July 06]*
15. Explain the different types of optical fibers. *[V.T.U.(O.S.) July 04, March 2001]*
16. Discuss the different types of optical fibers with suitable diagrams. *[V.T.U. June 08, July 07]*
17. With neat diagrams sketch the different types of modes of propagation in an optical fiber.
[V.T.U. Jan 06]
18. With a neat diagram explain numerical aperture, and ray propagation in an optical fiber. Describe the types of optical fibers and modes of transmission. *[V.T.U. March 99.]*

19. With neat diagrams explain the different types of optical fibers. [V.T.V. (O.S.), Jan 07]
20. Describe the different types of optical fiber, along with the typical core and cladding diameter, refractive index profile, and mode propagation sketches. [V.T.U. Jan 08]
21. What is attenuation in an optical fiber. [V.T.U. Jan 07, Jan 06]
22. Explain the attenuation mechanisms. [V.T.U. Jan. 07]
23. Mention the factors contributing to the fiber losses. [V.T.U. Jan 06]
24. What are the advantages of optical communications over other conventional types of communication? [V.T.U. March 99.]
25. Explain fiber-optic communication. Describe point to point communication system using optical fibers with the help of a block diagram, [V.T.U. July 04]
26. Discuss the point to point optical fiber communication system and mention its advantages over the conventional communication systems. [V.T.U., Jan 03]
27. Discuss the advantages and disadvantages of an optical communication system over conventional communication system. [V.T.U., Feb. 05]
28. Describe/Explain: [V.T.U. Aug 99]
 - (i) Principle of propagation of Optical fiber.
 - (ii) Numerical aperture.
 - (iii) Point to point communication in optical fibers.
 - (iv) Advantages of optical communication.
29. With neat figure derive an expression for N.A in an optical Fiber. [VTU June 2009]
30. Give a brief account of SQUID. [VTU June 2009]
31. Explain Meissner effect. [VTU Jan 2009]
32. Obtain an expression for numerical aperture and arrive the condition for propagation. [VTU Jan 2009]
33. What is Superconductivity? Describe type I and type II super conductors. [VTU Jan 2008]
34. Explain the different types of optical fiber, along with the refractive index profile and mode propagation sketches. [VTU Jan 2008]
35. Discuss the three different types of optical fibers. [VTU June 2008]
36. Discuss BCS theory of super conductivity. [VTU June 2008]
37. Write short note on Maglev vehicles. [VTU June 2008]
38. Describe how Cooper pairs are formed and explain the salient features of superconductivity. [VTU June 2007]
39. Explain the mechanism of light propagation in optical fiber. Discuss the different types of optical fibers with suitable diagrams. [VTU June 2007]

40. What is Meissner effect? Explain the BCS theory of superconductors. [VTU June 2010]
41. Derive the expression for numerical aperture of an optical fibre. [VTU June 2010]
42. Explain in brief Type-I and Type-II super conductors. How does a super conductor differ from a normal conductor? [VTU Jan 2007]
43. What is attenuation in an optical fibre? Explain the attenuation mechanisms. [VTU Jan 2007]
44. Describe the point to point communication system, with the help of a block diagram. [VTU Jan 2010]
45. Discuss BCS theory of superconductor. Explain SQUID. [VTU Jan 2010]

II. Multiple Choice Questions

- Numerical aperture of an optical fiber depends on
 - Diameter of the Fiber
 - Acceptance angle
 - Critical angle
 - n_{core} material
- The width of the energy gap of a super conductor is maximum at
 - T_c
 - 0K
 - $\frac{T_c}{2}$
 - $\frac{T_c}{3}$
- Which of the following is correct?
 - Cladding is for providing greater strength
 - Core has higher R.I. than cladding
 - Cladding has higher R.I. than core
 - None
- Fractional index changes of optical Fiber for R.I of core and cladding are 1.563 and 1.498 is
 - 0.00415
 - 0.0415
 - 0.043
 - 0.004
- The temperature at which super conductivity occurs is called
 - Low temperature
 - Super temperature
 - Critical temperature
 - High temperature
- Super conductivity phenomenon can be explained on the basis of
 - BCS theory
 - CCS theory
 - DCS theory
 - MCS theory
- Meissner effect will take place in
 - Solid
 - Super conducting magnet
 - Magler vehicle
 - MRI

9. Loss of power during transmission through optical fiber is called.....
 - (a) Power loss
 - (b) Energy loss
 - (c) Attenuation
 - (d) Modification.
10. Superconductor in superconducting state behaves as
 - (a) Monovalent metals
 - (b) Ferromagnetic materials.
 - (c) Good conductors at room temperature
 - (d) Diamagnetic materials.
11. A superconducting material, on being subjected to the critical field, changes to
 - (a) Critical conductivity
 - (b) Superconducting which is independent of temperature
 - (c) Normal state
 - (d) Remains uninfluenced
12. Fractional index change of optical fiber and refractive index of core are 0.00515 and 1.533 respectively. The cladding refractive index is
 - (a) 1.492
 - (b) 1.525
 - (c) 1.499
 - (d) 1.511
13. Attenuation in the optical fiber causes due to
 - (a) Absorption
 - (b) Scattering
 - (c) Dispersion
 - (d) All the three
14. In a single mode fibre, the diameter of the core is nearly equal to
 - (a) 125 μm
 - (b) 100 μm
 - (c) 50 μm
 - (d) 10 μm
15. The numerical aperture of an optical fibre is 0.2 when surrounded by air. The acceptance angle when the fibre is in water of refractive index 1.33 is
 - (a) $8^{\circ}21'$
 - (b) $8^{\circ}65'$
 - (c) $0^{\circ}11'$
 - (d) None of these
16. The loss of power by the optical signal through the optical fibre is mainly due to
 - (a) Rayleigh scattering
 - (b) Raman scattering
 - (c) Wein's scattering
 - (d) All of these
17. When the type-I superconducting material is placed in an external magnetic field, it
 - (a) attracts the magnetic lines
 - (b) enhances the magnetic field lines
 - (c) repels the magnetic field lines
 - (d) does not influence magnetic field of lines
18. Optical fiber manufacturing method : OVD stands for _____
 - (a) Optical Vapor Deposition
 - (b) Outside Vapor Deposition
 - (c) Oxide Vapor Deposition
 - (d) None of these

19. The size of the acceptance cone is a function of _____
 (a) The refractive index difference between the fiber's core and cladding
 (b) The size difference between the fiber's core and cladding
 (c) Velocity of light propagating through it.
 (d) All of these.
20. Single-mode fiber has a _____ Numerical Aperture
 (a) Small (b) Large
 (c) Zero (d) None of these
21. In optical fiber, the term V is _____
 (a) Normalised frequency (b) Dimensionless fiber parameter
 (c) Used to calculate the spot size, the cutoff wavelength and even chromatic dispersion
 (d) All of these
22. 1. An optical fiber will be single-moded at the given wavelength if _____
 (a) $V \leq 2.405$ (b) $V \geq 2.405$
 (c) $V = 2.405$ (d) $V \leq 0$
23. Attenuation in optical fiber is caused primarily by _____
 (a) Scattering (b) Absorption
 (c) Both scattering and absorption (d) None of these
24. Charles Kao has been awarded the Nobel Prize in Physics in 2009 for _____
 (a) Discovering Optical fiber (b) Using optical fiber for optical communication
 (c) Promoting the idea that the attenuation in optical fibers could be reduced below 20 dB/Km.
 (d) Discovering BCS theory of superconductivity
25. The discovery of _____ has reduced the cost of long distance optical communication by decreasing number of repeaters.
 (a) Erbium-doped fiber amplifier
 (b) Wavelength division multiplexing
 (c) Manufacture of silica-glass fibers with high purity
 (d) None of these

III. Numerical Problems

1. Calculate the numerical aperture, relative refractive index difference, V -number and number of modes in an optical fiber of core diameter 50 μm core and cladding refractive indices 1.41 and 1.40, at wavelength 820 nm. [V.T.U Jan 06]

Ans: N.A = 0.168, $\Delta n = 0.007$, $V = 32$, No of modes = 512

2. A multimode step-index fiber with core diameter $80 \mu\text{m}$ and relative refractive index difference of 1.5% is operating at $0.85 \mu\text{m}$. If the core refractive index is 1.48, calculate the number of guided modes.
- Ans:** The number of modes = 2825.
3. Calculate the number of modes that an optical fiber would transmit given the following data: $n_{\text{core}} = 1.50$, $n_{\text{clad}} = 1.48$, core radius = $50 \mu\text{m}$, wavelength of light = $1 \mu\text{m}$. [V.T.U., June 08, July 07]
- Ans:** The number of modes = 2941.
4. Calculate the numerical aperture of the given optical fiber if the refractive indices of the core and cladding are 1.623 and 1.522 respectively. [V.T.U., Aug 2001]
- Ans:** N.A. = 0.564
5. The numerical aperture of an optical fiber is 0.2 when surrounded by air. Determine the refractive index of its core given the refractive index of cladding as 1.59. Also find the acceptance angle when it is in a medium of refractive index. 1.33. V.T.U. Feb. 05
- Ans:** $n_1 = 1.60$, $\theta_0 = 8.65^\circ$
6. Calculate the number of modes that can propagate inside an optical fiber, given $n_{\text{core}} = 1.53$, $n_{\text{clad}} = 1.50$, core radius = $50 \mu\text{m}$, $\lambda = 1 \mu\text{m}$. V.T.U. July 05.
- Ans:** 95
7. The attenuation of light in an optical-fiber is estimated at 2.2 dB/km. What fractional initial intensity remains after 2 km & 6 km? V.T.U. July 06
- Ans:** $(P_{\text{out}}/P_{\text{in}}) = 0.363, 0.0479$ at the end of 2 km and 6 km respectively.
8. An optical signal loses 85% of its power after traversing a fiber length 400 m. What is the fiber loss? V.T.U. July 07
- Ans:** $\alpha = 1.7645$
9. A glass clad fiber is made with core glass refractive index 1.5 and cladding is doped to give a fractional index difference of 0.0005. Determine (a) the cladding index, (b) the critical internal reflection angle, (c) the external critical acceptance angle, (d) the numerical aperture.
- Ans:** $n_2 = 1.499$, $\theta_c = 87.9^\circ$, $\theta = 2.72^\circ$, N.A. = 0.0474
10. An optical fiber has clad of refractive index 1.50 and numerical aperture 0.39. Find the refractive index of the core and the acceptance angle. **Ans:** $n_1 = 1.54$, and $\theta = 22.96^\circ$
11. A Fiber 500m long has an input power of 8.6 mW and out put power 7.5mW. What is the loss specification in cable? [VTU June 2009]
12. The angle of acceptance of an optical fiber is 30° when kept in air. Find the angle of acceptance when it is in a medium of refractive index 1.33. [VTU Jan 2009]
13. Calculate the numerical aperture, fractional index change and V-number for a fiber of core diameter $40 \mu\text{m}$ and with refractive indices of 1.55 and 1.50 respectively for core and cladding. The wavelength of the propagating wave is 1400 nm. Assume that the fiber is in air. [VTU Jan 2008]

14. Calculate the number of modes an optical fiber will transmit given the following data $n_{\text{core}} = 1.50$, $n_{\text{clad}} = 1.48$, core radius = $50 \mu\text{m}$, wavelength of light = $1 \mu\text{m}$. [VTU June 2008]
15. Calculate the number of modes an optical fiber can transmit, given the following data: wavelength of light = $1 \mu\text{m}$, radius of the core = $50 \mu\text{m}$, Refractive index of the core = 1.50, Refractive index of the cladding 1.48. [VTU June 2007]
16. An optical fiber has core R.I. 1.5 and R.I. of cladding is 3% less than the core index. Calculate the numerical aperture, angle of acceptance and internal critical acceptance angle. [VTU June 2010]
17. The attenuation of an optical fibre is -3.6 dB/km . What is the fraction of light intensity that remains after (i) 1km (ii) after 3 km? [VTU Jan 2007]
18. An optical glass fibre of refractive index 1.50 is to be clad with another glass to ensure internal reflection that will contain light travelling within 5° of the fibre axis. What maximum index of refraction is allowed for the cladding? [VTU Jan 2010]

Answers to Multiple Choice Questions

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

CRYSTAL STRUCTURES

OBJECTIVES

The concepts and phenomenon introduced in Chapter III - VI can be readily understood by knowing the atomic arrangements in the solids. The properties of materials depend on the internal arrangement of atoms. Crystallography is the science which gives the information regarding the internal arrangement of atoms or molecules in solids. This chapter is dedicated to introduce the reader to the basic concepts of crystal physics. The main objectives of this chapter is to study

- Definition of Space lattice, Bravais lattice, Unit cell, Primitive cell and Lattice parameters
- Seven crystal systems and 14 Bravais lattices
- Direction and planes in a crystal, Miller indices and interplanar spacing
- Co-ordination number of cubic structure, Number of atoms per unit cell, Relation between Atomic radius and Lattice constant, and Atomic packing factor
- Bragg's Law and Bragg's X-ray spectrometer
- Crystal structures of NaCl and diamond.

7.1 INTRODUCTION

There are three states of the matter namely solid, liquid and gaseous state. In gaseous state the interaction length between the molecules or the atoms is large, of the order 30\AA . Whereas in the liquid, the interaction length is less compared to that of gaseous state and usually the liquids take the shape of the container. On contrary to gas and liquids the solids are having very less interaction length and each and every atoms or molecules are tightly held by hydrogen bonds. Every solid has its own shape and this external shape differ from solids to solids. Further, there are two types of solids, crystalline and amorphous. The solids which possess long range three dimensional ordering are known as crystals. Thus a crystal may be defined as a solid which possesses long range, three dimensional atomic or molecular arrangements. The physical property of amorphous solid invariant with the direction and are considered as isotropic materials. But in the case of crystal the directional property differs and hence most of the crystals are non-isotropic. In order to understand the structure and property relation one need to know the arrangement of atoms or molecules in three dimensional lattices. It is very difficult to predict the crystal structure of any compound without having determined the structure by X-ray or neutron diffraction technique.

7.2 SPACE LATTICE

A crystal structure is built of infinite repetition of identical atoms or group of atoms in three dimensions. A group of atoms is called the basis or motif. The set of mathematical points to which the basis is attached is called a lattice. A **crystal lattice or space lattice** is an infinite pattern of lattice points in three dimensions, each of which must have the same surroundings in the same orientation. Space lattice can also be defined as a well defined repeating unit (motif or basis) and the each motif is associated to a lattice point so that the overall lattice is a three dimensional array of lattice points which are geometrically identical (Fig. 7.1). A lattice is a mathematical concept. The crystal structures can be built up from a lattice by placing basis or motif (an atom or a group of atoms) at each lattice point.

$$\text{Crystal structure} = \text{Lattice} * \text{basis (Motif)}$$

Where the symbol * may be taken to mean 'associated with'

It is possible to describe the crystal structure of a simple metal as well as that of a complex protein in terms of the same lattice. In the case of simple metallic crystals the number of atoms allocated to each lattice point is just one and in the case of a protein crystal the number of atoms allocated to each lattice point may be thousands. Since the lattice is only a geometric representation, it is possible to have many different crystals which have same lattice but different basis or motifs.

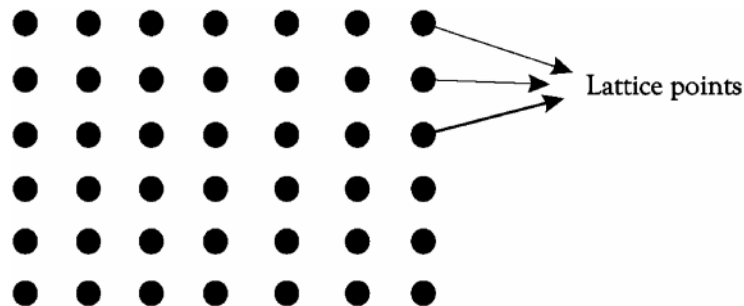


Figure 7.1 *Two dimensional space lattice or plane lattice*

7.2.1 Bravais Lattice

The array of equivalent lattice points in two or in three dimensions is referred as Bravais lattice. If all the equivalent lattice points are replaced by motifs, the overall structure represents the crystal structure or space lattice itself. The array of non-equivalent lattice points is referred as non-Bravais lattice.

In Fig. 7.1, each lattice points are replaced by a motif which contains three different objects (Fig. 7.2) (triangle, filled + and filled circle). Each of the objects can be considered as an each type of atom. All the three objects as a whole they repeat in two dimensions in a regular interval and hence they are equivalent, represents the Bravais lattice. Similarly, consider only one type of the object then one can still achieve the equivalence. But if we consider different objects in a single lattice point or motifs then

those objects are nonequivalent and periodicity is lost in the two dimensional lattice and are regarded as non-Bravais lattice.

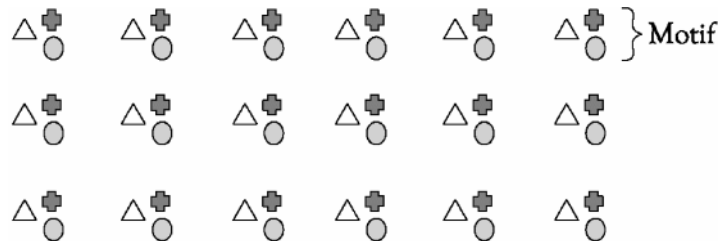


Figure 7.2 Bravais lattice

Basis vector and translational vector

A vector is a mathematical quantity having both magnitude and direction. A vector having unit magnitude is generally referred as a unit vector. A set of non-collinear unit vectors are used to define a coordinate system. Let us call these vectors as basis vectors as they give magnitude and direction of separation between two identical lattice points. If we chose three basis vectors, \vec{a} , \vec{b} and \vec{c} to define a right-handed, orthogonal, three dimensional Cartesian co-ordinate systems then any vector \vec{T} which gives the position and direction of the any identical lattice point in three dimensional lattices can be represented as

$$\vec{T} = u\vec{a} + v\vec{b} + w\vec{c}$$

Where, \vec{T} is the translational vector or lattice vector and u , v , and w are integers.

Let us consider a two dimensional lattice (plane lattice) as shown in Fig. 7.3. Consider \vec{a} and \vec{b} are the two basis vectors oriented along AB and AC directions, respectively. The position of the lattice point D can be represented by a combination of basis vector \vec{a} and \vec{b} as $\vec{T} = \vec{a} + \vec{b}$. Therefore the coordinates of the lattice point D with respect lattice point A is (1,1). Any lattice point in a plane lattice can be obtained by the integer (u and v) linear combinations of basis vectors \vec{a} and \vec{b} . One should note here that the length of basis vectors need not be same and similarly the angle between the two vectors need not be 90° always, but the two basis vectors \vec{a} and \vec{b} must be non-collinear. Similarly any lattice point in a three dimensional lattice can be represented by the lattice vector. The coordinates of the lattice point in three dimension is represented by (u,v,w) . Based on the concept of translational vector, the space lattice is a geometrical image of the operation of the translational operators on the lattice point at the origin.

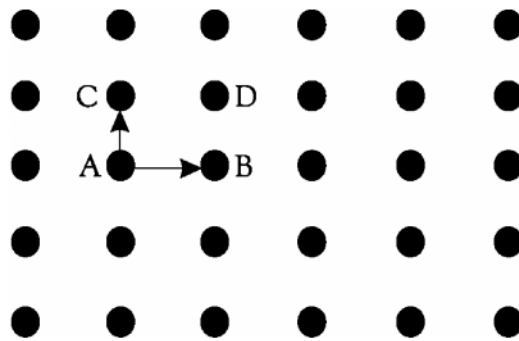


Figure 7.3 Plane lattice

7.2.2 Unit Cell

The parallelepiped-shaped volume which, when reproduced by close packing in three dimensions, gives the whole crystal structure or space lattice itself is called the *unit cell*. *Unit cell is also defined as the smallest geometrical volume in a space lattice, defined by three basis vectors, which on translation along three basis vector directions yields the complete crystal structure or space lattice itself.* It is well to note that the unit cell may not be an entity which can be uniquely defined. For convenience and understanding let us consider a two dimensional lattice (plane lattice). A two-dimensional lattice is shown in Fig. 7.4, which can be thought of as a portion of the arrangement of atoms within a crystal. Several possible choices of shape and origin of unit cell can be made depending on the easy convenience of representing symmetry of the space lattice. The possible choices of unit cells are shown in Fig. 7.4 and they are all perfectly acceptable in that reproducing the unit cells in a close-packed two-dimensional array gives the correct atomic arrangement. However, in this case there is one rectangular unit cell and this choice of unit cell conveys more readily the special rectangular repeat features of the overall pattern.

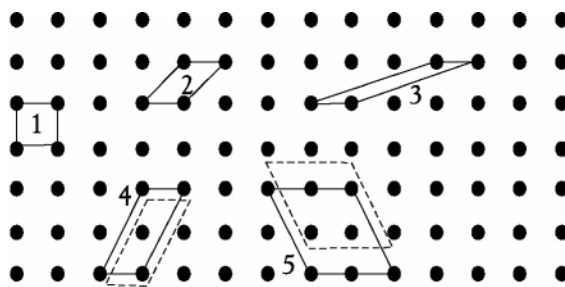


Figure 7.4 Unit cell

7.2.3 Primitive Cell

All fundamental unit cells associated with a single lattice point in it are called primitive cells or P-cells. A primitive cell is a one in which lattice points are present only at the edges (or corners) of the unit cell. Similarly if the unit cells are associated with more than one lattice point are referred as non-primitive or multi unit cells. A non-primitive cell is a one in which there are lattice points present in the unit cell in addition to the lattice points at the edges of the unit cell.

In the above Fig. 7.4, there are five choices of representing unit cell and all yields a same space lattice on repetition along basis vector directions. Let us check one by one whether these choices of unit cells are primitive or not. For example, the unit cell 5 associated with a total of 4 lattice points. Four lattice points at the edges of the unit cell contributing about $1/4^{\text{th}}$ to unit cell i.e $1/4 \times 4 = 1$, two lattice points at the center of the unit cell and the contribution from them is 2 and remaining one due to the two lattice points contributing about $1/2$ to the unit cell, each situated between the two lattice points at the edges of unit cell as shown in the Fig. 7.4. Therefore there are 4 lattice points associated with a unit cell and therefore the unit cell 5 is non-primitive cell. The same can be realized by moving the unit cell slightly away from the lattice points as shown in the Fig. 7.4 with dashed lines. The number of lattice points associated with the dashed line unit cell is 4, which is similar to the calculated number of lattice points; hence unit cell 5 is non-primitive. The similar type of calculation and operation can be adapted to the remaining set of unit cells. The unit cell 1, 2 and 3 are primitive because the number of lattice points associated with these unit cells is one and the unit cell 4 is non-primitive due to number of lattice points associated with it are 2.

7.2.4 Lattice Parameters

As we discussed earlier there are many number of ways of choosing \vec{a} , \vec{b} and \vec{c} vector, which are called basis vectors and the choice of them are completely arbitrary and any number of unit cell can be constructed. However, for crystallographic convention it is better to choose vectors resulting as small a unit cell as possible and the choice of unit cell should reveal the underlying symmetry of the lattice.

Basically the parallelepiped formed by the three basis vectors \vec{a} , \vec{b} and \vec{c} , defines the unit cell of the lattice, with edges of length a, b and c, is selected as unit cell.

The size of the unit-cell is described in terms of its unit-cell parameters. These are the edge lengths and the interfacial angles of the unit-cell. Therefore, the unit cell parameters is defined as a set of six parameters, lengths of the three non-collinear basis vectors and three interfacial angles, that together defines a unit cell.

Let \vec{a} , \vec{b} and \vec{c} are non-collinear basis vectors and let α , β and γ be the interfacial angle between basis vectors \vec{b} and \vec{c} , \vec{a} and \vec{c} and \vec{a} and \vec{b} , respectively (Fig. 7.5). These interfacial angles are also known as crystallographic angles or opposite angles.

The axial distances and angles are measured from one corner to the cell, i.e. a common origin. It is a useful convention (and helps to avoid confusion) if the origin is taken as the 'back left-hand corner' of the cell, the *a*-axis pointing forward (out of the page), the *b*-axis towards the right and the *c*-axis

upwards. This convention also gives a right-handed axial system. If any one of the axes is reversed (e.g. the b -axis towards the left instead of the right), then a left-handed axial system results.

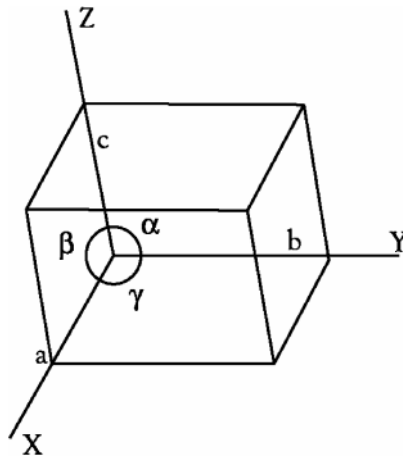


Figure 7.5 *Unit cell*

7.3 CRYSTAL SYSTEMS

The systematic work of describing the space lattices was done initially by Frankenheim, who, in 1835, proposed that there were fifteen space lattices. Among the fifteen suggested by Frankenheim, two of the proposed lattices were identical and it was first pointed out by Bravais in 1848. Hence, to this day, the fourteen space lattices are usually, and are called Bravais lattices. These 14 Bravais lattices fall into seven crystal systems, depending on the overall symmetry of the unit cell. They are

- (1) Cubic
- (2) Tetragonal
- (3) Orthorhombic
- (4) Monoclinic
- (5) Triclinic
- (6) Rhombohedra (or Trigonal) and
- (7) Hexagonal.

The lattice parameter for all seven crystal systems along with 14 types of Bravais lattice and lattice symbols are given in Table 7.1. The lattice points here are presented as thick filled circles and these circles centers are exactly placed at the edges where three basis vectors meet. But one should note here

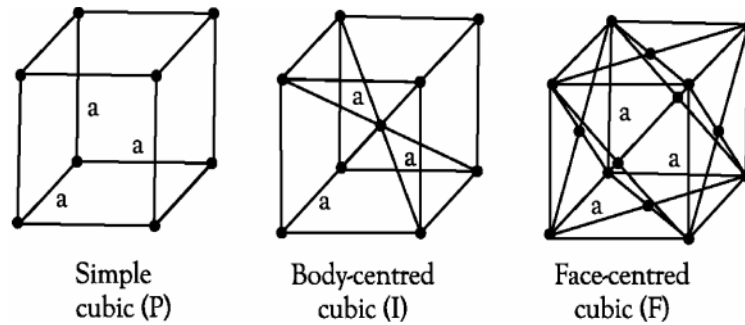
that the size of the filled circles doesn't corresponds or take care of the size of the atoms and in principle the atoms are in contact with the nearest surrounding neighbor atoms in the space lattice.

Table 7.1 Crystal systems and the 14 Bravais Lattices

| Seven systems | Axes and angles | 14 Bravais Lattices | Lattice Symbols |
|--------------------------|--|---------------------|-----------------|
| Cubic | $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ | Primitive | P |
| | | Body centered | I |
| | | Face centered | F |
| Tetragonal | $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ | Primitive | P |
| | | Body centered | I |
| Orthorhombic | $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ | Primitive | P |
| | | Body centered | I |
| | | Base face centered | C |
| | | Face centered | F |
| Trigonal or rhombohedral | $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ | Primitive | R |
| | | | |
| Hexagonal | $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$ | Primitive | P |
| | | | |
| | | | |
| Monoclinic | $a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$ or $(\alpha = \beta = 90^\circ \neq \gamma)$ | Primitive | P |
| | | Base face centered | C |
| Triclinic | $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$ | Primitive | P |
| | | | |

Cubic system

For cubic system, all the axes lengths are equal and all the crystals axes are perpendicular to each other. In this system there are three types of Bravais lattices are possible namely simple cubic (SC) (P), Body-centered cubic (BCC) (I) and Face-centered cubic (FCC) (F).

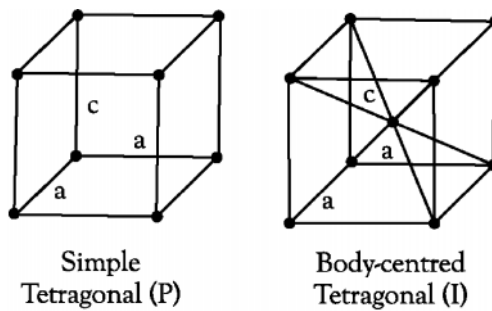


$$a = b = c, \quad \alpha = \beta = \gamma = 90^\circ$$

Figure 7.6 Cubic crystal systems

Tetragonal system

The two axes have equal length and all the axes are mutually perpendicular to each other. There are two types of tetragonal Bravais lattices are possible namely simple (P) and body centered (I) tetragonal lattice.

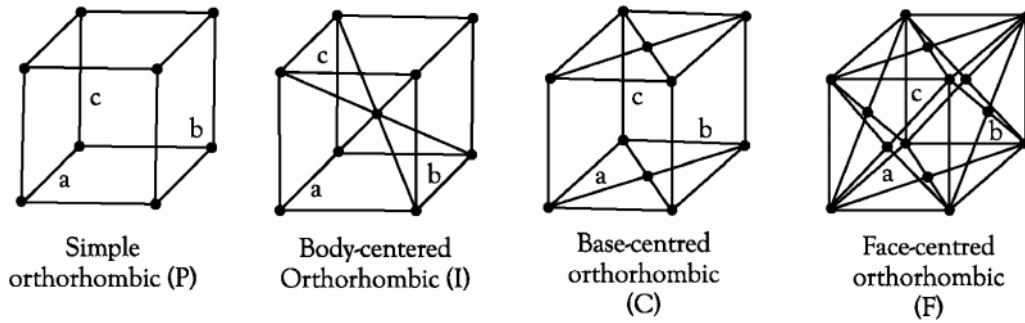


$$a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$

Figure 7.7 Tetragonal crystal systems

Orthorhombic system

All the axes lengths are unequal and all the axes are perpendicular to each other. There are four possible orthorhombic Bravais lattices namely, simple (P), body-centered (I), face-centered (F) and base face centered (C).

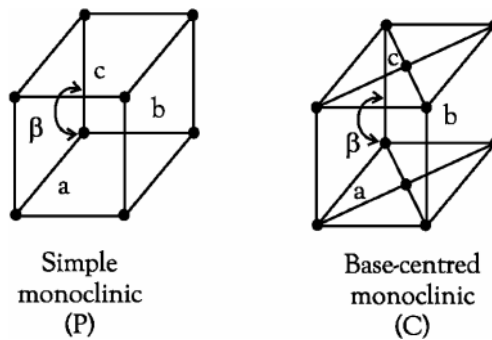


$$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$$

Figure 7.8 Orthorhombic crystal system

Monoclinic system

All the axes lengths are unequal and the angles $\alpha = \gamma = 90^\circ$ and $\beta \neq 90^\circ$. Monoclinic has two types of Bravais lattices namely, simple (P) and base-face centered (C).

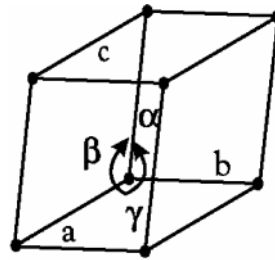


$$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$$

Figure 7.9 Monoclinic crystal system

Triclinic system

All the three axes length are unequal and all the axes angles are unequal and are not perpendicular to each other.



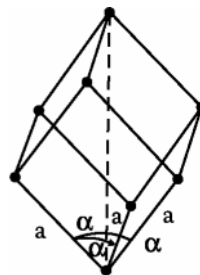
Triclinic
(P)

$$a \neq b \neq c, \alpha \neq \gamma \neq \beta \neq 90^\circ$$

Figure 7.10 *Triclinic crystal system*

Rhombohedral or Trigonal system

All axes lengths are equal and the interfacial angle should be equal to each other, but other than 90° .



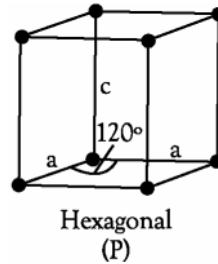
Rhombohedral
(R)

$$a = b = c, \alpha = \gamma = \beta \neq 90^\circ$$

Figure 7.11 *Rhombohedral crystal system*

Hexagonal system

The two axes lengths are equal and one of the interfacial angle $\gamma = 120^\circ$ and other two interfacial angles are equal to 90° .



$$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$$

Figure 7.12 Hexagonal crystal system

7.4 DIRECTION AND PLANES IN A CRYSTAL

7.4.1 Directions in a Crystal

Any lattice point T can be represented by the equation

$$\vec{T} = u\vec{a} + v\vec{b} + w\vec{c}$$

Where u , v and w are integers and \vec{a} , \vec{b} and \vec{c} are basis vectors.

A vector from the origin to the lattice point \vec{T} defines a direction in space and since this direction is related to the integers u , v and w , one defines the directions based on the values of integers. Further the vector represented by (u, v, w) and (hu, hv, hw) are parallel and are therefore in the same direction. The direction in space corresponding to the vectors is written in square brackets, without using commas to separate the digits, as $[uvw]$. For example $[213]$ and it should be read as 'two one three'.

7.4.2 Planes in a crystal and Miller indices.

The facets of a well formed crystal or internal planes through a crystal structure are specified in terms of Miller Indices, h , k and l , written in round brackets, (hkl) . The same terminology is used to specify planes in a lattice. Miller indices, (hkl) , represent not just one plane, but the set of all identical parallel lattice planes. The values of h , k and l are the reciprocals of the fractions of a unit cell edge, a , b and c respectively, intersected by an appropriate plane. This means that a set of planes that lie parallel to a unit cell edge is given the index 0 (zero) regardless of the lattice geometry. Thus a set of planes that pass across the ends of the unit cells, cutting the a -axis at a position $1/a$, and parallel to the b - and c -axes of the unit cell has Miller indices (100) , (Fig. 7.13a). The same principles apply to the other planes shown. The set of planes that lies parallel to the a - and c -axes, and intersecting the end of each unit cell at a position $1/b$ have Miller indices (010) , (Fig. 7.13b). The set of planes that lies parallel to the a - and b -axes, and intersecting the end of each unit cell at a position $1/c$ have Miller indices (001) , (Fig. 7.13c), and planes cutting the a -, b - and c -axes at $1/a$, $1/b$ and $1/c$ will be (111) .

A set of three integers which are used to represent the plane are referred as Miller indices.

A set of planes is defined by three integers h , k , and l known as plane indices or Miller indices. The steps that should be followed to determine the miller indices is given below.

1. Find the intercept of the planes along three basis vectors.
2. Either reduce the fractional intercepts to set of integers p , q and r or express the intercepts as fractional multiples of basis vector lengths
3. Take the reciprocals
4. Find the least common multiple (LCM) of the denominator and multiply this LCM to above ratios yields set of three integers h , k and l referred as Miller indices.

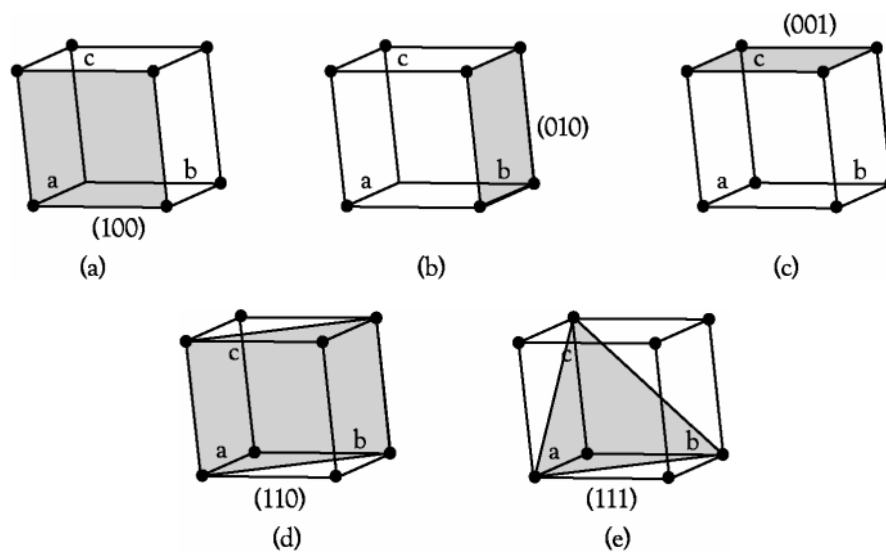


Figure 7.13 Crystal planes

7.4.3 Expression for Interplanar Spacing

Let us consider two parallel planes ABC and $A'B'C'$. Let x , y and z be the intercepts of the plane ABC along three basis vector directions. Let us consider $A'B'C'$ be the imaginary plane passing through the origin and is parallel to ABC plane. If one draw a normal from origin to crystal plane ABC then distance of separation between these two planes is OP , where OP is referred as interplanar distance denoted by $d_{(hkl)}$. Let us consider the unit vector OP makes an angle θ_1 , θ_2 and θ_3 with respect to X , Y and Z axes. By considering space lattice is orthogonal, the OP is normal to the plane and x , y and z will be the hypotenuses to the three right angled triangles. All these triangles have common adjacent side OP .

Therefore, one can write interplanar spacing as

$$d_{(hkl)} = x \cos \theta_1 = y \cos \theta_2 = z \cos \theta_3$$

Form the procedure of finding the Miller indices we have

$$h = a/x, k = b/y \text{ and } l = c/z$$

substitute for x, y and z in the above equation. We get

$$d_{(hkl)} = (a/h)\cos\theta_1 = (b/k)\cos\theta_2 = (c/l)\cos\theta_3$$

But for orthogonal coordinates we know that

$$\cos^2\theta_1 + \cos^2\theta_2 + \cos^2\theta_3 = 1$$

Substitute for $\cos\theta$ value in the above equation yields.

$$d_{(hkl)}^2 \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

Therefore

$$d_{(hkl)} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad \dots(7.1)$$

The above equation is the expression for interplanar distance.

For cubic case all the cell lengths are same and the above equation reduces to

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \dots(7.2)$$

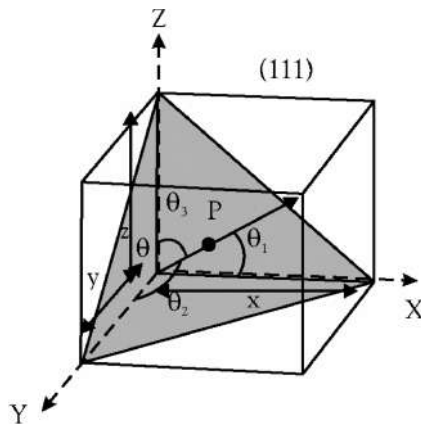


Figure 7.14 Inter planar spacing

7.5 CO-ORDINATION NUMBER

The coordination number is defined as the number of nearest neighbors surrounding the central or a given atom within the space lattice.

7.5.1 Coordination Number of Cubic Crystal Structure

- Simple cubic (SC):** The coordination number for simple cubic lattice is 6. Four lattice points which are in plane with the origin atom and the remaining two lattice points are out of the plane.
- Body centered cubic (BCC):** The coordinate number for BCC is 8. There are 8 lattice points present at the edges of the primitive cell and are having equal distance from the lattice point at the body center.
- Face centered cubic lattice (FCC):** The co-ordination number for FCC structure is 12. Four atoms are in plane with the atom under consideration and four atoms to right hand side and the remaining four atoms to left hand side.

7.5.2 Number of Atoms Per Unit Cell

The number of atoms present in a unit cell can be evaluated by the contribution of the individual atom to the unit cell.

- Simple cubic (SC) cell:** SC has each lattice points placed at corners of the unit cell. Each corner atoms lies at the meeting point of eight unit cells. Therefore the contribution from the atom present at corner to unit cell is $1/8^{\text{th}}$ part of atom and there are 8 corners. Therefore the total number of lattice point present in simple cubic is $1/8 \times 8 = 1$. i.e only one atom present in a simple cube.
- Body centered cubic (BCC) lattice:** In BCC, in addition to the eight lattice points at the eight corners there is one lattice point situated at the center of the cell which is not at all shared by any other unit cell. Therefore the number of lattice points present in BCC is

$$= 1 + (1/8 \times 8) = 1 + 1 = 2.$$

- Face centered cubic (FCC) cell:** In FCC structure, there are 8 atoms at the corners contributing $1/8^{\text{th}}$ to the unit cell. There are 6 atoms at the face center of the six planes of the cube contributing about $1/2$ to unit cell. Therefore the total number of atoms present in FCC is

$$= 1/8 \times 8 + 1/2 \times 6$$

$$= 1 + 3 = 4$$

The total number of lattice points present in FCC is 4.

7.5.3 Relation Between Atomic Radius and Lattice Constant

Let us consider that the all the elements present in space lattice are of the same type and are having spherical shape. It is possible to write an expression relating lattice constant and atomic radius.

- (a) **Simple cubic:** unit cell is assumed to be constructed of eight atoms stacked as shown in Fig. 7.15. The distance between the two atoms in a simple cubic is a and is equal $2R$, where R is the radius of the atom.

Therefore for simple cubic the relation between the lattice parameter and atomic radius is given by

$$a = 2R$$

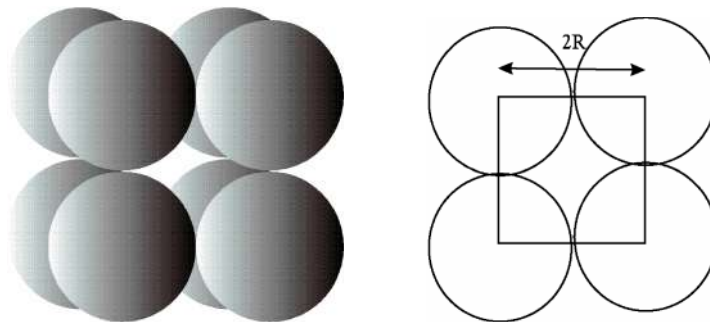


Figure 7.15 Simple cubic packing

- (b) **Body centered cubic lattice:** The packing of body centered cubic lattice is shown in Fig. 7.16. The relation between the lattice parameter and atomic radius can be obtained by geometrical analysis.

The diagonal length is equal to 4 times the atomic radius R . i.e $AC=4R$

From the geometry of the cube,

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

But

$$AB^2 = a^2 + a^2$$

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

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

Therefore

$$a = 4R / \sqrt{3}$$

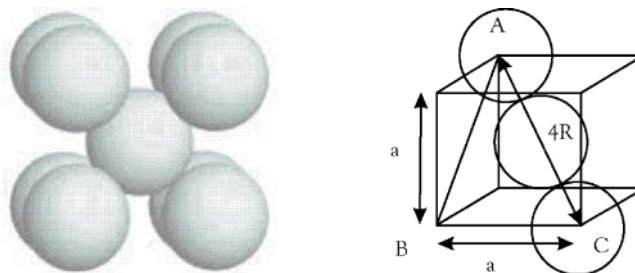


Figure 7.16 Body centered cubic structure

- (c) **Face centered cubic:** The atom present at face center touches four atoms which are in plane and the atoms present at corner do not touch each other. A top view of the packing diagram is shown in Fig. 7.17. The relation between the lattice parameter and atomic radius can be obtained from the crystal geometry as follows

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

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

$$4R = \sqrt{2a}$$

Therefore,

$$a = 4R/\sqrt{2}$$

or

$$a = 2\sqrt{2}R$$

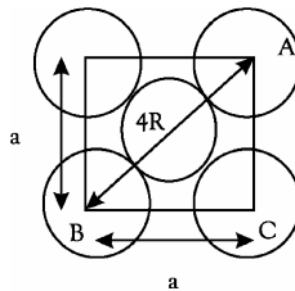


Figure 7.17 Face centered cubic structure

7.6 ATOMIC PACKING FACTOR

Atomic packing factor (APF) is the ratio of the total volume of the atoms present in one unit cell to that of total volume of the unit cell.

Let us assume that the atoms has spherical shape and therefore the volume is given by $= (4/3)\pi R^3$

The volume of the unit cell for a cubic case is a^3

Total volume of the atoms present in one unit cell = $n \times (4/3)\pi R^3$

Where n is the number of atoms present in unit cell which is different for different lattice settings.

Now, the atomic packing factor is given by

$$\text{Atomic Packing factor} = \frac{\text{total volume of the atoms present in unit cell}}{\text{total volume of the unit cell}} = \frac{n \times (4/3)\pi R^3}{a^3}$$

(a) Simple cubic

Number of atom present in simple cubic is 1 and $a=2R$

Substitute in the above equation we get

$$\begin{aligned}\text{Atomic packing fraction for simple cubic} &= \frac{n \times (4/3)\pi R^3}{a^3} = \frac{1 \times (4/3)\pi R^3}{(2R)^3} \\ &= \frac{(4/3)\pi R^3}{8R^3} = (1/6)\pi\end{aligned}$$

$$\text{APF} = 0.52$$

(b) **Body centered cubic**

Number of atoms present in a unit cell is 2 and for BCC $a = 4R/\sqrt{3}$

$$\text{Atomic packing fraction for BCC} = \frac{n \times (4/3)\pi R^3}{a^3} = \frac{2 \times (4/3)\pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}}{8}\pi$$

$$\text{APF} = 0.68$$

(c) **Face centered cubic**

Number of atoms in a unit cell is 4 and for FCC $a = 2\sqrt{2}R$

$$\text{Atomic packing fraction for FCC} = \frac{4 \times (4/3)\pi R^3}{(2\sqrt{2}R)^3} = \frac{1}{3\sqrt{2}}\pi$$

Therefore APF for FCC is = 0.74

7.7 BRAGG'S LAW

The easiest example of scattering yielding structural information is that of Bragg scattering of a wave from a set of partially reflecting equally spaced parallel planes. An incident wave will be diffracted by the set of planes, its intensity being modulated by constructive or destructive interference. For an infinite set of such planes (with infinitesimal reflection coefficient) the only surviving reflection is one for which there is constructive interference between waves reflected by each set of neighboring planes. Thus, the difference in path length between waves reflected from adjacent planes separated by a distance d must be an integral multiple of the wavelength λ and This leads to Bragg's law,

$$2d\sin\theta = n\lambda \quad \dots(7.4)$$

where n is the order of diffraction and θ is the glancing angle with respect to crystal plane and d is the interplanar separation.

7.7.1 Determination of Crystal Structure by Bragg's X-ray Spectrometer

The experimental setup of the Bragg diffractometer is shown in Fig. 7.18. There are three major components in Bragg diffractometer namely X-ray generator, sample holder and a detector. A beam of electron is accelerated through a potential difference in the range 10-50 kV. The accelerated electron beam is

made to fall on metal target, T, which is typically made up of Cu, Mo, W, Co or Cr, where the kinetic energy of the accelerated electrons are converted into X-rays and heat.

Thus produced X-rays are made to pass through a slit in order to get a fine beam of X-rays which are made to fall on the sample. The sample, S, is mounted on a stage that can be rotated around an axis normal to plane of the paper. A detector D is placed at a distance of r from the sample. The angle between the sample plane and the X-ray beam direction is taken as θ . When a sample rotates by an angle of θ , the detector rotates around the same axis by an angle of 2θ to collect the Bragg reflection. This experimental configuration is known as a $\theta - 2\theta$ diffractometer.

The detector measure the number of X-ray photon (intensity) I which are scattered from the sample over an angle of 2θ with respect to incident X-ray beam direction. The plot of scattered X-ray intensity I as a function of the angle 2θ is shown in Fig. 7.18 and is referred as the powder diffraction sample. Different crystal samples gives rise to its own finger print of X-ray diffraction pattern which made easy to identify the newly formed compounds.

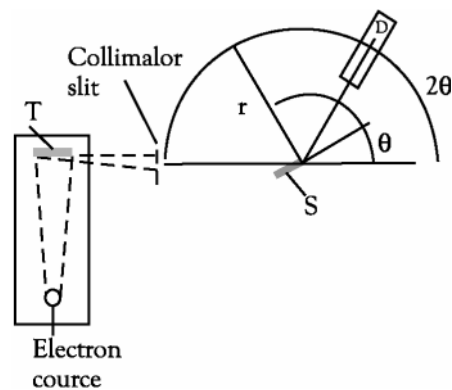


Figure 7.18 Experimental setup of Bragg diffractometer

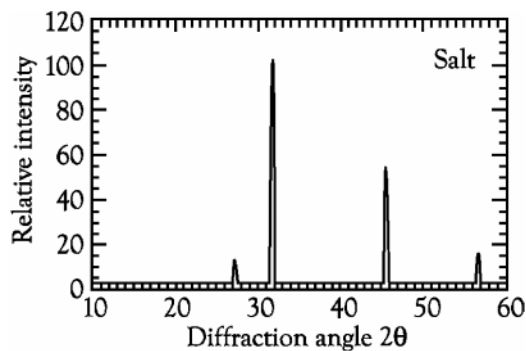


Figure 7.19 Powder diffraction pattern

7.7.2 Crystal Structures of NaCl

There are four sodium and four chlorine atoms in the unit cell which takes alternative position in the crystal structure. For all materials with the halite structure, the number of molecules present in one unit cell is 4 ($Z=4$). In the NaCl structure, each atom of sodium is surrounded by six atoms of chlorine and similarly the each atom of chlorine is surrounded by six atoms of sodium. A perspective view of the halite structure is shown in Fig. 7.20. This structure is adopted by many oxides, sulphides, halides and nitrides with a formula MX.

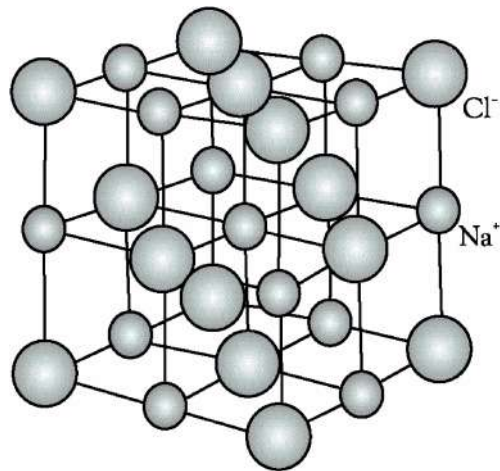
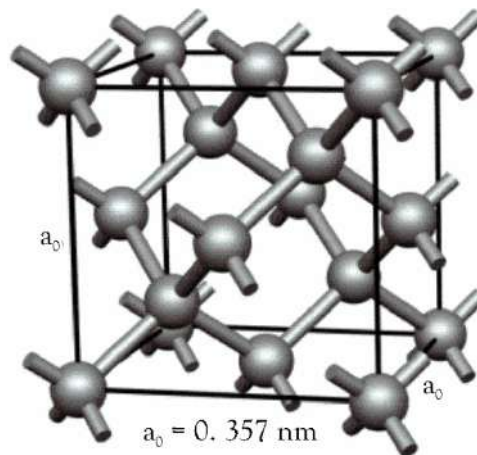


Figure 7.20 FCC structure of NaCl crystal

7.7.3 Crystal Structure of Diamond



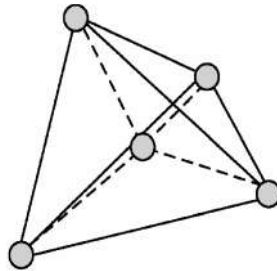


Figure 7.21 (a) unit cell of Diamond Crystal, (b) carbon atoms forming the tetrahedron structure

Let us consider two unit cells of FCC structure. Super impose one FCC structure on the other. Now fixing one unit cell, move the other unit cell by $\frac{1}{4}$, $\frac{1}{4}$ and $\frac{1}{4}$ of the side length along x, y and z direction respectively, results in diamond structure. The diamond structure can be described as two interpenetrating fcc structures that are displaced relative to one another along the main diagonal. The position of the origin of the second fcc structure, expressed in terms of the basis vectors, is $(\frac{1}{4} \frac{1}{4} \frac{1}{4})$. The four carbon atoms together forms tetrahedron structure as shown in Fig. 7.21. The nearest neighbor distance in the diamond structure is $\frac{\sqrt{3}}{4}a$. Since there are 8 atoms in a unit cell of diamond, the

packing factor is $\frac{\sqrt{3}}{16}\pi$ or 0.34. The elements which crystallize similar to the structure of diamond are Germanium (Ge) and Silicon (Si).

SOLVED PROBLEMS

1. Draw the following planes in a cubic cell $[312]$, $\bar{1}\bar{1}\bar{1}$

Given that:

Miller indices of planes are $[312]$, $\bar{1}\bar{1}\bar{1}$

$$a) [312] = [hkl] = \left[\begin{array}{ccc} a & b & c \\ x & y & z \end{array} \right]$$

By reversing the procedure followed for calculating the Miller indices, one can calculate the intercept of the plane

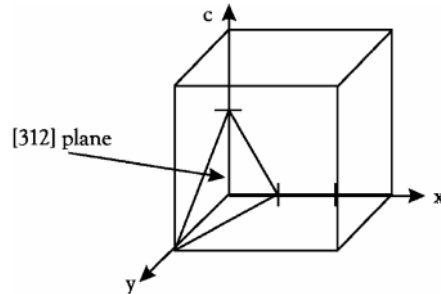
- (i) Express given Miller indices as a fraction

$$[hkl] = [312] = \left[\begin{array}{ccc} a & b & c \\ x & y & z \end{array} \right] = \left[\begin{array}{ccc} 3 & 1 & 2 \\ 1 & 1 & 1 \end{array} \right]$$

- (ii) Take the reciprocal

$$\left[\begin{array}{ccc} x & y & z \\ a & b & c \end{array} \right] = \left[\begin{array}{ccc} 1 & 1 & 1 \\ 3 & 1 & 2 \end{array} \right]$$

i.e., the intercepts $x=(1/3)a$, $y=1b$ and $z=(1/2)c$



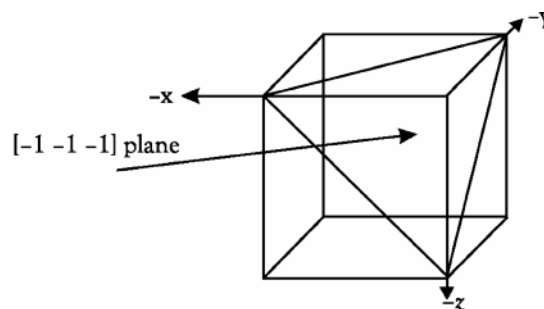
$$a) \quad [\bar{1}\bar{1}\bar{1}] = [hkl] = \left[\frac{a}{x} \frac{b}{y} \frac{c}{z} \right]$$

$$[hkl] = [\bar{1}\bar{1}\bar{1}] = \left[\frac{a}{x} \frac{b}{y} \frac{c}{z} \right] = \left[\frac{-1}{1} \frac{-1}{1} \frac{-1}{1} \right]$$

(iii) Take the reciprocal

$$\left[\frac{x}{a} \frac{y}{b} \frac{z}{c} \right] = \left[\frac{1}{-1} \frac{1}{-1} \frac{1}{-1} \right] = [-1 \ -1 \ -1]$$

i.e., the intercepts $x = -1a$, $y = -1b$ and $z = -1c$



2. Calculate the Miller indices of the plane whose intercepts are $(5/3)a$, $(3/2)b$ and $(\infty)c$.

Given that:

(i) Intercept of the planes

$$[x, y, z] = \left[\frac{5a}{3}, \frac{3b}{2}, \infty c \right]$$

(ii) Expressing these intercept as fractional multiples of magnitude of basis vectors

$$\left[\frac{x}{a}, \frac{y}{b}, \frac{z}{c} \right] = \left[\frac{5}{3}, \frac{3}{2}, \frac{\infty}{1} \right]$$

(iii) Take the reciprocal

$$\left[\frac{a}{x}, \frac{b}{y}, \frac{c}{z} \right] = \left[\frac{3}{5}, \frac{2}{3}, \frac{1}{\infty} \right] = \left[\frac{3}{5}, \frac{2}{3}, 0 \right]$$

(iv) Find the LCM and multiply LCM to fractions to get integers

The LCM is 15

$$[hkl] = [9, 10, 0]$$

The miller indices of the given plane is [9 10 0]

3. A monochromatic X-ray beam of wavelength 1.5 \AA undergoes second order Bragg reflection from the plane (2 1 1) of cubic crystal at a glancing angle of 54.38° . Calculate the lattice constant. (May/June 2010)

Given that:

X-ray wavelength $\lambda = 1.5 \text{ \AA} = 1.5 \times 10^{-10} \text{ m}$

Glancing angle $\theta = 54.38^\circ$

Order of diffraction $n = 2$

Miller indices $h = 2, k = 1, l = 1$

To calculate:

Lattice constant of cubic crystal $a = ?$

The interplanar distances for set of planes (2 1 1) can be calculated from the Bragg equation

i.e.,
$$2d_{(hkl)} \sin \theta = n\lambda$$

or
$$d_{(hkl)} = \frac{n\lambda}{2 \sin \theta}$$

$$d_{(211)} = \frac{2 \times 1.5 \times 10^{-10}}{2 \sin 54.38^\circ} = 1.845 \times 10^{-10} \text{ m}$$

The expression for interplanar distance for the cubic crystal is given by

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

or
$$a = d_{(hkl)} \sqrt{h^2 + k^2 + l^2}$$

$$a = 1.845 \times 10^{-10} \sqrt{2^2 + 1^2 + 1^2}$$

$$a = 4.52 \times 10^{-10} \text{ m} = 4.52 \text{ \AA}$$

The lattice constant of cubic crystal $a = 4.52 \text{ \AA}$

4. Calculate the glancing angle for incidence of X-rays of wavelength 0.58 \AA on the plane (1 3 2) of NaCl which results in second order diffraction maxima taking the lattice as 3.81 \AA .

Given that:

$$\text{Lattice constant } a = 3.81 \text{ \AA} = 3.81 \times 10^{-10} \text{ m}$$

Miller indices of the plane (1 3 2) $\Rightarrow h = 1, k = 3, l = 2$

Order of diffraction $n = 2$

Wavelength of X-ray $\lambda = 0.58 \text{ \AA} = 0.58 \times 10^{-10} \text{ m}$.

To calculate:

Glancing angle $\theta = ?$

We know that

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{(132)} = \frac{3.81 \times 10^{-10}}{\sqrt{1^2 + 3^2 + 2^2}}$$

$$d_{(132)} = 1.018 \times 10^{-10} \text{ m}$$

Glancing angle can be calculated from the Bragg equation

$$2d_{(hkl)} \sin \theta = n\lambda$$

or

$$\sin \theta = \frac{n\lambda}{2d_{(hkl)}}$$

\Rightarrow

$$\theta = \sin^{-1} \left(\frac{n\lambda}{2d_{(hkl)}} \right)$$

$$\theta = \sin^{-1} \left(\frac{2 \times 0.58 \times 10^{-10}}{1.018 \times 10^{-10}} \right)$$

$$\theta = 34.73^\circ$$

The glancing angle $\theta = 34.73^\circ$

5. The minimum order of Bragg's reflection occurs at an angle of 20° in the plane [212]. Find the wavelength of X-ray if lattice constant is 3.615 \AA . (June/July 2009)

Given that:

Glancing angle $\theta = 20^\circ$

For minimum order of diffraction $n = 1$

Lattice constant $a = 3.613 \text{ \AA} = 3.615 \times 10^{-10} \text{ m}$

Miller indices of a given plane is [212] $\Rightarrow h = 2, k = 1, l = 2$

To calculate:

Wavelength of X-ray $\lambda = ?$

The interplanar distance for set of [212] planes is given by

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{(212)} = \frac{3.615 \times 10^{-10}}{\sqrt{2^2 + 1^2 + 2^2}} = 1.205 \times 10^{-10} \text{ m}$$

Wavelength of X-ray can be calculated using Bragg equation as follows

$$2d_{(hkl)} \sin \theta = n\lambda$$

or

$$\lambda = \frac{2d_{(hkl)} \sin \theta}{n}$$

$$\lambda = \frac{2 \times 1.205 \times 10^{-10} \times \sin 20^\circ}{1} = 0.824 \times 10^{-10} \text{ m}$$

$$\lambda = 0.824 \times 10^{-10} \text{ m} = 0.824 \text{ \AA}$$

The wavelength of X-ray is $\lambda = 0.824 \text{ \AA}$

6. In a cubic unit cell the distance between the two atoms present at the coordinates (100) and (011) is 5.8 \AA . A monochromatic electron beam of unknown wavelength undergoes second order Bragg reflection from the plane (025) at a glancing angle of 45.95° . Calculate the wavelength of the electron beam.

Given that:

Miller indices of the given plane is (025) $\Rightarrow h = 0, k = 2$ and $l = 5$

Glancing angle $\theta = 45.95^\circ$

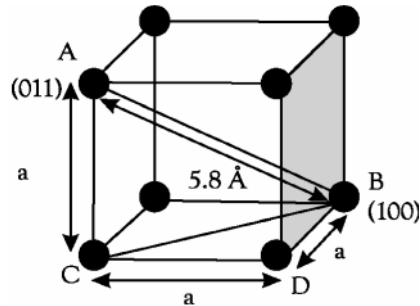
The distance between the atoms present at coordinates (100) and (011) is 5.8 \AA

Order of Bragg reflection $n = 2$

To calculate:

Wavelength of electron beam $\lambda = ?$

The coordinates of the given atoms can be represented as shown below



The lattice parameter can be calculated as follows

$$AB^2 = CB^2 + AC^2$$

But $CB^2 = CD^2 + DB^2$

$$CB^2 = a^2 + a^2$$

$$\Rightarrow AB^2 = 2a^2 + a^2$$

$$AB^2 = 3a^2$$

$$\Rightarrow a = \frac{AB}{\sqrt{3}} = \frac{5.8 \times 10^{-10}}{\sqrt{3}} = 3.348 \times 10^{-10} \text{ m}$$

The expression for interplanar distance for the cubic crystal is given by

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{(025)} = \frac{3.348 \times 10^{-10}}{\sqrt{0^2 + 2^2 + 5^2}}$$

$$d_{(025)} = 0.622 \times 10^{-10} \text{ m}$$

The electron beam wavelength can be calculated using Bragg equation as

i.e $2d_{(hkl)} \sin \theta = n\lambda$

or $\lambda = \frac{2d_{(hkl)} \sin \theta}{n}$

$$\lambda = \frac{2 \times 0.622 \times 10^{-10} \times \sin 45.95^\circ}{2}$$

$$\lambda = 0.447 \times 10^{-10} \text{ m}$$

The wavelength of the incident electron beam $\lambda = 0.447 \text{ \AA}$

EXERCISES

I. Descriptive Type Questions

- 1 Write a note on unit cell, basis vector, space lattice and primitive cell.
- 2 Write a note on Bravais lattice and non Bravais lattice.
- 3 Describe the procedure to find the Miller indices of a given plane.
- 4 Derive an expression for interplanar spacing for a tetragonal lattice.
- 5 Write neat labeled diagrams of seven Crystal systems and mention the lattice parameters.
- 6 What is a Bravais lattice? Draw the diagrams of 14 Bravais lattices.
- 7 Write a note on Bragg's Law.
- 8 Describe the structures of NaCl and Diamond with neat diagrams.
- 9 Draw all base centered and face centered lattice among 14 Bravais lattices and mention the lattice parameters.
- 10 Write a note on Bragg's X-ray spectrometer.
11. Derive an expression for inter planar spacing in terms of miller indices. (VTU June 2009)
12. With neat figure, explain crystal structure of NaCl. (VTU June 2009)
13. How do you find miller indices of a given plane. (VTU Jan 2009)
14. Derive an expression for interplaner spacing in terms of miller indices. (VTU Jan 2009)
15. Define coordination number and packing factor. Calculate the packing factor for SC and BCC structures. (VTU Jan 2008)
16. Describe how Bragg's spectrometer is used for determination of crystal structure. (VTU Jan 2008)
17. Explain how Miller indices are derived. Derive an expression for interplanar spacing of a crystal in terms of Miller indices. (VTU June 2008)
18. Explain the structure of NaCl. (VTU June 2008)
19. Define lattice points, Bravais lattice and primitive cell. Explain in brief the seven crystal systems with neat diagrams. (VTU June 2007)
20. Explain with neat sketch the diamond crystal. (VTU June 2007)
21. Explain how Bragg's X-ray spectrometer can be used to determine the inter planar spacing. (VTU June 2007)
22. Define unit cell and primitive cell. Describe crystal structure of diamond. (VTU June 2010)
23. Derive Bragg's law. (VTU June 2010)
24. Define crystal lattice, unit cell and primitive cell. (VTU Jan 2007)
25. What is atomic packing factor? Work out atomic packing-factors for simple cubic, FCC and BCC structures. (VTU Jan 2007)

26. Discuss the Bravais lattice and any five crystal systems with the help of illustrations.
(VTU Jan 2010)
27. Define coordination number and packing factor. Calculate the packing factor for sc, fcc and bcc structures.
(VTU Jan 2010)
28. Derive expression for interplanar spacing in terms of Miller indices
29. Explain the crystal structure of NaCl

II. Multiple Choice Questions

- The relation between atomic radius and lattice constant in FCC structure is _____
 (a) $a = 2r$ (b) $2\sqrt{2}r$
 (c) $a = \frac{\sqrt{3}r}{4}$ (d) $\frac{4r}{\sqrt{3}}$
- APF of diamond crystal structure is _____
 (a) 0.68 (b) 0.74
 (c) 0.52 (d) 0.34
- A crystal of Tetragonal lattice is _____
 (a) $a = b = c$ (b) $a \neq b \neq c$
 (c) $a = b \neq c$ (d) $a \neq b = c$
- For every rotation by an angle θ in Bragg's spectrometer, detector turns by an angle _____
 (a) θ (b) 3θ
 (c) $\theta/2$ (d) 2θ
- The coordination number in the case of simple cubic crystal structure is _____
 (a) 12 (b) 6
 (c) 2 (d) 1
- Which of the following metal crystallizes in fcc structure _____
 (a) Aluminium (b) Zinc
 (c) Sodium (d) Calcium chloride
- The number of molecules present in unit cell of sodium chloride is _____
 (a) 5 (b) 2
 (c) 4 (d) None of these.
- The Miller indices of the plane parallel to x and y axis are _____
 (a) (100) (b) (010)
 (c) (001) (d) (111)

9. Nearest neighbor distance between two atoms in case of bcc structure is _____
- (a) $(a\sqrt{3})/2$ (b) $2a/\sqrt{3}$
(c) $(a\sqrt{2})/2$ (d) $2a/\sqrt{2}$
10. The co-ordination number in case of simple cubic crystal structure is _____
- (a) 12 (b) 8
(c) 2 (d) 6
11. The crystal with lattices a is _____
- (a) Cubic (b) Hexagonal
(c) Orthorhombic (d) Tetragonal.
12. A plane intercepts at a, b/2, 2c in a simple cubic unit cell. The miller indices of the plane are _____
- (a) (214) (b) (241)
(c) (421) (d) (124)
13. Which one of the following crystal is an example of monoclinic? _____
- (a) SnO_4 (b) NaCl
(c) CaSO_4 (d) CuSO_4
14. In a simple cubic lattice the ratio $d_{100} : d_{110} : d_{111}$ is _____
- (a) 6 : 3 : 1 (b) $\sqrt{3} : \sqrt{6} : 1$
(c) $6 : 3 : \sqrt{2}$ (d) $\sqrt{6} : \sqrt{3} : \sqrt{2}$
15. Which one of the following Bravais lattices is not found in cubic crystal? _____
- (a) Simple cube (b) Face centered
(c) Body centered (d) Base centered
16. The packing fraction of diamond crystal structure is _____
- (a) 34% (b) 52%
(c) 68% (d) 74%
17. A crystal of hexagonal lattice is _____
- (a) $a \neq b \neq c$ (b) $a = b = c$
(c) $a \neq b = c$ (d) $a = b \neq c$
18. Inter atomic distance between Na and Cl is _____
- (a) 2.81 Å (b) 5.62 Å
(c) 6.62 Å (d) 5.50 Å

19. All types of Bravais lattices observed in _____
(a) Rhombohedra (b) Orthorhombic
(c) Triclinic (d) Monoclinic
20. For every rotation by angle θ in Bragg's spectrometer, detector turns by an angle _____
(a) θ (b) 3θ
(c) 4θ (d) 2θ
21. The array of equivalent lattice points in two or in three dimensions is referred as _____
(a) Motif (b) Bravais lattice
(c) Unit cell (d) Plane lattice
22. All fundamental unit cells associated with a single lattice point in it are called _____
(a) Motif (b) primitive cells
(c) Both (a) & (b) (d) None of these
23. Coordination number of FCC structure is _____
(a) 12 (b) 8
(c) 6 (d) 16
24. The total number of lattice points present in BCC is _____
(a) 12 (b) 8
(c) 6 (d) 2
25. Atomic packing fraction for BCC structure is _____
(a) 0.74 (b) 0.68
(c) 0.34 (d) 0.54
26. The intercepts of the plane with miller indices (9 10 0) is _____
(a) $(5/3, 3/2, \infty)$ (b) $(3/2, 2/3, \infty)$
(c) $(0, 1/2, 3/2)$ (d) none of these
27. The relation between the lattice constant and atomic radius of carbon atom in Diamond is _____
(a) $a = \frac{R\sqrt{3}}{4}$ (b) $a = 2R$
(c) $a = \frac{4R}{\sqrt{3}}$ (d) none of these
28. For a tetragonal unit cell, the plane (1 0 1) is parallel to _____
(a) parallel to x-y plane (b) parallel to y-z plane
(c) parallel to x-z plane (d) parallel to y-axis

29. The total number of atoms present in a unit cell of NaCl is _____
- (a) 4 (b) 6
(c) 12 (d) none of these
30. The cell length of the cubic structure is $3.348 \times 10^{-10}\text{m}$. The interplanar distance between the set of (0 2 5) planes is _____
- (a) $0.31 \times 10^{-10}\text{m}$ (b) $0.1 \times 10^{-10}\text{m}$
(c) $0.53 \times 10^{-10}\text{m}$ (d) $0.622 \times 10^{-10}\text{m}$

III. Numerical Problems

- Draw the following planes in a cubic unit cell $(0\bar{2}1)$, $(\bar{1}\bar{1}3)$ and $(3\bar{2}1)$
- Draw the following planes in the simple cubic cell (122), (143), (195) and (257).
- Calculate the Miller indices of a plane with intercepts $\frac{3a}{5}$, $\frac{2b}{3}$ and the same plane is parallel to c -axis.
- Give the sketch representing the unit cell of tetragonal lattice, $a = b = 2\text{\AA}$, $c = 4\text{\AA}$. Calculate the interplanar distance for (213) plane and verify the result geometrically. Draw a plane in the unit cell having Miller indices (213).
- When an element X is crystallized, it exhibited atomic arrangement in the crystal structure similar to that of Diamond crystal structure. If the distance between the X atoms present at coordinates (000) and $\left[\frac{1}{4}\frac{1}{4}\frac{1}{4}\right]$ is 3.5\AA , calculate the interplanar spacing for the planes (314).
- The inter atomic distance in a crystal possessing the structure similar to NaCl structure is 2.9\AA . Calculate the X-ray wavelength which undergoes second order reflection from the plane (312) at a glancing angle of 38.45° .
- The atomic diameter for the element which crystallizes in body centered cubic lattice is 4.2\AA . Calculate the X-ray wavelength which undergoes second order diffraction from a plane (314) at glancing angle of 43.4° .
- The minimum order of Bragg's reflection occurs at angle of 20° in the plane [2 1 2]. Find the wavelength of X-rays if lattice constant is 3.615\AA . (VTU June 2009)
- Calculate the glancing angle for incidence of X-rays of wavelength 0.7\AA on the plane (132) of NaCl which results in second order diffraction maxima taking the lattice as 3.85\AA .
- An X-ray beam of wavelength 0.7\AA undergoes minimum order Bragg reflection from the plane (302) of a cubic crystal at glancing angle 35° . Calculate the lattice constant. (VTU Jan 2008)
- X rays are diffracted in the first order from a crystal with d spacing $2.82 \times 10^{-10}\text{m}$ at a glancing angle 6° . Calculate the wavelength of X-rays. (VTU June 2008)

12. A monochromatic X-ray beam of wavelength 1.5 \AA undergoes second order Bragg reflection from the plane (211) of a cubic crystal, at a glancing angle of 54.38° . Calculate the lattice constant.
(VTU June 2010)
13. Calculate the glancing angle on the cube.(132) of NaCl, having lattice spacing 3.81 \AA , corresponding to the second order diffraction for x-rays of wavelength 0.58 \AA .
(VTU Jan 2007)
14. The minimum order of Bragg's reflection occurs at angle 20° in the plane [212]. Find the wavelength of X-ray if lattice constant is 3.615 \AA

Answers to Multiple Choice Questions

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

MATERIAL SCIENCE

OBJECTIVES

This chapter introduces to two topics, first one is the nano-technology and the second one is the ultrasonics. The main emphasis of this chapter is to give the introduction to the latest and emerging technology through the development of Nano-Science. The Nano-science deals the phenomenon related to materials having the size of several nanometers. As one reduces the dimensions of the materials new effects were observed depending on the size and shape of the nano materials. The objective of this section is to study

- Nano-science and Nano-technology, Opportunities & Challenges of Nano-technology, and Categories of nano-technology
- Nano-materials, Shapes of Nano-materials, Methods of preparation of Nano-materials, and Characterization
- Wonders of Nano-technology: Discovery of Fullerene and carbon Nanotubes
- Applications of Nano-technology
- Ultrasonic Waves & Non-destructive testing of materials, and Measurements of velocity in solids and liquids

8.1 INTRODUCTION TO NANO-SCIENCE AND NANO-TECHNOLOGY

8.1.1 What is Nano-technology ?

Nano-technology is an advanced technology, which deals with the design and synthesis of nano-particles, processing of nano-materials and devices, and their usage in various fields of science & technology. Normally, nano-materials are the particles of size ranging from 1 nm to 100 nm. To visualize the size of nano-materials, consider an Oxygen ion of normal size of 0.14 nm so that the group of about 7 oxygen ions form 1 nm size which is the lower limit (1 nm) of nano-material. Similarly the group of about 700 oxygen ions in spatial dimension forms the upper limit (100 nm) of nano-material. Similarly, for comparison, 10 nanometers is 1000 times smaller than the diameter of a human hair. Materials in nano-scale show surprising physical, chemical, biological, mechanical, and electrical properties compared to same materials at higher scale. Hence the phenomena occurring on 1 - 100 nm length scale are of

interest to physicists, chemists, biologists, electrical and mechanical engineers, and computer scientists, making research in nanotechnology a frontier activity in materials science.

Nano-technology is often referred to as a *general-purpose technology*. That's because in its advanced form it will have significant impact on almost all industries and all areas of society. It offers better built, longer lasting, cleaner, safer, and smarter products for the home, for communications, for medicine, for transportation, for agriculture, and for industry in general.

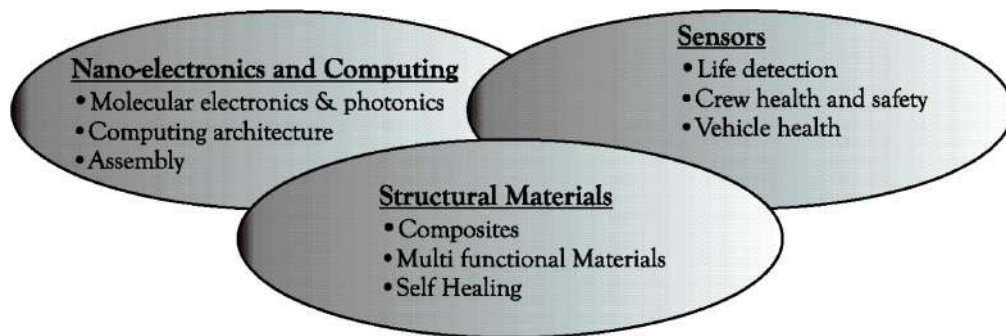
Nano-technology not only will allow making many high-quality products at very low cost, but it will allow making new nanofactories at the same low cost and at the same rapid speed. This unique ability to reproduce its own means of production is why nano-technology is said to be an *exponential* technology. It represents a manufacturing system that will be able to make more manufacturing systems—factories that can build factories—rapidly, cheaply, and cleanly. The means of production will be able to reproduce exponentially, so in just a few weeks a few nano-factories conceivably could become *billions*. It is a revolutionary, transformative, powerful, and potentially very dangerous—or beneficial—technology. Thus in nano-technology, the atoms and molecules become the building blocks called *mesoscopic state*.

The term 'nano-technology' was first used by the Japanese scientists Norio Taniguchi (1912-1999) in his paper in 1974 on production technology that creates objects and features on the order of a nanometer. The American engineer K. Eric Drexler (b. 1955) is credited with the development of molecular nanotechnology, leading to nanosystems machinery manufacturing. The invention of scanning tunneling microscope in the 1980s by IBM Zurich scientists and then the atomic force microscope allowed scientists to see materials at an unprecedented atomic level.

8.1.2 Why Nano-technology ?

- Advanced miniaturization is a key thrust area to enable new science and exploration missions.
 - Ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed.
- Revolutions in electronics and computing will allow reconfigurable, autonomous, “thinking” spacecraft.
- Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new space architectures.
 - Networks of ultra small probes on planetary surfaces.
 - Micro-rovers that drive, hop, fly, and burrow.
 - Collection of micro-spacecraft making a variety of measurements.
- Safe, Affordable Aviation
- Human Exploration and Colonization of Space
- Evolution of Universe and Life
- Nanoelectronics and Computing
 - Petaflop computing

- Ultrahigh density storage 10^{15} bytes/cm²
- Sensors
 - Sensor Web
 - Robot Colony
- Integration of computing, memory, sensing and communication
- Structural Materials
 - Microspacecraft
 - Self-healing, multifunctional materials



8.1.3 Opportunities and Challenges of Nano-technology

For Chemists and Chemical Engineers

- Novel synthetic routes and processing of nanomaterials
- New types of molecular nanostructures and supramolecular assemblies with varied nanoarchitectures
- Self-assembled periodic and a periodic nanostructures to induce multifunctionality and cooperative effects
- Chemistry for surface modifications to produce nanotemplates
- One-pot syntheses that do not require changing reaction vessels
- Scalable production to make large quantities economically

For Physicists

- Quantum electrodynamics to study novel optical phenomena in nanocavities
- Single photon source for quantum information processing
- Nanoscale nonlinear optical processes

- Nanocontrol of interactions between electrons, phonons and photons
- Time-resolved and spectrally resolved studies of nanoscopic excitation dynamics

For Device Engineers

- Nanolithography for nanofabrication of emitters, detectors, and couplers
- Nanoscale integration of emitters, transmission channels, signal processors, and detectors, coupled with power generators
- Photonic crystal circuits and microcavity-based devices
- Combination of photonic crystals and plasmonics to enhance various linear and nonlinear optical functions
- Quantum dot and quantum wire lasers
- Highly efficient broadband and lightweight solar panels that can be packaged as rolls
- Quantum cutters to split vacuum UV photons into two visible photons for new-generation fluorescent lamps and lighting.

For Biologists

- Genetic manipulation of biomaterials for photonics
- Biological principles to guide development of bio-inspired photonic materials
- Novel biocolloids and biotemplates for photonic structures
- Bacterial synthesis of photonic materials

For Biomedical Researchers

- Novel optical nanoprobes for diagnostics
- Targeted therapy using light-guided nanomedicine
- New modalities of light-activated therapy using nanoparticles
- Nanotechnology for biosensors

8.1.4 Categories of Nano-technology

On tracking the nano evolution, it has been stated that no matter what the market outcomes in the near or long term, nanoscience will never be an industry into itself but a science of many avenues of application, and possibility that could redefine the direction of several industries. This insight allows one to recognize that nanotechnology is not “a technology” but “a set of technologies,” yielding a set of technical breakthroughs that will seep into many different markets. Within such a framework, the world of nanotechnology may be divided into three broad categories: nanotools, nanodevices, and nanostructured materials.

(1) Nano-tools

Nano-tools are devices that manipulate matter at the nano or atomic regime. Devices such as atomic force microscopes, scanning probe microscopes, atomic-layer-deposition devices and nanolithography tools, can manipulate matter in the atomic or molecular regime. Some other nano-tools include fabrication techniques; analysis and metrology instruments; and software for nano-technology research and development. They are used in lithography, chemical vapor deposition (CVD), 3-D printing, and nano-fluidics. Nano-fluidics, the study of nanoscale fluid behavior, for example, the study of dynamics of droplets adsorbed onto surfaces under shearing is mostly used in areas such as medical diagnostics and biosensors.

(2) Nano-devices

Nanodevices are any complete system with nanostructured components that carries out as assigned function other than manipulating nano-matter. The first nano-devices on the market were quantum dot fluorescent biodetectors. Nano-devices are used as accelerometers in automotive airbags. Many other promising applications are in development such as nanoelectric memory devices, nanosensors and drug delivery systems. Components to nanodevices will include nanomaterials, semiconducting organic molecules, polymers and high-purity chemicals and materials.

(3) Nano-structured Materials

Nano-structured materials are materials with a microstructure, the characteristic length scale of which is on the order of a few (typically 1-100) nanometers. The microstructure refers to the chemical composition, the arrangement of the atoms (the atomic structure), and the size of a solid in one, two, or three dimensions. Effects controlling the properties of nano-structured materials include size effects (where critical length scales of physical phenomena become comparable with the characteristic size of the building blocks of the microstructure), changes of the dimensionality of the system, changes of the atomic structure, and alloying of components (e.g., elements) that are not miscible in the solid and/or the molten state.

The synthesis, characterization and processing of *nanostructured materials* are part of an emerging and rapidly growing field. Research and development in this field emphasizes scientific discoveries in the generation of materials with controlled microstructural characteristics, research on their processing into bulk materials with engineered properties and technological functions, and introduction of new device concepts and manufacturing methods.

8.2 NANO-MATERIALS

Nano-materials is a field which takes a materials science-based approach to nanotechnology. It studies materials with morphological features on the nanoscale, and especially those which have special properties stemming from their nanoscale dimensions. Some of the special properties of nano-materials are :

1. Due to increased ratio of surface area to volume in nanoscale materials, new quantum mechanical effects are possible. For example, the “quantum size effect” where the electronic properties of

solids are altered with great reductions in particle size. This effect does not come into play by going from macro to micro dimensions. However, it becomes pronounced when the nanometer size range is reached.

2. The small size of nano-materials ensures that many atoms, perhaps half or more, will be near to the surface. Hence in nano-materials, surface properties such as energy levels, electronic structure, and reactivity can be quite different from bulk material, and give rise to quite different material properties.
3. A certain number of physical properties also alter with the change from macroscopic systems. Novel mechanical properties of nano-materials is a subject of nanomechanics research.
4. Catalytic activities of nano-materials also reveal new behaviour in the interaction with biomaterials.
5. Materials reduced to the nanoscale can suddenly show very different properties compared to what they exhibit on a macroscale, enabling unique applications. For instance, opaque substances become transparent (copper); inert materials attain catalytic properties (platinum); stable materials turn combustible (aluminum); solids turn into liquids at room temperature (gold); insulators become conductors (silicon).
6. Materials such as gold, which is chemically inert at normal scales, can serve as a potent chemical catalyst at nanoscales. Much of the fascination with nano-technology stems from these unique quantum and surface phenomena that matter exhibits at the nanoscale.

Current knowledge of science at the nanoscale comes from developments in disciplines such as chemistry, physics, life sciences, medicine and engineering. There are several areas in which nanoscale structures are under active development or already in practical use :

1. In materials science, nano-particles allow for the making of products with mechanical properties very different from those of conventional materials and can also improve surfaces by adding new friction, wear or adhesion properties.
2. In biology and medicine, a greater understanding of the functioning of molecules and of the origin of diseases on the nanometre scale has led to improvements in drug design and targeting.
3. Nano-materials are also being developed for analytical and instrumental applications, including tissue engineering and imaging.
4. A wide variety of nanoscale materials and coatings are already in use in **consumer products** such as cosmetics and sunscreens, fibers and textiles, dyes, and paints.
5. The smallest components of a computer chip are on a nanoscale.
6. The constant drive towards miniaturization in **electronic engineering** has led to devices that are well within the nanometre range. Data storage devices based on nanostructures provide smaller, faster, and lower consumption systems.
7. Optical devices have also benefited from this trend and new types of microscopes have been invented, that can produce images of atomic and molecular processes at surfaces.

8.3 SHAPES OF NANO-MATERIALS

In nano-materials, the size and shape of the very small domains that compose the bulk material affect its properties. The dependence of the physical property (such as color or conductivity) on the size and shape of the nanoscale domains is often a result of *surface* and *interface interactions*.

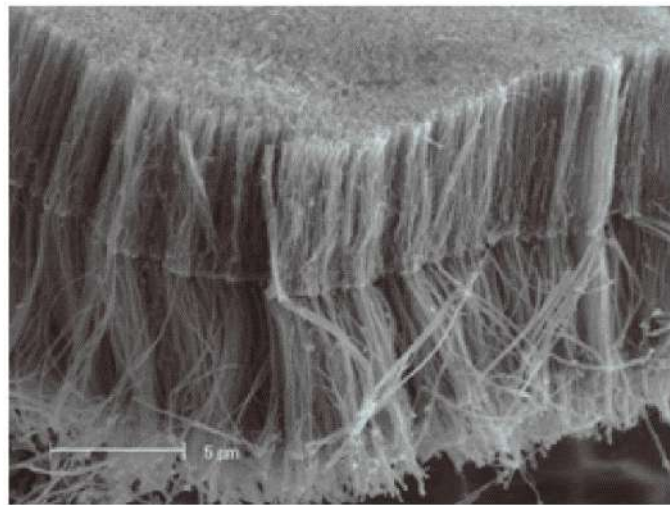


Figure 8.1 *A tower of multiwalled carbon nanotubes*

Materials that are comprised of many small structures often have a very large surface area. The reason is that the surface areas of the many small structures together contribute to a very large surface area of the bulk material. For example, if the size of a shoe box were to be split up into 2 nm spheres, these spheres would correspond to the area of 10,000 football fields. It is not surprising that when the surface area is so large, the physical properties are dominated by surface interactions.

Nano-materials come in many varieties. A few examples of materials that exhibit interesting properties on the nanoscale are carbon nano-tubes, inorganic nano-wires, dendrimers, nano-particles, quantum dots, nano-plates and **nano-composites**.

1. Carbon Nanotubes

Carbon nanotubes were discovered in 1991 by Sumiyo Iijima, a Japanese scientist working at the NEC Corporation. A carbon nanotube (CNT) is a tubular form of carbon with a diameter as small as 0.4 nm and length from a few nanometers up to a millimeter (Fig. 8.1). The length-to-diameter ratio of a carbon nanotube can be as large as 28,000,000:1, which is unequalled by any other material. Usually nanotubes are formed by graphene sheet (Fig. 8.2).

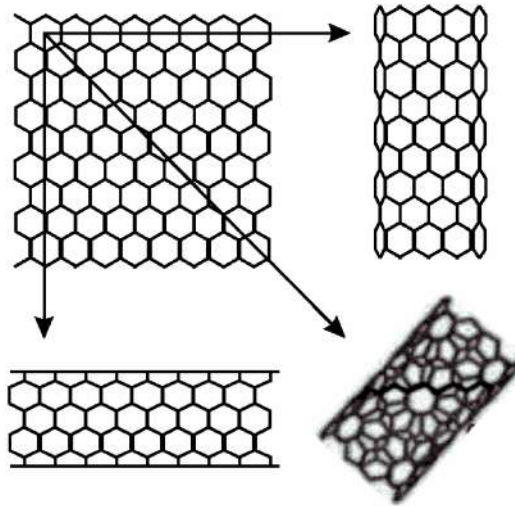


Figure 8.2 A sheet of graphene rolled to show formation of different types of single-walled carbon nanotubes

Carbon exists in several forms; graphite and diamond are the most familiar. Graphene is the basic structural element of some carbon allotropes including graphite, carbon nanotubes and fullerenes. It can also be considered as an infinitely large aromatic molecule, the limiting case of the family of flat polycyclic aromatic hydrocarbons called graphenes. Graphene is a one-atom-thick planar sheet of sp^2 -bonded carbon atoms that are densely packed in a honeycomb crystal lattice. It can be visualized as an atomic-scale chicken wire made of carbon atoms and their bonds. The name comes from graphite + ene; graphite itself consists of many graphene sheets stacked together. The carbon-carbon bond length in graphene is about 0.142 nm.

To imagine how a carbon nanotube looks like, think about taking a single layer of a graphite sheet, cutting it into a small piece of any size, and rolling it like you would roll a cigar. The result is a single-wall carbon nanotube (SWCNT) shown in Fig. 8.3. If we take multiple layers of a graphite sheet and roll them like a cigar, then we get a multiwall carbon nanotube (MWCNT). Carbon nanotubes are available in Arm chair, Wavy, and Zig-zag structure.

Carbon Nanotubes are grown in laboratories, often using a process called chemical vapor deposition. Though many sophisticated commercial growth reactors are available, carbon nanotubes can be made in a standard chemistry laboratory. A quartz tube about 1 inch in diameter serves as the growth reactor and is inserted inside a tube furnace (a tube furnace is a standard heating device for conducting syntheses and purifications). The nanotube is grown on a silicon wafer that placed at a central location inside the quartz tube. A thin layer of iron or nickel or cobalt is applied to the silicon wafer to serve as a catalyst to grow the nanotubes. A hydrocarbon such as methane (high purity form of natural gas) or ethane or acetylene is sent through the reactor tube which is heated to 750-900°C by the furnace.

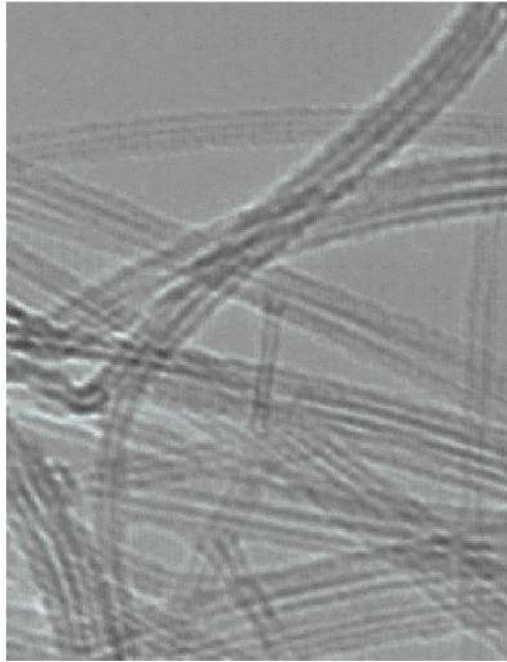


Figure 8.3 *Single-walled carbon nanotubes*

In a few minutes, the silicon wafer appears black, indicating that it is covered with nanotubes. Depending on growth conditions (temperature, type of gas, thickness of catalyst etc), single-wall or multi-wall carbon nanotubes are found on the silicon wafer. These can be viewed using powerful microscopes such as a *scanning electron microscope* or a *transmission electron microscope*.

In addition to unique electronic properties, single wall carbon nanotubes exhibit extraordinary mechanical properties. They are a hundred times stronger than steel at one-sixth of its weight. Their ability to carry current and heat along the axial direction is extraordinary, and therefore has the potential to replace copper wires as conductors.

The exciting properties of carbon nanotubes have led to wide ranging studies across the world for their use in high strength but low weight composites, body armor, conducting polymers, electrostatic discharge protection, computer chips, chemical and biosensors and many other applications.

2. Inorganic Nanowires

Inorganic materials cover the entire span of the periodic table. Examples range from elemental semiconductors (silicon, germanium), metals (copper, aluminum), to compounds such as gallium arsenide, and all kinds of oxides and nitrides. In the last three decades, these inorganic materials have been successfully grown in the form of *thin films* with a film thickness as small as 1 nm and as high as several microns (Fig. 8.4).

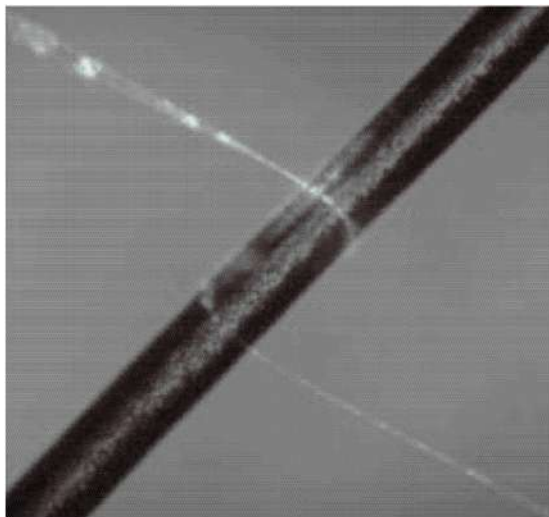


Figure 8.4 *A light-conducting silica nanowire wraps a beam of light around a strand of human hair. The nanowires are flexible and can be as slender as 50 nanometers in width, about one-thousandth the width of a hair*

Thin films are ubiquitous in products all around us, including computers, CDs, DVDs, cell phones, iPods, lasers (used in supermarket scanners as well as eye surgery), solar panels, and flat panel TVs. Recently there is interest in growing these same materials in the form of one dimensional nanowires rather than as two dimensional thin films.

Inorganic nanowires may have diameters of 1-50 nm and any desirable length, perhaps up to a micrometer. They offer interesting electronic, optical and other properties, and may be used in the future to link tiny components into small scale circuits. The properties of nanowires are projected to allow improved performance in existing products as well as development of new products.

Nanowires of silicon and germanium are useful in making future generation computer chips and memory devices. A variety of oxides such as zinc oxide, tin oxide, and indium tin oxide are now grown in the form of nanowires. Zinc oxide is being considered for ultraviolet (UV) lasers and light emitting diodes (LEDs). A variety of nitrides such as gallium nitride and aluminum nitride find applications in solid state lighting that may replace the inefficient filament light bulbs.

3. Dendrimers

Dendrimers are a special class of polymers. A *polymer* is a huge molecule made up of tens of thousands of repeating units called monomers. A monomer is a simple organic molecule which reacts with other monomers to form a large polymer. Polymers are ubiquitous in our lives, they represent a large class of natural and synthetic materials including textiles, rubber, tires, fishing net, stockings, sporting goods, and plastics.

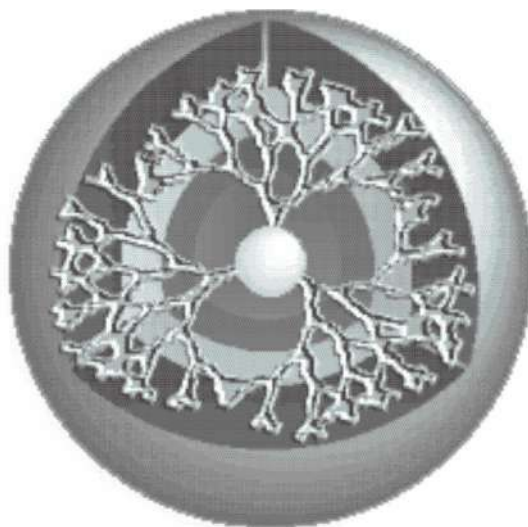


Figure 8.5 Image of dendrimers which are tree-like polymers with a cavity in the middle

The typical polymers run like linear chains, whereas, dendrimers are tree-like polymers (Fig. 8.5). They branch out from a central core, exhibiting a dense surface surrounding a relatively hollow core. They are a series of chemical shells built on a small core molecule. The size is typically not more than 15 nanometers but the molecular weight is large.

Since the central core of a dendrimer is hollow, it can be used to trap or store “guest molecules.” The interior and the core of dendrimers can thus be tailored for different applications. One area that has attracted interest is biomedical applications. In these applications the guest molecules are drugs, candidates for gene therapy or cancer therapy, or antimicrobial and antiviral agents. Another area of interest is the synthesis of organic *light emitting polymers*.

4. Nano-particles

Nanoparticles (sized between 1 and 100 nanometers) are considered a bridge between bulk materials and atomic or molecular structures. A bulk material has constant physical properties regardless of its size, but often this is not the case at the nano scale.

One of the important characteristics of nano-particles is their large ratio of surface area to volume (compared to bulk materials). This property can be illustrated by the following thought experiment: consider a cube of edge $W=1$ meter, and cut it into two pieces, thereby exposing additional ‘faces’ of the material. That is, new visible or usable areas are added while the total volume remains the same. Repeat this exercise until all particles reach a size of approximately one nanometer. The result is a group of small particles with enormous surface area which occupy the same volume we started with. There are nano-materials which exhibit a surface area equivalent to a football field for just a few grams of weight.

Large surface area makes some nano-particles highly soluble in liquids. This property found applications in paints, pigments, medicine pills, and cosmetics. A 30 nanometer iron particle has 5% of its atoms on the surface while the remaining reside inside. However, a 3 nm particle has 50% of its atoms on the surface. Fig. 8.6 illustrates how surface area increases as the size is reduced. The atoms on the surface, which are not bonded on one side, are far more active than the atoms residing inside (which are bonded all around, thus they are “satisfied”). An increase in surface area therefore leads to an increase in reactivity.

Particle size can also affect the *color* of the material, with applications in the production of inks, for example for glossy magazines where color schemes are of great interest. Large surface areas are also attractive for a process called *adsorption*. Adsorption occurs when a gas or liquid solution accumulates on the surface of a solid or a liquid (adsorbent), forming a film of molecules or atoms. Large surface areas increase adsorption. This process is useful in applications such as catalytic converters, water purification devices, waste recovery technologies, and manufacturing of deodorants, perfumes, varnishes and adhesives.

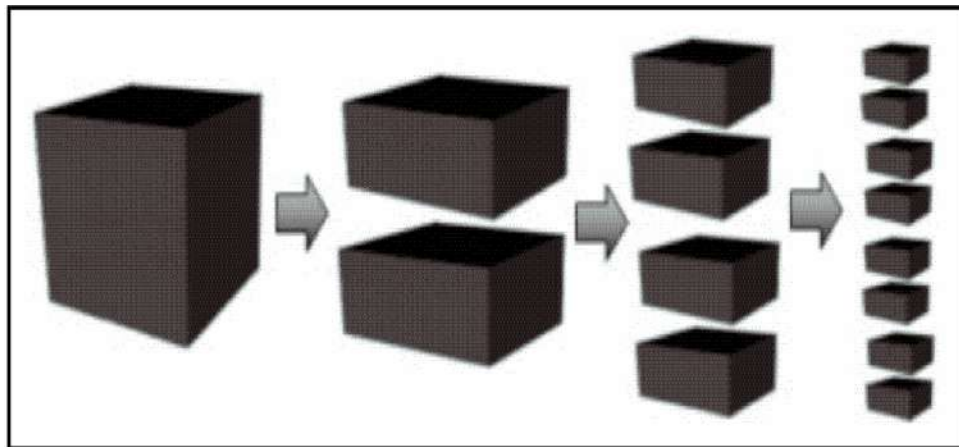


Figure 8.6 This image illustrates how surface area increases as the size is reduced

Once nano-particles are produced, it is desirable that they maintain their small dimensions. However, in some cases, agglomeration of small particles into a bigger lump has been observed. When this happens, most of the advantages of using nanoparticles are lost. Scientists are looking into preventing agglomeration, for example by using surface coatings that prevent the union of particles.

5. Quantum Dots

Quantum dots are used for drug delivery, multicolored display, quantum dot lasers (Fig. 8.7), etc. A quantum dot is a tiny structure made of a solid material. It is so tiny (typically consisting of 1,000-10,000 atoms) that an electron inside it is severely restricted in its movement. Now, when an electron's motion is so severely constrained, its kinetic energy can assume only certain allowed values that are determined by the size and shape of the dot, as well as the material making up the dot.

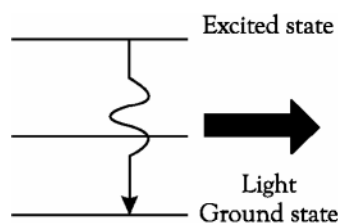


Figure 8.7 Light is emitted when an electron in a quantum dot decays from an excited state to a ground state

Gallium arsenide (GaAs) is a popular material out of which quantum dots can be made, because the effective mass of an electron and the shape of the crystal correlate at room temperature to form desirable properties. Note that 1 nanometer = 10^{-9} meter, which is roughly 100,000 times smaller than the thickness of human hair. Since atoms in GaAs are spaced approximately 0.5 nm apart, a quantum dot contains about 25,000 atoms.

One important property of quantum dots is their exceptionally large surface-to-volume ratios. In the case of a cube of edge W , this ratio is $6/W$; in the case of a sphere of diameter D , the ratio is $6/D$. The ratio increases as the dimension of the dot (W or D) becomes smaller. For a basketball of diameter 0.1 m, the ratio is 60 m^{-1} , but for a quantum dot of diameter 10 nanometers (10^{-8} m), the ratio is $6 \times 10^8 \text{ m}^{-1}$, which is ten million times larger. The large surface-to-volume ratio of the quantum dot is used in chemical and biological sensors. The sensing activity typically takes place only on the surface and not in the interior; therefore it pays to have a large surface-to-volume ratio. It may be beneficial to replace a large sensing particle with several tiny particles or quantum dots.

To understand this even better, note that the volume of the basketball is 10^{21} times larger than that of the quantum dot we just described, so the basketball can be broken up into 10^{21} quantum dots. The combined surface area of all these dots is 10^7 times larger than that of the basketball. Therefore, breaking up the basketball into quantum dots, results in a sensor that is *ten million times more effective*. That is why quantum dots are so important in applications such as sensing, targeted drug delivery, and catalysis - all of which require a large surface-to-volume ratio.

Quantum dots are also useful in multi-colored displays (Fig. 8.7). They emit light when an electron inside the dot undergoes a transition from a higher energy (excited) state to a lower energy (ground) state. The color of the emitted light depends on the difference in the energies of the final and initial states as well as the size of the dot. Therefore, quantum dots of different sizes will emit different colored light. This is the basis of multicolored display.

Fabricating quantum dots with good control over size, material purity, and placement on a given surface is not an easy task. Two approaches are common: the “top-down approach” where a large piece of material is chiseled down to a small quantum dot using the process of lithography and etching. A slight variation of this approach is *electrostatic delineation of quantum dots* where metal pads are placed on a thin layer of material. A negative potential is applied to the pads, which drives away the electrons from underneath, leaving a small puddle of electrons in the center, which form a quantum dot.

The second approach is “bottom up” and is known as self-assembly. Here, spontaneous congregation of atoms into structures of well defined size (of a few nanometers) and shape form quantum dots.

Directed self assembly is a refinement of the process, where the spontaneous congregation is allowed to proceed on a patterned substrate that offers preferred sites for nucleation of quantum dots. This is also referred to as *template-based self assembly* since the patterned substrate acts as a template for spatially ordering the quantum dots.

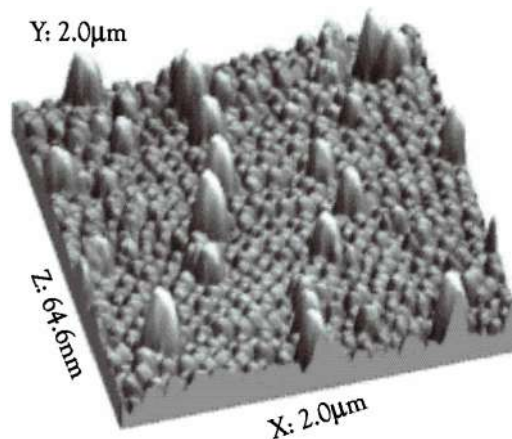


Figure 8.8 An atomic force micrograph of Lanthanum Monosulfide quantum dots formed by pulsed laser deposition of the material on a porous alumina film

Fig. 8.8 shows an example where a material was deposited on a porous ceramic film containing a quasi-periodic array of pores. The deposited atoms congregated on the island between the pores to form a spatially ordered array of pyramidal quantum dots.

Quantum dots can also be synthesized by selectively electrodepositing materials within the pores. This process would result in an array of quantum dots embedded in an insulating ceramic matrix. The bottom up technique is cheaper than the top down technique and usually results in higher quality product since it is also ‘gentle’ and less invasive.

Quantum dots are fascinating entities that are increasingly making their way into a large assortment of commercial and defense related products. Rapid advancements are being made in perfecting the synthesis methods and one can expect to see quantum dots permeate the marketplace within the next decade or so.

6. Nano-composites

Nano-composites are materials with a nanoscale structure that improve the macroscopic properties of products. Typically, nano-composites are clay, polymer or carbon, or a combination of these materials with nano-particle building blocks.

Nano-composites, materials with nanoscale separation of phases can generally be divided into two types: multilayer structures and inorganic/organic composites. Multilayer structures are typically formed by gas phase deposition or from the self-assembly of monolayers. For example, inorganic/organic composites can be formed by sol-gel techniques, bridging between clusters, or by coating nano-particles, in polymer layers. Nano-composites can greatly enhance the properties of materials. For example, ppm level impurities can result in the formation of nanoscale aluminide secondary phases in aluminum alloys, increasing their strength and corrosion resistance. Magnetic multilayered materials are one of the most important aspects of nano-composites as they have led to significant advances in storage media.

7. Nanoplates

Until recently, thin coatings on a substrates have not been considered as nano-objects, but simply as thin films, because typically they have been more than 100 nm thick. Exceptions are Langmuir films (a class of organic monolayer/multi-layer films), transferred to solid substrate using the Langmuir-Blodgett and Langmuir-Schaefer techniques and these films are of only few nanometer thick. Such Langmuir films are also called nanoplates.

8.4 METHODS OF PREPARATION OF NANOMATERIALS

Nano-technology is dependent on nanostructures that require creation and characterization. Two fundamentally different approaches for the controlled generation of nanostructures have evolved. On one hand there is growth and self assembly, from the **bottom up approach**, involving single atoms and molecules. On the other hand, there is the **top-down approach** in which the powerful techniques of lithography and etching start with large uniform pieces of material and generate the required nanostructures from them. Both methods have inherent advantages. Top down assembly methods are currently superior for the possibility of interconnection and integration, as in electronic circuitry. Bottom-up assembly is very powerful in creating identical structures with atomic precision, such as the supramolecular functional entities in living organisms. The main route of bottom-up formation of nano-particles in the gas-phase is by a chemical reaction leading to a non-volatile product, which undergoes homogeneous nucleation followed by condensation and growth. Recently, this has become an important pathway for the industrial production of nanoparticle powders, which may be of metals, oxides, semiconductors, polymers and various forms of carbon, and which may be in the form of spheres, wires, needles, tubes, platelets or other shapes.

Some of the methods used in the preparation of nano-materials are :

- Atomic Layer Deposition
- Physical Vapor Deposition
- Polymers for Electrospinning
- Self Assembly & Contact Printing
- Sol-Gel Processing
- Mechanical Deformation

8.4.1 Sol-gel Method

The sol-gel process is a wet-chemical technique (also known as Chemical Solution Deposition) widely used recently in the fields of materials science and ceramic engineering. Such methods are used primarily for the fabrication of materials (typically a metal oxide) starting from a chemical solution (*sol*, short for solution) which acts as the precursor for an integrated network (or *gel*) of either discrete particles or network polymers.

Typical precursors are metal alkoxides and metal chlorides, which undergo hydrolysis and polycondensation reactions to form either a network “elastic solid” or a colloidal suspension (or dispersion)—a system composed of discrete (often amorphous) submicrometer particles dispersed to various degrees in a host fluid. Formation of a metal oxide involves connecting the metal centers with oxo (M-O-M) or hydroxo (M-OH-M) bridges, therefore generating metal-oxo or metal-hydroxo polymers in solution. Thus, the sol evolves towards the formation of a gel-like diphasic system containing both a liquid phase and solid phase whose morphologies range from discrete particles to continuous polymer networks.

In the case of the colloid, the volume fraction of particles (or particle density) may be so low that a significant amount of fluid may need to be removed initially for the gel-like properties to be recognized. This can be accomplished in any number of ways. The most simple method is to allow time for sedimentation to occur, and then pour off the remaining liquid. Centrifugation can also be used to accelerate the process of phase separation.

Removal of the remaining liquid (solvent) phase requires a drying process, which is typically accompanied by a significant amount of shrinkage and densification. The rate at which the solvent can be removed is ultimately determined by the distribution of porosity in the gel. The ultimate microstructure of the final component will clearly be strongly influenced by changes implemented during this phase of processing. Afterwards, a thermal treatment, or firing process, is often necessary in order to favor further polycondensation and enhance mechanical properties and structural stability via final sintering, densification and grain growth. One of the distinct advantages of using this methodology as opposed to the more traditional processing techniques is that densification is often achieved at a much lower temperature.

The precursor sol can be either deposited on a substrate to form a film (e.g. by dip-coating or spin-coating), cast into a suitable container with the desired shape (e.g. to obtain a monolithic ceramics, glasses, fibers, membranes, aerogels), or used to synthesize powders (e.g. microspheres, nanospheres). The sol-gel approach is a cheap and low-temperature technique that allows for the fine control of the product's chemical composition. Even small quantities of dopants, such as organic dyes and rare earth metals, can be introduced in the sol and end up in uniformly dispersed in the final product. It can be used in ceramics processing and manufacturing as an investment casting material, or as a means of producing very thin films of metal oxides for various purposes. Sol-gel derived materials have diverse applications in optics, electronics, energy, space, (bio)sensors, medicine (e.g. controlled drug release) and separation (e.g. chromatography) technology.

The interest in sol-gel processing can be traced back in the mid-1880s with the observation that the hydrolysis of tetraethyl orthosilicate (TEOS) under acidic conditions led to the formation of SiO_2 in the form of fibers and monoliths. Sol-gel research grew to be so important that in the 1990s more than 35,000 papers were published worldwide on the process.

8.4.2 Other Methods

- (i) **Physical vapour deposition:** Atom clusters are typically synthesized via vapour deposition which is essentially evaporation of a solid metal followed by rapid condensation to form nanosized clusters. The resulting powder is essentially agglomerates of the nano-sized atom clusters. The powder can be used as fillers for composite materials or consolidated into bulk materials. The cluster assembly method can be used to produce ceramic or metal nanostructured powders.
- (ii) **Chemical Synthesis:** Both metals and ceramics can be produced using a variety of chemical approaches such as sol-gel or thermal decomposition. These methods provide large quantities of nano-sized agglomerates at low cost. Chemical processes allow effective control.
- (iii) **Mechanical Deformation:** A common method of producing nanostructured powders is through mechanical deformation, i.e. milling or shock deformation. These processes produce nano-structured materials. The nanometer sized grains nucleate within the dissociation cell structures located in the shear bands. The final grain size is a function of the amount of energy input during the milling as well as time, temperature during milling and milling atmosphere. Thus through mechanical milling, it is possible to produce nanostructured powders of systems which are otherwise immiscible.

8.5 CHARACTERIZATION

The first observations and size measurements of nano-particles were made during the first decade of the 20th century. They are mostly associated with the name of Zsigmondy who made detailed studies of gold sols and other nanomaterials with sizes down to 10 nm and less. He published a book in 1914. He used ultramicroscope that employs a *dark field* method for seeing particles with sizes much less than light wavelength.

There are traditional techniques developed during 20th century in Interface and Colloid Science for characterizing nanomaterials. These methods include several different techniques for characterizing particle size distribution. This characterization is imperative because many materials that are expected to be nano-sized are actually aggregated in solutions. Some of methods are based on light scattering. Other apply ultrasound, such as ultrasound attenuation spectroscopy for testing concentrated nano-dispersions and microemulsions.

There is also a group of traditional techniques for characterizing surface charge or zeta potential of nano-particles in solutions. This information is required for proper system stabilization, preventing its aggregation or flocculation. These methods include microelectrophoresis, electrophoretic light scattering and electroacoustics.

8.6 WONDERS OF NANOTECHNOLOGY: DISCOVERY OF FULLERENE AND CARBON NANOTUBES

Carbon is one of the commonest substances on Earth and it is widely distributed in nature. All life is carbon-based, and this gives rise to the description of the chemistry of carbon compounds as Organic. Carbon was probably the first element that man was aware of since it is produced in the form for charcoal from burned wood. Charcoal, used in early cave painting and by the artists today, consists of very small crystals of graphite, one of two forms of carbon. The other form is diamond, which is

especially famous for its hardness and its high dispersion of light. These properties make diamond valuable in jewel industry as well as in other industrial applications. Until the late twentieth century, graphite and diamond were the only known allotropes of carbon. Fullerenes were first discovered in 1985 in an apparatus designed by Prof. Rick Smalley to produce atomic clusters of the non-volatile element. The discovery of this new form of pure carbon, and the insight that led to the interpretation of the magic number features in the observed mass spectra in terms of hollow carbon molecules, led to the award of the Noble Prize in Chemistry to Curl, Kroto and Smalley in 1996.

8.6.1 Discovery of Fullerenes

The discovery of C_{60} has a long and very interesting history. In 1970, Eiji Osawa realized that a molecule made up of SP^2 hybridized carbons could have the soccer structure. He therefore made the first proposal for C_{60} . But this prediction turned out to be incorrect later. In 1985, Professor Kroto, from University of Sussex, UK, met Professor Curl, from Rice University, at a conference on molecular structure in Austin, Texas. Kroto went back to Houston with Curl, who introduced him to Smalley and showed him around the lab. They arranged to examine a special kind of carbon produced in a cluster beam apparatus of Smalley. After discounting various highly improbable structures, they concluded that the molecule must be a cage, and Smalley succeeded in building it out of his paper and tape. The paper including describing this work was submitted to *Nature*, on September 12th, 1985. They named C_{60} as Buckminsterfullerene, because of the similarity of the structure to be geodesic structures widely credited to R. Buckminster Fuller. Because of this work, Kroto, Smalley, and Curl were awarded the Nobel Prize in Chemistry in 1996 as mentioned before.

However, in 1990, Wolfgang Kratschmer of Heidelberg University and Donald Huffman of the University of Arizona discovered a really simple way to produce solid fullerenes by arc-vaporization of graphite in a helium environment. Since then, the field of fullerenes developed rapidly and made an impact in many different scientific areas.

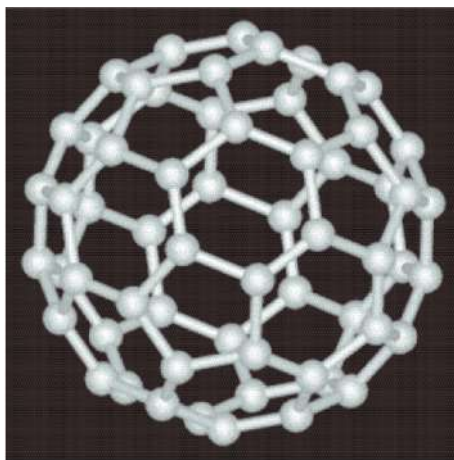


Figure 8.9 Structure of C_{60} (Fullerene)

Properties of Fullerenes

Unlike graphite or diamond, fullerenes are closed-cage carbon molecules, consisting of a number of five-membered rings and six-membered rings. In order to make a closed cage, all the fullerene molecules should have the formula of C_{20+m} , where m is an integer number. For example: the structure of C_{60} is a truncated icosahedron, which looks like a soccer ball with 12 pentagons and 20 hexagons (Fig. 8.9). The bonds in C_{60} are having two different kinds. The reason for this is that it would increase strain to have a double bond in a pentagon. As a result, the length of a bond in a pentagon is 1.45\AA , that of a bond between pentagons is 1.40\AA . As the size increases, the solubility of fullerene decreases. At room temperature, the solubility of C_{60} is about 2.8 mg/ml in toluene. As the size increases, the heat of sublimation of fullerene increases. For C_{60} , the value is 43.3 Kcal/mol. C_{60} is unstable at higher temperatures and measurable decomposition can be observed about 830K. The process of decomposition is faster in the presence of oxygen.

Preparation of Fullerenes

Fullerenes can be prepared in simple processes. Graphite rods are vaporized in an atmosphere of inert gas, helium the best, by passing a high electric current through them. This produces a light condensate called fullerene soot, which contains a variety of different fullerenes. The fullerenes can be extracted by a number of different solvent. Toluene is the most widely used due to its low cost, low boiling point and relatively large capacity of carrying fullerenes. Separation and purification can be achieved by column chromatography.

Applications of Fullerenes

Because of their unique structures and properties, fullerenes draw lots of attention from physicists, chemists and engineers, who are trying to find some potential applications of these new carbon structures. Nowadays, scanning probe microscopy (SPM) is one of the most important tools in the field of surface chemistry. Carbon nanotube, which has small diameter and high aspect ratio, is a ideal material that can be used as tips in SPM, such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM). It is reported that nanotubes attached tip can be used to enhance SPM resolution to nanoscale. In these research works, nanotubes were attached on conventional Si tips under a microscope by acrylic adhesive. However, this method is difficult to control the length of the tip, and it is always difficult to get a strong and reliable attachment. In 1999, a new method to make carbon nanotube tips for SPM was reported. In this method, nanotubes were prepared by conventional arc discharge method. After purification, they were aligned by electrophoresis on the knife edge of a disposable razor. Then one single nanotube was transferred onto a Si tip and it was attached onto the Si tip by the deposition of carbon. In order to compare the nanotube tip and conventional Si tip, both tips were used to image DNA molecules by AFM. As a result, the image produced by nanotube tip showed a factor of two lateral resolution improvement than the image by the conventional tip.

These manual methods of producing nanotube tips, though produce some good results, is very time consuming. A new method called chemical vapor deposition (CVD) was developed to make the production of nanotube tips more practical. The fabrication of nantube tips by CVD can overcome the limitations that manual methods have. So it is a preferred method to produce nanotube tips.

Overall, the advantage of the nanotube tips over conventional Si tips is high lateral resolution due to its high aspect ratio and small diameter. It is also more mechanically flexible, so it can be elastically buckled without any damage to the tip. It has long life time because it won't be broken by an accidental contact on the surface. It can be applied to image some structure with steep sidewalls, such as silicon trenches.

Fullerenes and their derivatives are also applied to coat materials on some chemical sensors, such as quartz crystal microbalance (QCM) and surface acoustic wave sensors (SAW). Both QCM and SAW have a key component called piezoelectric crystals, which are well known to be very sensitive to mass changes on their surface. Thus, they can be applied for trace quantitative analysis. Because of its affinity to organic molecules, fullerenes C_{60} and its derivatives can be coated onto piezoelectric crystal and applied as a chemical sensor for organic molecules. In studies carried out by Shih, J.S. et al., they prepared a kind of fullerene derivatives called fullerene C_{60} -cryptand and then spin coated them onto both sides of the piezoelectric crystal of a chemical sensor. The sensor was used to detect organic molecules such as propanol, butanol, ethanol and methanol. As the organic molecules adsorbed on to the fullerene derivative film, the oscillating frequency of the piezoelectric crystal decreases, the change is proportional to the concentration of the adsorbent. In this way, the concentration can be determined.

8.6.2 Discovery of Nanotubes and Nanoparticles

In addition to fullerenes and endohedral fullerenes, carbon nanotubes are another kind of carbon materials that can be produced by vaporizing graphite rods under specific conditions. These tubes can be synthesized in relatively large quantities and has been predicted for many applications. Basically, nanotubes are elongated fullerenes, they are made up by hexagons as well as pentagons in the end caps in order to close the tube. Arranging the pentagon in different ways can give different shape to the caps. The shapes of the outer caps is parallel to that of the inner ones. Because nanotubes are elongated fullerenes, as fullerenes can be either empty (single-wall nanotube, SWNT) or nested (multi-wall nanotube, MWNT). MWNTs are usually straight, while SWNTs are more flexible (Fig. 8.10).

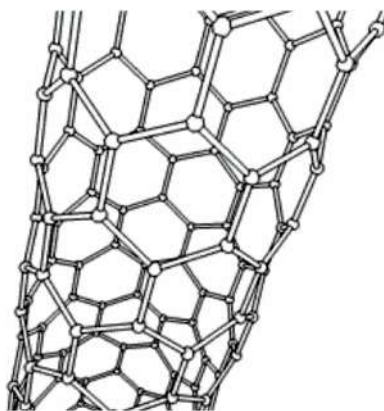


Figure 8.10 Model of a rotating carbon nanotube shows its 3D structure

After Iijima reported that carbon nanotubes could be deposited on the cathode of a fullerene-soot generator, Ebbesen and Ajayan published a paper on how to make large quantities of nanotubes. They also got a particular type of carbonaceous deposit formed on the cathode of their apparatus. Under some further study, they conclude that certain interior region contained large quantities of carbon nanotubes as well as nanoparticles. The nanoparticles are normally tens of nm in diameter and consist of many concentric graphite layers. Ebbesen and coworkers have reported the separation of nanotubes from nanoparticles by heating mixture of nanotubes and nanoparticles in pure oxygen. It is worth pointing out that although fullerenes, nanotubes and nanoparticles can form in the same environment and they also have similar formation process, nanotubes and nanoparticles form in significant yield under a broader range of conditions than fullerenes do.

Molecular sensors based on semiconducting single-walled carbon nanotubes (SWNT) are also developed. The electrical resistance of this SWNT changes dramatically when it is exposed to gas molecules such as NO_2 and NH_3 . For the NO_2 case, the conductance of the SWNT increases by about three orders of magnitude when 200 ppm NO_2 is introduced. For the NH_3 , using the same SWNT, the conductance decreases 100-fold when it is exposed to an Argon flow with 1% NH_3 . Combining with their small size, room temperature operation and high sensitivity, carbon nanotube sensors should be a promising chemical sensors.

Because of their high aspect ratios, carbon nanotubes can be also used as a field emission source. At 1995, an electron gun based on field emission for a film of aligned carbon nanotubes was made by Dr. W. A. de Heer and coworkers. The schematic diagram of the electron source is shown at Fig. 8.11. It consists of three important components. First Component (a) is a carbon nanotube film on a polytetrafluoroethylene (PTFE) substrate. Second Component (b) is a perforated mica sheet with a thickness of $20\mu\text{m}$ and a hole of 1mm in diameter. Third Component (c) is an electron microscopy copper grid, which covers the hole in Second component.

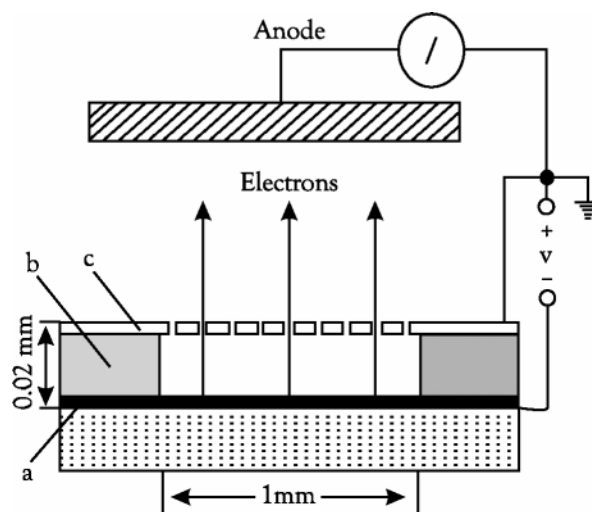


Figure 8.11 Schematic diagram of the CNT electron source

Scientists are now trying to make field emission displays (FED) using carbon nanotubes as field emission electron sources. FEDs is similar to the conventional television cathode ray tubes (CRT). But the big difference is that each pixel has its own electron source. This difference allows FEDs to be made only several millimeter thick and still have the same picture quality as conventional CRTs. Compared to other kinds of flat panel display, such as LCD and Plasma, FEDs are more power saving, cheaper to make and having wide view angles.

The discoveries of fullerenes and carbon nanotubes have opened a new chapter on the physics and chemistry of carbon. So far, the physical and chemical properties of fullerenes and carbon nanotubes are still under investigation. More research are needed to be done to confirm the suitability of some important application. Some potential applications will need more time for them to become reality.

8.7 APPLICATIONS OF NANOTECHNOLOGY

Nano-particles are now being used in the manufacture of scratchproof eyeglasses, crack- resistant paints, anti-graffiti coatings for walls, transparent sunscreens, stain-repellent fabrics, self-cleaning windows and ceramic coatings for solar cells. Nano-particles can contribute to stronger, lighter, cleaner and “smarter” surfaces and systems.

8.7.1 General Applications

Nano-technology has applications in areas such as information and communications, materials and manufacturing, biomedical, energy and environmental, transportation, and consumer goods.

1 Information and Communications

Nano-technology has enabled many advances in computer memory, increasing storage size, reducing power consumption, and increasing speed. These three factors will enable sophisticated computer controlled devices in the future.

Nano-RAM (or NRAM) is a random access memory that uses carbon nanotubes to determine the state of the memory element, comprising an information bit. This memory is a non-volatile device meaning that its cells maintain their information regardless of whether or not power is supplied to the system (the carbon nanotubes keep their mechanical position whether or not power is supplied). NRAM (which is a proprietary computer memory technology) has been projected to be of very high density and low cost.

2 Materials and Manufacturing

Materials and manufacturing deal with the application of knowledge relating to composition, structure and processing of materials to their properties and applications.

In the last few years there was significant increase in the development of *composite materials* with excellent properties. Composite materials are engineered materials which are made from two or more constituent materials with significantly different physical or chemical properties. Nano-technology has emerged as a key technology used in fabrication of composite materials.

Though “top-down” fabrication methods are still used, nano-technology has empowered a “bottom-up” approach to modify the material properties at nanoscale level.

3 Biomedical Applications

Nano-technology is expected to have a significant impact on improving the quality of health care through early and reliable diagnostics of diseases, better drugs, targeted drug delivery, improved implants, and other applications.

Biosensors are fabricated using a combination of nanomaterials, novel device fabrication and advanced signal processing techniques and are being developed for early detection of several life threatening illnesses. These sensors use carbon nanotubes or silicon nanowires which can host the probe molecule that seeks to identify the signature of a particular condition or illness. Nanobiosensors using this approach are expected to be mass-produced using techniques developed by the computer chip industry.

Nano-technology will also play an important role in therapeutics. Two areas where nanotechnology is expected to make an impact are *synthesis of improved drugs* using principles of nanotechnology, and *targeted drug delivery*. Specifically, a certain family of molecules known as *dendrimers* are considered as candidates for effective delivery of drugs. These large polymers have a pouch-like configuration at their centers which can be used to host drugs inside the molecules that carry them to their destination.

Individuals who need artificial parts in their body like legs, limbs, ligaments or organs, can expect more reliable and rejection-proof substitutes using nano-materials, better composites using nanotubes, nano-particles, and other nano-materials with desirable mechanical properties. Some of the desirable properties include better response to electrical and other forces. These would contribute to the development of reliable, durable artificial components.

4 Energy and Environmental Applications

Skyrocketing oil prices, concerns about the environment from increasing greenhouse emissions, and the desire to save the planet from environmental disasters, have turned wide attention to alternative energy sources and to the need to increase the energy efficiency of the systems.

The alternative light sources include fluorescent lamps, high-intensity discharge lamps, and light-emitting diodes (LEDs). Nano-technology innovations are applied intensively to reduce the cost of producing some of the alternative light bulb designs.

Nano-materials are beginning to play a prominent role in developing other alternative energy technologies. Much of the solar cells produced worldwide today rely on bulk crystalline technology which competes with the computer industry for the silicon raw material. This is not a desirable situation, since both solar energy and computer electronics are critical technologies with high demand and expanding volumes. Alternative research directions include novel nanomaterials such as quantum dots to increase efficiency; and production of solar cells on flexible substrates (like plastic, thin metal sheets). Lightweight and high strength composites for *wind turbine blades* are being developed using nanocomposites to harness wind energy.

Environmental pollution of air, soil and water, including the impact of toxic waste in landfills, is a major concern across the world. Using nano-technology, scientists are designing new catalysts for waste remediation, and for conversion of toxic gases into benign components. These designs take advantage of the large surface area of nano-materials and of the novel properties and reactivity that arise at the

nanoscale. New, efficient filters to trap mercury, heavy metals and other hazardous substances are developed, using carbon nanotubes and other nano-materials.

5 Transportation Applications

One of the major contributions that nano-technology can make in the transportation sector is lighter weight and high strength composite materials (“composites”) for the construction of airplanes and automobiles.

Composites are created from two or more materials with significantly different physical or chemical properties. These properties remain distinct within the finished structure. The promise of *nano-composites* is that they will be lighter and stronger than other kinds of widely used composites.

After decades of research and development, composites were first used in civil aviation when Boeing unveiled its 777 airplane in the mid 1990s. Until then, aluminum and other metals were used for airplane bodies. In the next generation of planes (e.g., the Boeing 787 Dreamliner), nearly 50% of the material in use is composites.

Among the leading candidates to become the nanocomposites of choice are *Carbon nanotube based nanocomposites* and *polymer clay nanocomposites*. Nanocomposites are expected offer higher fuel savings to the aerospace industry because of their lighter weight (at strength levels similar or better when compared to those of currently-used materials). The use of nanocomposites also allows for more comfortable journey for airline passengers, since higher cabin pressure and humidity levels are possible; composites suffer less than metals from material fatigue and corrosion.

Some of the other benefits expected from developments in nanotechnology for the aerospace industry are wear-resistant and corrosion-resistant coatings, de-icing coatings, wear-resistant tires, better protection against lightning, sensor networks for monitoring vehicle health, and improved navigation and communication systems.

In the automotive sector, the biggest thrust is to develop alternatives to gasoline and diesel powered engines. Researchers are looking into efficient storage of hydrogen into nanoporous materials that would enable hydrogen powered cars. Other nano-enabled benefits in the automotive sector include high strength and light weight components, paintable polymers, anti-fouling paints, ultraviolet light (UV) protective coatings, corrosion protection, and organic light emitting diodes (LEDs) for panel lighting and instrumentation.

Many transportation applications use *multifunctional material*. While the major function of the structure is often load-bearing, additional properties of the material are desirable. Such properties involve: electrical characteristics (conducting or insulating); thermal characteristics (conducting or insulating); health effects (monitor, control); sensing (physical variables such as stress, strain); reaction to environmental effects (ice, rain, contaminants); stealth (managing or suppressing electromagnetic or visible radar signatures); and actuation.

6 Consumer Goods Applications

Nano-technology is emerging from the science laboratory into the marketplace, and is used today in the design and manufacturing of many commercial devices and systems. Among the fields affected

by nanotechnology are medical and environmental applications, food production and processing, energy (storage, conversion and saving), information and communication, and improvements to textile and automotive products.

Applications of nano-technology in *medicine* include the development of *contrast agents* for cell imaging. These agents assist in visualization of cells, and contribute to biomedical research and to medical diagnostics (detection and classification of diseases). Nano-technology had also affected *drug delivery systems* and there are designs that call for the use of *nanorobots* to repair damage and detect abnormalities inside the human body.

Nano-technology is being used for creating *fabrics* with enhanced properties such as stain, dirt, and water resistance. The fabric used in these applications contains tiny nano-whiskers or fiber-like structures that are connected to a common center. The whiskers are hydrophobic and hence they repel water by causing it to form droplets. The droplets are larger than the spacing between whiskers, therefore remaining on top of the fabric allowing it to be brushed or wiped.

Nano-technology has improved *fresh water filtration* through the use of Nanopores (small pores in an electrically insulating membrane that can be used as a single-molecule detector). Nanopores have been developed that are so small that they can filter the smallest contaminant. Water purifications systems that use such pores often incorporate ultraviolet (UV) resistant materials so that the water passing through can be radiated to destroy contaminants such as pesticides, solvents, and microbes. Nanopores can be fabricated with great precision, allowing for effective filtration with minimal effect on the flow rate through the system.

The contribution of nano-technology to information and communication is in providing new methods for *data storage*, enabling the design of novel semiconductor and *optoelectronic devices* as well as *integrated circuits*. Nano-technology is used in the design of *displays* and *human-computer interfaces*. One of the areas of applications is the development of *smaller platforms for video games*.

8.7.2 Other Applications

1. **Abrasives:** Nano-materials exhibit superior effectiveness in critical abrasive and polishing applications when properly dispersed. The ultra-fine particle size and distribution of properly dispersed products is virtually unmatched by any other commercially-available abrasives. The result is a significant reduction in the size of surface defects as compared to conventional abrasive materials.
2. **Catalyst:** Nano-materials possess enhanced catalytic abilities due to their highly stressed surface atoms which are very reactive.
3. **Cosmetics:** Nano-products facilitate the creation of superior cosmetic products. Nano-products provide high UV attenuation without the use of chemicals, provide transparency to visible light when desired, and can be evenly dispersed into a wide range of cosmetics vehicles to provide non-caking cosmetic products.
4. **Electronic Devices:** Nano-products can provide new and unique electrical and conduction properties for use in existing and future technologies.

5. **Magnetics:** Nano-products can provide new and unique magnetic properties for use in existing and future technologies.
6. **Pigments & Coatings:** Nano-products facilitate the creation of superior pigments and coatings. Nano-products provide high UV attenuation, provide transparency to visible light when desired, and can be evenly dispersed into a wide range of materials. Nano-products can also provide more vivid colors that will resist deterioration and fading over time.
7. **Structural Ceramics:** Nano-products can be used in the production of ceramic parts. The ultra-fine size of the particles allows near-net shaping of ceramic parts via super plastic deformation which can reduce production costs by reducing the need for costly post-forming machining.

8.7.3 Advantages of Nano-materials

1. Nano-materials are three-dimensional solids composed of nanometer-sized grains, or crystallites. Their ultra-fine grain size and properties can be exploited to make 'next-generation' super strong materials.
2. The mechanism of plastic deformation in nano-crystalline materials may be different and so may lead to novel mechanical properties.
3. High strength or hardness has been observed in many nano-materials.

8.7.4 Limitations of Nano-materials:

In most cases, nano-materials have very low ductility, i.e., they fail when their shape is changed. Some nano-materials become brittle when a force or deforming load is applied. Strength and ductility are usually opposing characteristics: the higher the strength, the lower the ductility, and vice versa.

This correlation is associated with the nature of plasticity: the more difficult it is for dislocations to appear and to move, the stronger but brittle and less ductile is any crystalline material.

8.8 ULTRASONIC WAVES & NON-DESTRUCTIVE TESTING OF MATERIALS :

8.8.1 Ultrasonic Waves

Ultrasonic waves are sound waves whose frequencies are higher than human audibility limit, i.e., 20 KHz. Ultrasonic waves are commonly produced using the principle of Piezoelectricity. Ultrasonic waves travel with different velocities in different materials, and in solids it propagates both in the form of transverse waves and longitudinal waves. Since transverse waves can not exist in liquids, ultrasonic waves propagate only in the form of longitudinal wave in liquids. Propagation of these waves through material medium depends on elastic properties and the density of the medium. Ultrasonic waves are used for nondestructive testing of materials. Nondestructive method is a technique used to test a material/product for its defects/flaws without causing any damage to it.

8.8.2 Ultrasonic Method of Non-destructive Testing

Principle:

When ultrasonic wave is incident on a material medium, a part of incident wave is reflected back and the remaining part is transmitted into the material medium.

Consider an ultrasonic wave travelling in a medium of density ρ_1 and incident to second medium of density ρ_2 . If I_1 is the intensity of ultrasonic wave in first medium and I_2 is the intensity of reflected beam from the interface and v_1 and v_2 are the velocities of waves in first and second medium respectively, then the ratio of the reflected and incident intensities is given by,

$$I_2/I_1 = [(\rho_1 v_1 - \rho_2 v_2)/(\rho_1 v_1 + \rho_2 v_2)]^2 \quad \dots(8.1)$$

Since

$$v_1 = v_2,$$

$$I_2 = I_1 [(\rho_1 - \rho_2)/(\rho_1 + \rho_2)]^2 \quad \dots(8.2)$$

Hence, the intensity of reflected wave is basically dependent on the difference between ρ_1 & ρ_2 for a given intensity incident wave. Thus, if the wave is travelling from high density medium to low density medium (or vice versa), then an intense reflection of the wave occurs at the boundary of separation. By knowing the time elapse between incident and reflected wave, and the velocity of wave in that medium, the distance at which the change in density occurred can be measured. By knowing such change in density inside the material at a place it is not expected to occur is a direct indication of the presence of defect/flaw. The signal due to a reflected wave is called echo.

Experimental Procedure:

The experimental arrangement contains (1) Pulse generator (2) Piezoelectric crystal Transmitter, (3) Piezoelectric crystal Receiver, (4) Signal amplifier and (5) Cathode Ray Oscilloscope as shown in Fig. 8.12.

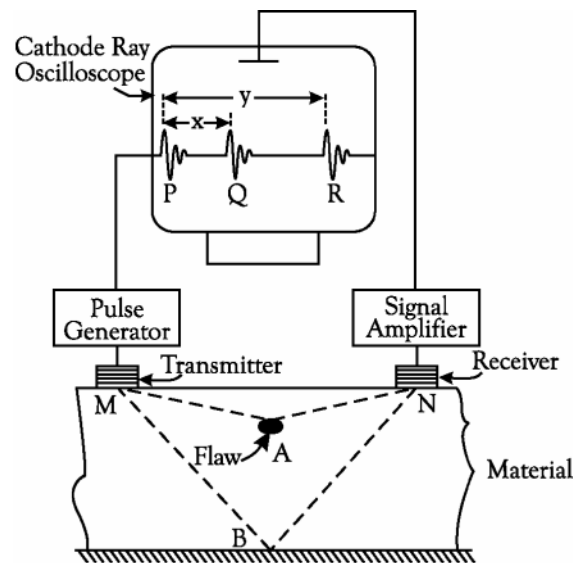


Figure 8.12 Experimental set-up for ultrasonic non-destructive testing

The time base of the CRO is connected to the pulse generator. The pulse generator produces pulses each comprising of electric oscillations of ultrasonic frequency. The a.c. field so produced is applied to a piezoelectric crystal. The crystal executes mechanical vibrations of the same frequency as that of the pulse waves. The piezoelectric crystal is kept in perfect body contact with the specimen since, the pulse energy suffers great amount of dissipation by any air gap present within the contact region. A thin film of oil spread between the two, ensures elimination of air gaps. Thus the vibrations of the crystal are transmitted efficiently into the body of the specimen, and the crystal performs the function of transmitter of ultrasonic pulsed beam. Also, at the same intensity the pip 'P' appears as the source signal on the screen. The beam suffers reflection at places wherever there is change in density.

The change in density occurs wherever there is discontinuity in the material of the specimen. The discontinuity occurs at A, the site of the flaw, and also at the boundaries like the side face 'B'. A part of the injected beam is reflected at A. It reaches the receiver at N. The receiver is also a piezoelectric crystal kept in tight contact with the specimen, and is set into mechanical vibrations by the reflected beam reaching it. By the piezoelectric effect, a feeble alternating electric voltage is induced across the crystal. This voltage acts as an echo signal and fed into the signal amplifier whose output is fed into CRO.

The echo appears as the pip 'Q' on the CRO screen. Similarly some part of the beam is reflected at B and picked up also by the receiver. Since it had travelled a longer distance to reach the receiver, its echo appears later than 'Q', as a pip 'R' on the screen. After this cycle of events, the transmitter will be ready to inject the next pulse into the specimen. Since there are no electric oscillations in the time interval between generation of any two consecutive pulses, the transmitter remains dormant during that interval.

Let 'x' and 'y' be the distances of the echoes Q and R respectively from the source pulse P. With the help of the time base calculation of CRO, the lengths 'x' and 'y' can be determined.

The values of 'x' and 'y' are proportionate measures of the path distances MAN and MBN. The specimen is studied by placing the transmitter and receiver at various places on it, which provides a set of values of x and y. The size of the flaw and its location in the specimen are determined on the basis of the values of x and y so obtained.

Advantages:

1. It is a reliable and fast method of non-destructive testing
2. The minimum flaw size which can be detected is equal to about 0.1% of the distance from the transmitter probe to the defect.
3. Sensitivity of ultrasonic flaw detection increases with increase in frequency of ultrasonic waves.
4. Ultrasonic inspection provides high speed operation at low cost.
5. This method is suitable in industry for initial detection of major defects in big castings.

Limitations:

1. Since ultrasonic inspection is sensitive to surface roughness, machining of castings will be required in some cases.

2. The interpretation of oscillograph trace is not easy in complex castings. The waves reflected from corners and other surfaces may give wrong indication of defects.

Applications:

Ultrasonic method of non-destructive testing can be used in detection of defects/flaws in,

- (1) Metallic sheets or plates, to check irregularities or discontinuities developed during their fabrication.
- (2) Concrete structures, in the form of imperfections or obstruction.
- (3) Heavy metal castings, and
- (4) Rails and massive axels of railway engines.

The test is sensitive enough to detect the cracks of the order of one hundredth part of a millimeter in the material.

8.9 MEASUREMENTS OF VELOCITY IN SOLIDS AND LIQUIDS

8.9.1 Measurements of Velocity of Ultrasonic Waves in Solid

The velocity of ultrasonic waves in a solid can be measured by pulse-echo method. The set-up used will be essentially same as the one described in the non-destructive testing of materials. In the set-up, a quartz crystal cut for producing longitudinal waves is utilized in the transmitter. The material, in which the velocity of ultrasonic waves is to be measured, is used as the specimen. The frequency of the pulse generator is adjusted to match the natural frequency of the crystal. The generator then sends the pulses at periodic intervals into the specimen. Every time the pulse is injected, it travels through the specimen and a part of it gets reflected from the opposite face. The receiver then responds to the reflected echoes. The pulse remainders keep bouncing between the opposite ends of the specimen attenuating with time. Accordingly the receiver sends signals which will be seen as a train of echoes on the CRO screen (Fig. 8.13). The time 't' between any two echoes is the length of the time required for the pulse to travel through the specimen & back to the transducer. The amplitude decays exponentially with time.

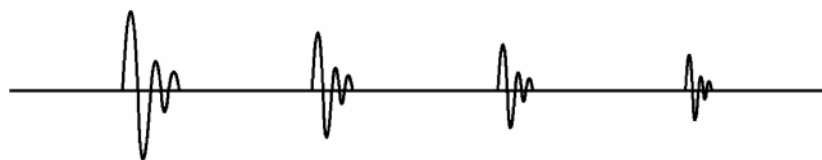


Figure 8.13 *Echo pulses on CRO screen*

It is possible to estimate the distance d travelled between the transmitter and the reflecting end by knowing the dimension of the specimen. This is also equal to the distance between the receiver and the reflecting end. Using d and t it is possible to calculate the longitudinal velocity V_L of ultrasonics in the specimen using the relation,

$$V_L = \frac{2d}{t} \quad \dots(8.3)$$

Using the same procedure, the transverse or the shear velocity V_s of the ultrasonics in the specimen can be determined by using a piezoelectric crystal that issues transverse waves for the transmitter in the set-up.

8.9.2 Determination of Elastic Constants in Solids

It may be shown that the speeds of longitudinal and shear waves of ultrasonic are given by,

$$V_L = \sqrt{\frac{E(1-\sigma)}{\rho(1+\sigma)(1-2\sigma)}} \quad \dots(8.4)$$

And
$$V_s = \sqrt{\frac{E}{2\rho(1+\sigma)}} = \sqrt{\frac{n}{\rho}} \quad \dots(8.5)$$

where,

E is the Young's modulus,

σ is the poisson's ratio,

ρ is the density of the solid,

n is the rigidity modulus.

Solving Eqns. (8.4) and (8.5), we get,

$$\sigma = \frac{1 - 2\left(\frac{V_s}{V_L}\right)^2}{2 - 2\left(\frac{V_s}{V_L}\right)^2} \quad \dots(8.6)$$

$$E = 2\rho V_s^2 (1 + \sigma) \quad \dots(8.7)$$

and
$$n = \rho V_s^2 \quad \dots(8.8)$$

Thus, knowing V_L and V_s for a solid, σ , E , and n of the solid can be calculated.

The velocity of ultrasonic waves in a few solids is given in Table 8.1.

Table 8.1 Velocity of ultrasonic waves in a few solids

| Material | Logitudinal velocity (km/s) | Transverse or shere velocity km/s) |
|-----------------|-----------------------------|------------------------------------|
| Aluminium | 6.42 | 3.04 |
| Gold | 3.24 | 1.20 |
| Nickel | 6.04 | 3.00 |
| Steel | 5.79 | 3.1 |
| Rubber Neoprene | 1.6 | . |

8.9.3 Measurements of Velocity of Ultrasonic Waves in Liquid

Experimental Set-up:

The experimental set up consists of a piezoelectric X-cut quartz crystal placed in between two plates in a watertight encapsulation provided with two leads that are connected to the plates inside (Fig. 8.14). The natural frequency of oscillation of the crystal is known as data.

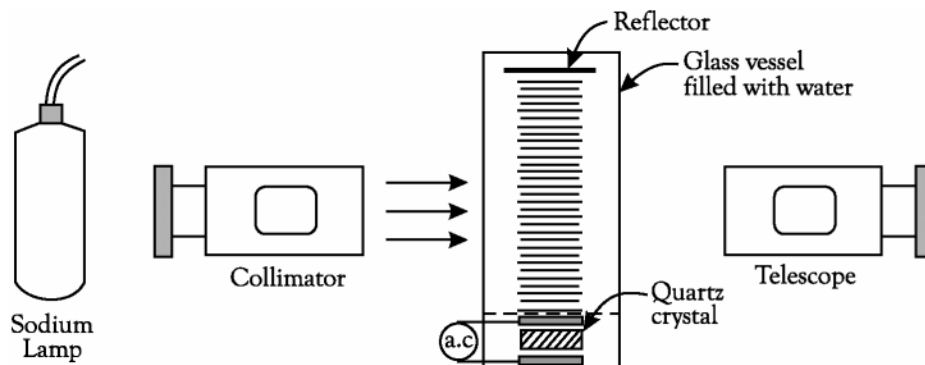


Figure 8.14 Experimental set-up for measurements of velocity of ultrasonic waves in liquid

The given liquid is taken in a small transparent rectangular cell. After the preliminary adjustments of the spectrometer, the glass vessel filled with the given liquid is placed on the spectrometer turn table with its length normal to the incident beam from the collimator. The crystal is suspended at one end inside the liquid with its vibrating plane perpendicular to the end side of the cell. There will be a movable metallic plate called reflector held by a support at the other end of the cell with its plane parallel to the end side.

The leads in the crystal are connected to the oscillator. The frequency of the oscillator is varied. When its frequency becomes equal to the crystal natural frequency of vibration, the crystal starts giving

resonant vibrations, during which time its amplitude becomes maximum. The pressure waves generated due to the vibration, start from the crystal and propagate through the liquid and then get reflected from the reflector. These reflected waves superimpose on the direct waves from the crystal. As a result, a standing wave pattern will be formed between the crystal and the reflector. In the standing wave, there will be nodes and antinodes.

At nodes, the liquid will be under maximum compression which renders its density to become high due to which it becomes almost opaque to the incident light. On the other hand, at antinodes, the liquid will be pushed away due to intense vibrations and rarefies the liquid. Thus the nodes & antinodes create regions of maximum & minimum density for the liquid causing opaque & clear regions at perfectly regular intervals. Thus the liquid turns essentially into a grating & hence referred to as acoustic grating. When the parallel beam of light is incident normally on this acoustic grating, it undergoes diffraction and gives rise to diffraction line when observed through a telescope. There will be a central maxima at the center on either side of which, the first order lines appear symmetrically and next the second order lines, and so on.

Theory:

We know that, if d is the grating constant and λ_L is the wavelength of light, then for normal incidence, the equation for diffraction is,

$$d \sin \theta_n = n\lambda_L$$

where θ_n is the angle of deviation of the spectral line of order n .

Since the grating constant is the distance between consecutive opaque lines, it corresponds to the distance between corresponding nodes, which must be equal to half the wavelength λ_u of the ultrasonic waves as per the theory of standing waves.

$$d = \frac{\lambda_u}{2} \quad \text{and} \quad \frac{\lambda_u}{2} \sin \theta_n = n\lambda_L$$

$$\lambda_u = \frac{2n\lambda_L}{\sin \theta_n} \quad \dots(8.9)$$

Velocity v of a wave of wavelength λ and frequency f is given by,

$$v = f\lambda.$$

If f is the frequency of the ultrasonic wave, then it will be same as the frequency of vibration of the crystal (which is known).

\therefore Velocity of the ultrasonic wave v_u is,

$$v_u = f\lambda_u$$

$$v_u = \frac{2nf\lambda_L}{\sin \theta_n} \quad \dots(8.10)$$

Since n , f and λ_L are known, by measuring θ_n one can evaluate v_u the velocity of ultrasonic waves in the liquid.

8.9.4 Determination of Elastic Constant in Liquid

The elastic behaviour of a liquid is characterised by its bulk modulus K . It is related to the velocity v_u of the ultrasonic waves through the following equation.

$$v_u = \sqrt{\frac{K}{\rho}} \quad \dots(8.11)$$

where ρ is the density of the liquid.

$$K = v_u^2 \rho \quad \dots(8.12)$$

Hence K can be determined by knowing v_u & ρ .

The velocity of ultrasonic waves (in km/s) in certain liquids is given in Table 8.2.

Table 8.2 Velocity of ultrasonic waves in certain liquids

| Liquid | Longitudinal velocity (km/s) |
|-----------------|------------------------------|
| Distilled water | 1.497 |
| Benzene | 1.295 |
| Castor oil | 0.987 |
| Kerosene | 1.324 |
| Mercury | 1.450 |

SOLVED PROBLEMS

1. An ultrasonic generator of 0.06 MHz sends down a pulse towards the sea bed which returns after 0.75 s. The velocity of the waves in sea water is 1600 m/s. Compute the depth of the sea and the wavelength of the pulse.

Solution

In 1 second the waves travel a distance of 1600 m. Hence in 0.75 s the distance travelled is

$$1600 \times 0.75 = 1200 \text{ m}$$

$$\text{i.e.,} \quad 2L = 1200 \text{ m,} \quad L = 600 \text{ m}$$

$$\text{Again,} \quad \lambda = v/f = [1600/(0.06 \times 10^6)] = 26666.666/10^6 = 0.0266 \text{ m}$$

$$\text{or} \quad \lambda = 2.67 \text{ cm}$$

EXERCISES

I. Descriptive Type Questions

1. Write a note on nano-technology?
2. What are nano-materials ? Explain various shapes of nano-materials ?
3. Write a note on Discovery of Fullerene and carbon nanotubes
4. Explain various methods of preparation of Nano-materials ?
5. Explain the advantages, limitations, and applications of nano-materials?
6. What are ultrasonic waves? Describe ultrasonic waves propagation in solids.
7. What is non-destructive testing? Describe the principle & procedure employed in nondestructive method of testing by using ultrasonics. What are its practical applications?
8. Describe a method of measuring velocity of ultrasonic waves in solids.
9. Describe the experimental method for determination of velocity of ultrasonic waves in liquids and mention how the bulk modulus of the liquid could be evaluated.
10. Discuss the process of determination of elastic constants in solids.
11. What are nano materials? Write a note on carbon nano-tubes. *(VTU June 2009)*
12. Describe a method of measuring velocity of ultrasonic waves in liquid. *(VTU June 2009)*
13. Describe a method of measuring velocity of ultrasonic waves in solids. *(VTU Jan 2009)*
14. Explain nano tubes and its applications. *(VTU Jan 2009)*
15. Describe with theory a method of measuring velocity of ultrasonic waves in a Liquid and mention how the bulk modulus of the liquid could be evaluated. *(VTU Jan 2008)*
16. What are nano-materials? Write a note on carbon nanotubes. *(VTU Jan 2008)*
17. Mention the factors which affect the velocity of ultrasonic waves in solids. Give the experimental method of determination of velocity of ultrasonic waves in liquids. *(VTU June 2008)*
18. Write a brief note on
 - (i) Nanotechnology
 - (ii) Carbon nanotubes. *(VTU July 2007)*
19. What are ultrasonic waves? Describe a method of measuring the velocity of ultrasonic waves in solids. *(VTU July 2007)*
20. What is an acoustic grating? Explain how an acoustic grating is used to determine the velocity of ultrasonic waves in liquid. Also mention how the bulk modulus of a liquid can be evaluated. *(VTU July 2007)*
21. Explain density of states for various quantum structures. *(VTU June 2010)*

22. What is non destructive testing? Describe the method of measuring velocity of ultrasonic waves in solids. (VTU June 2010)
23. What are nano-materials? Write a note on carbon nanotubes. (VTU Jan 2010)
24. What is non-destructive testing? Explain with principle how flow in a solid can be detected by non-destructive method using ultrasonics? (VTU Jan 2010)
25. Discuss the variation of density of states for different quantum structures. (VTU Jan 2010)

II. Multiple Choice Questions

- The state of matter around the nano size is known as
 - solid State
 - liquid state
 - Plasma State
 - Mesoscopic State
- Carbon nano tubes are made up of
 - Graphite Sheet
 - Graphene Sheet
 - Honey
 - Plastic
- The bulk material reduced in three directions is known as
 - Quantum dot
 - Quantum Wire
 - Film
 - Quantum particle
- Ultrasonic waves are produced by
 - Electromagnetic induction
 - magnetostriction method
 - Piezoelectric
 - inverse piezoelectric
- Which one of these does not represent a type of carbon nano tube?
 - Arm chair
 - Wavy
 - Zig-zag
 - Arch discharge
- The bulk material reduced in two directions is known as
 - Quantum dot
 - Quantum wire
 - Film
 - Reduced structure.
- The ultrasonic waves are produced by
 - Electromagnetic induction
 - Electric tuning fork
 - Piezoelectric effect
 - Inverse piezoelectric effect.
- Which of the procedures is not employed to detect the internal flaws of a material?
 - Ultrasonic method
 - Magnetic method
 - Alpha ray method
 - Dynamic testing

9. The elastic behaviour of the liquid is characterized by its
(a) Young's modulus. (b) Modulus of rigidity
(c) Bulk modulus (d) Poisson's ratio
10. The relation between longitudinal velocity and transverse velocity of ultrasonics in the given material is
(a) Longitudinal velocity is same as transverse velocity
(b) Longitudinal velocity is greater than transverse velocity
(c) Transverse velocity is greater than longitudinal velocity
(d) Transverse velocity is double the longitudinal velocity.
11. Quantum dots are used for _____
(a) drug delivery (b) multi-coloured display
(c) quantum dot lasers (d) all the above
12. When material is reduced to nanoscale, which of the following is not true _____
(a) Gold turns into liquid at room temperature
(b) Gold being inert turns into a potent chemical catalyst
(c) Silicon being semiconductor turns into conductor
(d) Ductility of Iron increases
13. A constant testing of product without causing any damage is called
(a) Minute testing (b) Destructive testing
(c) Non destructive testing (d) Random testing.
14. When material is reduced to nanoscale, which of the following is not true _____
(a) Copper being opaque becomes transparent
(b) Platinum being inert material attains catalytic properties
(c) Aluminum being stable material turns combustible
(d) Silicon become insulator
15. If the reduction is in two direction the resultant structure will be in one dimension which is called
(a) Reduced structure (b) Thin wire
(c) Quantum wire (d) Enlarge structure
16. The signal due to a reflected wave is called
(a) Transmitted wave (b) Longitudinal wave
(c) Echo (d) Peaco

17. Carbon nano tubes are molecular structures of
(a) Graphite sheet (b) Graphene sheet
(c) Plastic (d) None.
18. Which of the following is not true in case of nano-materials ____
(a) Increased ratio of surface area to volume
(b) Altered surface properties compared to bulk material
(c) Increase in size compared to bulk material
(d) Some of the mechanical properties will be altered compared to bulk material
19. The ultrasonic's can exist only as longitudinal waves in
(a) Solid (b) Liquid
(c) Gases (d) All the above
20. The velocity of ultrasonic waves through the liquid is proportional to
(a) Bulk modulus (b) Density
(c) Volume (d) Rigidity modulus
21. Ultrasonic waves are sound waves whose frequencies are _____ human audibility limit.
(a) higher than (b) lower than
(c) within (d) far above
22. The relation between velocity of ultrasonic wave V_u and angle of deviation (θ_n) of the spectral line of order n is _____
(a) $V_u = \frac{2nf\lambda_L}{\sin\theta_n}$ (b) $V_u = \frac{2n\lambda_L}{\sin\theta_n}$
(c) $V_u = \frac{nf\lambda_L}{\sin\theta_n}$ (d) $V_u = \frac{2f\lambda_L}{\sin\theta_n}$
23. The velocity of ultrasonic waves in a solid can be measured by _____
(a) Pulse-echo method (b) Young's modulus method
(c) Piezoelectric method (d) Non-destructive method
24. The major limitation of nano-materials for useful applications is due to _____
(a) very low ductility (b) very low strength
(c) very small size (d) poor mechanical properties

25. The term 'nano-technology' was used first by the _____
- (a) Japanese scientist Norio Taniguchi
 - (b) American engineer K. Eric Drexler
 - (c) IBM Zurich scientists
 - (d) Japanese scientist Sumiyo Iijima

Answers to Multiple Choice Questions

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

MODEL QUESTION PAPER

MODEL QUESTION PAPER-I

Time : 3 Hrs.

Max. Marks : 100

- Note :**
1. Answer any FIVE full questions, selecting at least TWO questions from each part.
 2. Standard notations are used & Missing data may be suitably assumed.
 3. Answer all objective type questions only on OMR sheet, page 5 of answer book.
 4. Objective type questions, if answered on other than OMR sheet, will not be valued.

PART – A

1. (a) (i) An electron and a proton are accelerated through same potential. The ratio of de- Broglie wavelength λ_e/λ_p is
- (a) 1 (b) m_e/m_p
- (c) m_p/m_e (d) $\sqrt{\frac{m_p}{m_e}}$
- (ii) In a black body radiation Spectrum, the maximum energy peaks shifts towards the shorter wavelength side with the increase in temperature. This confirms
- (a) Stefan's law (b) Wein's law
- (c) Rayleigh-Jean's law (d) Planck's law
- (iii) The Compton wavelength is given by
- (a) $\frac{h}{m_0 c^2}$ (b) $\frac{h^2}{m_0 c^2}$
- (c) $\frac{h}{m_0 c}$ (d) $\frac{h^2}{2m_0 c}$
- (iv) If the group velocity of a particle is 3×10^6 m/s, its phase velocity is
- (a) 100 m/s (b) 3×10^6 m/s
- (c) 3×10^8 m/s (d) 3×10^{10} m/s (1×4 = 4)
- (b) What is Compton Effect? Derive an expression for the Compton shift.
- (c) Derive an expression for de-Broglie wavelength of an accelerated particle and also for the particles at thermal equilibrium.
- (d) Derive an expression for the de-Broglie wavelength from group velocity. (6+4+6)

2. (a) (i) The wave function is acceptable wave function if it is
 (a) Finite everywhere (b) Continuous everywhere
 (c) Single valued everywhere (d) All of these
- (ii) According to Max Born Approximation wave function as _____
 (a) Energy density (b) Particle density
 (c) Probability density (d) Charge density
- (iii) The wave function for the motion of the particle in a one dimensional potential box of length 'a' is given by ' $\psi_n = A \sin\left(\frac{n\pi x}{a}\right)$ ', where A is normalization constant. The value of A is
 (a) $\frac{1}{\sqrt{a}}$ (b) $\frac{2}{\sqrt{a}}$
 (c) $\sqrt{\frac{2}{a}}$ (d) $\sqrt{\frac{a}{2}}$
- (iv) The lowest quantized energy of a particle of mass m in a box of length L is given by
 (a) zero (b) $\frac{h^2}{8mL^2}$
 (c) $\frac{2h^2}{8mL^2}$ (d) $\frac{h^2}{2mL^2}$ (4×1=4)
- (b) State and explain Heisenberg's uncertainty principle and prove that nuclei do not contain electron.
- (c) Set up time independent wave equation?
- (d) Compute the first 4 permitted energy levels of an electron in a box of width 4 Å (6+6+4)
3. (a) (i) Ohms law relates to the electric field E, conductivity σ and current density J as
 (a) $J = E/\sigma$ (b) $\sigma.E^2$
 (c) $J = \frac{\sigma}{E}$ (d) $J = \sigma.E$
- (ii) The average drift velocity V_d of electrons in a metal is related to the electric field E, and collision time τ as
 (a) $\sqrt{\frac{eE\tau}{m}}$ (b) $\sqrt{\frac{m}{eE\tau}}$
 (c) $\frac{eE\tau}{m}$ (d) $\frac{m}{eE\tau}$

- (iii) If the Fermi energy of metal at 0°K is 5 eV, $f(E)$ for Fermi energy at $T > 0^\circ\text{K}$ is
 (a) 0.5 eV (b) 1 eV
 (c) 0.75 eV (d) 0 eV
- (iv) If the Fermi energy of silver is 5.5 eV, the Fermi velocity of conduction electron is
 (a) 0.98×10^6 m/s (b) 1.39×10^6 m/s
 (c) 2.46×10^5 m/s (d) None of these (1×4=4)
- (b) Give the expression for Density of states for conduction electron for unit volume of metal and obtain an expression for Fermi Energy
- (c) Discuss the various drawbacks of classical free electron theory of metals. What are the assumption made in quantum theory to overcome.
- (d) The mobility of the electron in gold wire is found to be 4.3×10^{-3} m²/Vs. if the resistivity of the gold wire is 2.4×10^{-8} W-m, calculate the electron concentration in the gold. (6+6+4)
4. (a) (i) If the distance between the plates of capacitor is increased double, the capacitance is
 (a) Doubled (b) Increased to four times
 (c) Halved (d) Constant
- (ii) For a given dielectric, the electron polarizability, α_e
 (a) Increases with temperature
 (b) Decreases with temperature
 (c) Independent of temperature
 (d) May increase or decrease with temperature.
- (iii) Which one of the following is necessarily the piezoelectric material?
 (a) Lead (b) Mica
 (c) Iron (d) Quartz
- (iv) The electronic polarization is also referred as
 (a) Orientational polarization (b) Migrational polarization
 (c) Optical polarization (d) ionic polarization
- (b) Derive the equation for internal field in case of solid or liquid dielectric for one dimensional, array of dipoles.
- (c) Describe the nature of hard and soft magnetic materials. Discuss their applications.
- (d) Sulphur is elemental solid dielectric whose dielectric constant is 3.4. Calculate electronic polarizability if its density is 2.07×10^3 kg/m³ and atomic weight is 32.07. (8+4+4)

PART – B

5. (a) (i) In He-Ne lasers, the ratio of He-Ne is in the order
(a) 1:10 (b) 1:1
(c) 10:1 (d) 100:1
- (ii) The emission of photon without being aided by any external agency is called
(a) Light amplification (b) Induced absorption
(c) Stimulated emission (d) Spontaneous emission
- (iii) Supply of energy to atoms for excitation is called
(a) Glowing (b) Bombarding
(c) incidenting (d) Pumping (1×4=4)
- (iv) Which of the following is not a laser property?
(a) Highly monochromatic (b) High directionality
(c) Very narrow band width (d) Highly divergent
- (b) Explain the construction and working of He-Ne Laser
- (c) Obtain an expression for energy density of radiation under equilibrium condition in terms of Einstein coefficient.
- (d) A laser beam with Power per pulse is 1 mw lasts 10 ns, if the number of photons emitted per pulse is 3.941×10^7 , calculate the wavelength of laser. (6+6+4)
6. (a) (i) The temperature at which super conductivity occurs is called
(a) Low temperature (b) Super temperature
(c) Critical temperature (d) High temperature
- (ii) The width of the energy gap of a super conductor is maximum at
(a) T_c (b) 0 K
(c) $\frac{T_c}{2}$ (d) $\frac{T_c}{3}$
- (iii) Super conductivity phenomenon can be explained on the basis of
(a) BCS theory (b) CCS theory
(c) DCS theory (d) MCS theory
- (iv) In a single mode fiber, the diameter of the core is nearly equal to (1×4=4)
(a) 125 μm (b) 100 μm
(c) 50 μm (d) 10 μm
- (b) Discuss the three different types of optical fibers
- (c) Derive the expression for numerical aperture of an optical fiber.

- (d) Calculate the numerical aperture, relative refractive index difference, V-number and number of modes in an optical fiber of core diameter 50 μm core and cladding refractive indices 1.41 and 1.40, at wavelength 820 nm. (6+4+4)
7. (a) (i) APF of diamond crystal structure is
 (a) 0.68 (b) 0.74
 (c) 0.52 (d) 0.34
- (ii) For every rotation by an angle θ in Bragg's spectrometer, detector turns by an angle
 (a) θ (b) 3θ
 (c) $\theta/2$ (d) 2θ
- (iii) The Miller indices of the plane parallel to x and y axis are
 (a) (100) (b) (010)
 (c) (001) (d) (111)
- (iv) The co-ordination number in case of simple cubic crystal structure is
 (a) 12 (b) 8
 (c) 2 (d) 6 (1×4=4)
- (b) Explain how Miller indices are derived. Derive an expression for interplanar spacing of a crystal in terms of Miller indices.
- (c) Explain the structure of NaCl and Diamond
- (d) Draw the following planes in the simple cubic cell (122), (143), (195) and (257). (6+4+4)
8. (a) (i) If the reduction is in two direction the resultant structure will be in one dimension which is called
 (a) Reduced structure (b) Thin wire
 (c) Quantum wire (d) Enlarge structure
- (ii) As per the scaling laws, the frequency of operation increases with
 (a) Decrease of size (b) Increase of size
 (c) Constant (d) None
- (iii) The ultrasonics can exist only as longitudinal waves in
 (a) Solid (b) Liquid
 (c) Gases (d) All the above
- (iv) The velocity of ultrasonic waves through the liquid is proportional to
 (a) Bulk modulus (b) Density
 (c) Volume (d) Rigidity modulus (1×4=4)
- (b) What are ultrasonic waves? Describe a method of measuring the velocity of ultrasonic waves in solids.
- (c) Explain density of states for various quantum structures.
- (d) What are nano-materials? Write a note on carbon nanotubes. (6+4+4)

MODEL QUESTION PAPER

MODEL QUESTION PAPER-II

Time : 3 Hrs.

Max. Marks : 100

- Note :**
1. Answer any FIVE full questions, selecting at least TWO questions from each part.
 2. Standard notations are used & Missing data may be suitably assumed.
 3. Answer all objective type questions only on OMR sheet, page 5 of answer booklet.
 4. Objective type questions, if answered on other than OMR sheet, will not be valued.

PART – A

1. (a) (i) Group velocity of wave is equal to

| | |
|------------------------|---------------------------|
| (a) V_{phase} | (b) V_{particle} |
| (c) Velocity of light | (d) None of these |
- (ii) If the momentum of a particle is increased to four times, then the de-Broglie Wavelength is

| | |
|-----------------------|-----------------------|
| (a) become twice | (b) become four times |
| (c) become one-fourth | (d) become ten times |
- (iii) The wave property of large, massive objects is not observed because _____

| | |
|-------------------------------------|---------------------------------|
| (a) their acceleration is too small | (b) their momenta are too small |
| (c) their speeds are too small | (d) none of these |
- (iv) If the group velocity of a particle is $3 \times 10^6 \text{m/s}$, its phase velocity is

| | |
|--------------------------------|-----------------------------------|
| (a) 100m/s | (b) $3 \times 10^6 \text{m/s}$ |
| (c) $3 \times 10^8 \text{m/s}$ | (d) $3 \times 10^{10} \text{m/s}$ |

(1×4=4)
- (b) Describe Davison and Germer Experiment
- (c) Derive an expression for de-Broglie wavelength from the group velocity.
- (d) A particle of mass $0.65 \text{ MeV}/c^2$ has free energy 120 eV . Find its de-Broglie, wavelength, c is the velocity of light.. (6+6+4)
2. (a) (i) The normalization of wave function is always possible, if

| | |
|--|---|
| (a) $\int_{-\infty}^{\infty} \psi \psi^* dx = \text{infinite}$ | (b) $\int_{-\infty}^{+\infty} \psi \psi^* dx = \text{finite}$ |
|--|---|

- (c) $\int_{-\infty}^{+\infty} \psi \psi^* dx = 0$ (d) All of these
- (ii) The ground state energy of an electron in an infinite well is 5.6 MeV. If the width of the well is doubled, the ground state energy is
 (a) $9.92 \times 10^{23} \text{J}$ (b) $4.48 \times 10^{22} \text{J}$
 (c) $2.24 \times 10^{22} \text{J}$ (d) None of these
- (iii) The wave function is acceptable wave function if it is
 (a) finite everywhere (b) Continuous everywhere
 (c) Single valued everywhere (d) All of these.
- (iv) The lowest quantized energy of a particle of mass m in a box of length L is given by
 (a) zero (b) $h^2/8mL^2$
 (c) $\frac{2h^2}{8mL^2}$ (d) $\frac{h^2}{2mL^2}$ (4×1=4)
- (b) State Heisenberg's uncertainty principle and discuss its physical significance
- (c) Solve the Schrodinger's wave equation for allowed energy values in case of a particle in a potential box.
- (d) An electron has a speed of $6 \times 10^5 \text{m/s}$ with an inaccuracy of 0.01%. With what fundamental accuracy can we locate the position of the electron? (4+8+4)
3. (a) (i) For ordinary metals, the resistivity versus temperature curve at $T = 0$,
 (a) has a positive intercept (b) has a negative intercept
 (c) goes through the origin (d) none of these
- (ii) The average drift velocity V_d of electrons in a metal is related to the electric field E , and collision time τ as
 (a) $\sqrt{\frac{eE\tau}{m}}$ (b) $\sqrt{\frac{m}{eE\tau}}$
 (c) $\frac{eE\tau}{m}$ (d) $\frac{m}{eE\tau}$
- (iii) If the Fermi energy of metal at 0°K is 5 eV, $f(E)$ for Fermi energy at $T > 0^\circ\text{K}$ is
 (a) 0.5 eV (b) 1 eV
 (c) 0.75 eV (d) 0 eV
- (iv) If the Fermi energy of silver is 5.5 eV, the Fermi velocity of conduction electron is
 (a) $0.98 \times 10^6 \text{ m/s}$ (b) $1.39 \times 10^6 \text{ m/s}$
 (c) $2.46 \times 10^5 \text{ m/s}$ (d) None of these (1×4=4)

- (b) Based on free electron theory, derive an expression for electrical conductivity of metals. How does electrical resistance change with impurity and temperature?
- (c) Describe Fermi-Dirac distribution and discuss the same for different temperature conditions.
- (d) A metal has Fermi energy 5.6 eV. Determine the energy for which the probability of occupancy is 0.25 at 450 K. (6+6+4)
4. (a) (i) Choose the correct relation
 (a) $E = E_0(\epsilon_r - 1)P$ (b) $P = \epsilon_0(\epsilon_r - 1)E$
 (c) $\epsilon_r = K - 1$ (d) $E = \epsilon_0(\epsilon_r - 1)E$
- (ii) The unit of dipole moment / unit volume is
 (a) Coulomb/metre (b) Coulomb/metre²
 (c) coulomb/metre³ (d) Coulomb
- (iii) In a solid or liquid dielectric with external applied electrical field, as the electronic polarizability α_e increases the interval field E_j
 (a) Increases (b) Reduces
 (c) Remains constant (d) none of these.
- (iv) The electronic polarization is also referred as
 (a) Orientational polarization
 (b) Migrational polarization
 (c) Optical polarization
 (d) Ionic polarization
- (b) Derive Clausius Mossuti equation for 3-dimensional cubic solid dielectric.
- (c) Describe the nature of hard and soft magnetic materials. Discuss their applications.
- (d) The atomic weight and density of sulphur are 32 and $2.08 \times 10^3 \text{ kg/m}^3$ respectively. The electronics polarizability of the atom is $3.28 \times 10^{-40} \text{ F-m}^2$. If sulphur solid has cubic structure, calculate its dielectric constant. (6+6+4)

PART – B

5. (a) (i) The life time of an atom on a metastable state is of the order
 (a) a few seconds (b) unlimited
 (c) a nano second (d) few milli second
- (ii) n_1 be the number density of lower energy E_1 , and n_2 be the number density of higher: energy E_2 , if $n_2 > n_1$ is called

- (a) Thick population. (b) Inverted population
 (c) Normal population (d) No population.
- (iii) The relation between Einstein's coefficients A and B is
- (a) $\frac{8\pi h \lambda^3}{c^3}$ (b) $\frac{8\pi h^2 \lambda^3}{c^3}$
 (c) $\frac{8\pi h \nu^3}{c^3}$ (d) $\frac{8\pi h \nu^3}{c^2}$
- (iv) Which of the following is not a laser property? (1×4=4)
 (a) Highly monochromatic (b) High directionality
 (c) Very narrow band width (d) Highly divergent
- (b) Describe the construction and working of Semiconductor laser.
 (c) Describe the recording and reconstruction processes in holography, with the help of suitable diagrams.
 (d) Find the number of modes of the standing waves and their frequency separation in the resonant cavity of length 1m of He-Ne laser operating at wavelength 632.8 nm. (6+6+4)
6. (a) (i) Meissner effect will take place in
 (a) Solid (b) Super conducting magnet
 (c) Magler vehicle (d) MRI
- (ii) Fractional index changes of optical Fiber for R.I of core and cladding are 1.563 and 1.498 is
 (a) 0.00415 (b) 0.0415
 (c) 0.043 (d) 0.004
- (iii) Super conductivity phenomenon can be explained on the basis of
 (a) BCS theory (b) CCS theory
 (c) DCS theory (d) MCS theory
- (iv) Attenuation in the optical fiber causes due to
 (a) Absorption (b) Scattering
 (c) Dispersion (d) All the three (1×4=4)
- (b) What is Superconductivity? Describe type I and type II super conductors.
 (c) Derive the expression for numerical aperture of an optical fiber.
 (d) An optical fiber has core R.I. 1.5 and R.I. of cladding is 3% less than the core index. Calculate the numerical aperture, angle of acceptance and internal critical acceptance angle. (6+6+4)

7. (a) (i) Nearest neighbour distance between two atoms in case of bcc structure is
- (a) $(a\sqrt{3})/2$ (b) $2a/\sqrt{3}$
(c) $(a\sqrt{2})/2$ (d) $2a/\sqrt{2}$
- (ii) In a simple cubic lattice the ratio $d_{100} : d_{110} : d_{111}$ is
- (a) 6: 3 : 1 (b) $\sqrt{3} : \sqrt{6} : 1$
(c) $6 : 3 : \sqrt{2}$ (d) $\sqrt{6} : \sqrt{3} : \sqrt{2}$
- (iii) The Miller indices of the plane parallel to y axis are
- (a) (100) (b) (010)
(c) (101) (d) (111)
- (iv) Which one of the following Bravais lattices is not found in cubic crystal?
- (a) Simple cube (b) Face centered
(c) Body centered (d) Base centered (1×4=4)
- (b) What is a Bravais lattice? Draw the diagrams of 14 Bravais lattices.
- (c) Define coordination number and packing factor. Calculate the packing factor for SC and BCC structures.
- (d) The minimum order of Bragg's reflection occurs at an angle 20° from [212] plane. Find the wavelength of X-ray if lattice constant is 3.615 \AA (6+6+4)
8. (a) (i) The state of matter around the nano size is known as
- (a) Solid State (b) Liquid state
(c) Plasma State (d) Mesoscopic State
- (ii) The bulk material reduced in three directions is known as
- (a) Quantum dot (b) Quantum Wire
(c) Film (d) Quantum particle
- (iii) Which one of these does not represent a type of carbon nano tube?
- (a) Arm chair (b) Wavy
(c) Zig-zag (d) Arch discharge
- (iv) The velocity of ultrasonic waves through the liquid is proportional to
- (a) Bulk modulus (b) Density
(c) Volume (d) Rigidity modulus (1×4=4)
- (b) Explain various methods of preparation of Nano-materials ?
- (c) What is non-destructive testing? Explain with principle, how flaw in a solid can be detected by non-destructive method, using ultrasonics.
- (d) What are nano-materials? Write a note on carbon nanotubes. (6+6+4)

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TEXTBOOK OF ENGINEERING PHYSICS

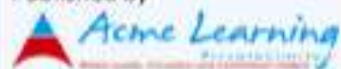
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