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A TEXTBOOK ON

ENGINEERING PHYSICS

Dr. Arun Khalkar

For F.Y.B.Tech students
As per the 2024 curriculum,
Pimpri Chinchwad College of Engineering (PCCOE), Nigdi, Pune.



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About the Author



Dr. Arun Khalkar is an accomplished educator and researcher with a distinguished academic journey and a passion for advancing scientific knowledge. He holds a Ph.D. in Nanoscience and Nanotechnology from Sungkyunkwan University (SKKU), South Korea, where he was awarded the prestigious BK-21 (Brain Korea-21) Fellowship for his exceptional research contributions.

Currently serving as an Assistant Professor of Engineering Physics in the Department of Applied Sciences and Humanities at Pimpri Chinchwad College of Engineering (PCCOE), Pune, India, Dr. Khalkar brings over 15 years of teaching experience at both national and international levels.

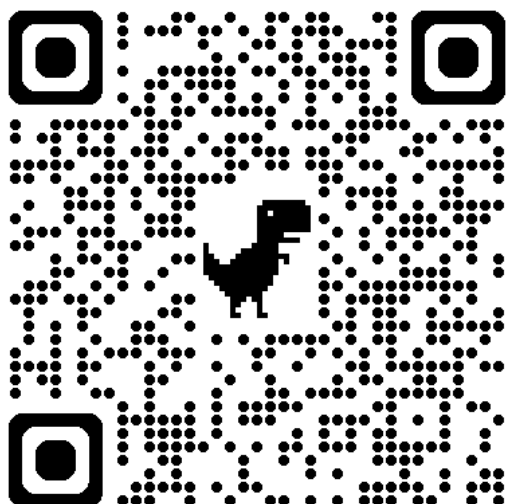
An ardent researcher, Dr. Khalkar has published more than 10 research papers in esteemed international journals and has presented his work at over 15 national and international conferences, including globally renowned platforms such as the IEEE Photovoltaic Specialists Conference (PVSC) in the USA, SKKU Solar Forum in Korea, and the Photovoltaic Science and Engineering Conference in China.

Beyond his academic achievements, Dr. Khalkar is deeply committed to mentoring and inspiring the next generation of innovators. He has guided over 50 students in Project-Based Learning (PBL), Mini Projects, and Basics of Innovation (MPBI), fostering creativity and practical skills among his students.

With his rich academic background and unwavering dedication to education and research, Dr. Arun Khalkar continues to inspire and contribute to the fields of nanotechnology, engineering physics, and beyond.

Author's webpage

For more details, please scan the QR code below to visit the author's webpage.





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PREFACE

Engineering Physics serves as a vital bridge between the fundamental principles of physics and their real-world applications in engineering and technology. This book is meticulously designed to cater to the academic needs of engineering students, providing a balanced understanding of foundational concepts and their practical applications. It aims to equip students with the knowledge and analytical skills essential for addressing contemporary challenges in science and technology.

The book is divided into four comprehensive units, each focusing on a crucial domain of physics that lays the groundwork for modern engineering:

Semiconductor Physics

This section delves into the behavior of semiconductors and conductors, starting with the Band Theory of Solids and Electrical Conductivity. Key topics include the derivation of the Hall Effect, Fermi-Dirac Probability Distribution, and the Fermi Level. The section also introduces the working principles of solar cells, their I-V characteristics, and the fundamentals of sensors, highlighting their characteristics, types, and applications.

Quantum Mechanics

This unit introduces the revolutionary concepts of wave-particle duality, the De Broglie hypothesis, and the Heisenberg Uncertainty Principle. It provides a thorough understanding of the wave function, probability interpretation, and Schrödinger's Time-Independent Wave Equation, along with applications such as the particle in a rigid box and tunneling effect. Practical implications are explored through topics like scanning tunneling microscopy (STM), emphasizing the transformative power of quantum mechanics in modern technology.

Magnetism and Superconductivity

Magnetism is discussed with a focus on phenomena like Magnetic Hysteresis, Giant Magnetoresistance (GMR), and the Magnetocaloric Effect. The section on Superconductivity introduces critical concepts such as zero electrical resistance, the Meissner Effect, and the BCS Theory. Advanced topics like Type I and II Superconductors, the Josephson Effect, and applications such as SQUIDs, superconducting magnets, and maglev trains are explored, showcasing the cutting-edge applications of superconductivity in engineering.

Introduction to Nanoscience

The fascinating field of nanoscience is presented with an emphasis on quantum confinement, the surface-to-volume ratio, and the unique properties of nanomaterials. Methods for the preparation of nanomaterials, including high-energy ball milling, physical vapor deposition, and colloidal synthesis, are described in detail. The section also discusses the transformative applications of nanomaterials in fields like medicine, energy, and defense, and introduces the emerging realm of quantum computing.

Throughout the book, theoretical concepts are reinforced with derivations, numerical problems, and practical applications. The content is presented in a clear and concise manner, supported by diagrams and examples, making it accessible to students and educators alike.

This book reflects the culmination of years of teaching and research experience, guided by the goal of making complex scientific principles approachable and relevant to engineering students. It is hoped that this text will not only help students excel academically but also inspire them to innovate and contribute to the fields of science and technology.

Finally, I extend my heartfelt gratitude to my mentors, colleagues, and students, whose insights and encouragement have been invaluable in the creation of this book. I also acknowledge the rapidly evolving nature of physics and engineering, and I encourage readers to explore beyond these pages, as the journey of learning never ends.

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Program:	B. Tech. (All Branches)					Semester: I /II	
Course:	Engineering Physics					Code:	BSH21BS03 BSH22BS03
Credits	Teaching Scheme (Hrs./Week)			Evaluation Scheme and Marks			
	Lecture	Practical	Tutorial	FA		SA	Total
				FA1	FA2		
2	2	-	-	10[20]	10[20]	30	50[70]
Prior knowledge of: 1. Atom, molecule and nuclei, 2. Current, electricity and magnetism, 3. Electromagnetic Induction is essential.							
Course Objectives: This course aims at enabling students, 1. To build strong conceptual understanding of Semiconductor Physics and Quantum Physics, 2. To explore advances in Physics with introduction of Nanotechnology and Superconductivity 3. To provide consciousness about the importance of Physics principles in various engineering applications							
Course Outcomes: After learning the course, the students should be able to: 1. Apply basics of semiconductor physics to explain the behavior of charge carriers inside a semiconductor 2. Distinguish wave behavior of a matter particle for the manipulation of the processes at quantum scale 3. Interpret properties of superconductors and their applications in advanced technologies 4. Summarize properties, preparation methods of nanomaterials and explore their applications in various engineering fields							
Detailed Syllabus							
Unit	Description						Duration [Hrs]
I	Semiconductor Physics Band Theory of solids, Electrical conductivity of conductors (qualitative), and semiconductors (Derivation), Numerical. Hall effect (with derivation) Numerical, Fermi Dirac probability distribution function, Fermi level (Definition), Fermi level variation with i) temperature and ii) doping concentration, Solar cell I-V characteristics, Basics of sensors, Characteristics of sensors-range, sensitivity, resolution, accuracy, repeatability types of sensors-Active and Passive sensors, Applications of sensors.						8
II	Quantum Mechanics Wave particle duality of radiation and matter, De Broglie hypothesis, De Broglie wavelength in terms of kinetic and potential energy, Numerical concept of wave packet, Properties of matter waves, Heisenberg's uncertainty principle, wave function and probability interpretation, well behaved wave function, Schrodinger's time independent wave equation, applications of independent wave equation to the problem of (i) particle in rigid box, (Derivation) Numerical. Tunneling effect, scanning tunneling microscope (STM)						7
III	Magnetism and Superconductivity Magnetism: Magnetic hysteresis loop, giant magneto-resistance (GMR), magneto caloric effect (only statement), adiabatic demagnetization. Superconductivity: Introduction, critical temperature, properties of superconductors-zero electrical resistance, persistent current, Meissner effect, critical magnetic field, Isotope effect, Numerical BCS theory, type I and II superconductors, low T _c and high T _c superconductors, Josephson effect, DC-SQUID-construction, working and applications, applications - superconducting magnets, maglev trains						7
IV	Introduction to Nanoscience Introduction, surface to volume ratio, quantum confinement, properties of nanomaterials- optical, electrical, mechanical, magnetic; methods of preparation of nanomaterials- bottom-up and top-down approaches, physical methods- high energy ball milling, physical vapor deposition; chemical method - colloidal route for synthesis of gold nanoparticle , Applications of nanomaterials in medical, energy, automobile, space, defense; introduction to quantum computing.						8
	Total						30



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CONTENT

UNIT 1: SEMICONDUCTOR PHYSICS

Band Theory of solids, Electrical conductivity of conductors (qualitative), and semiconductors (Derivation), Numerical. Hall effect (with derivation) Numerical, Fermi Dirac probability distribution function, Fermi level (Definition), Fermi level variation with i) temperature and ii) doping concentration, Solar cell I-V characteristics, Basics of sensors, Characteristics of sensors-range, sensitivity, resolution, accuracy, repeatability types of sensors-Active and Passive sensors, Applications of sensors.

UNIT 2: QUANTUM MECHANICS

Wave particle duality of radiation and matter, De Broglie hypothesis, De Broglie wavelength in terms of kinetic and potential energy, Numerical concept of wave packet, Properties of matter waves, Heisenberg's uncertainty principle, wave function and probability interpretation, well behaved wave function, Schrodinger's time independent wave equation, applications of independent wave equation to the problem of (i) particle in rigid box, (Derivation) Numerical. Tunneling effect, scanning tunneling microscope (STM).

UNIT 3: MAGNETISM AND SUPERCONDUCTIVITY

Magnetism: Magnetic hysteresis loop, giant magneto-resistance (GMR), magneto caloric effect (only statement), adiabatic demagnetization.

Superconductivity: Introduction, critical temperature, properties of superconductors-zero electrical resistance, persistent current, Meissner effect, critical magnetic field, Isotope effect, Numerical BCS theory, type I and II superconductors, low T_c and high T_c superconductors, Josephson effect, DC-SQUID-construction, working and applications, applications - superconducting magnets, maglev trains.

UNIT 4: INTRODUCTION TO NANOSCIENCE

Introduction, surface to volume ratio, quantum confinement, properties of nanomaterials- optical, electrical, mechanical, magnetic; methods of preparation of nanomaterials- bottom-up and top-down approaches, physical methods- high energy ball milling, physical vapor deposition; chemical method - colloidal route for synthesis of gold nanoparticle , Applications of nanomaterials in medical, energy, automobile, space, defense; introduction to quantum computing.



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UNIT 1: SEMICONDUCTOR PHYSICS

1. Introduction

- Semiconductor physics is at the heart of modern technological advancements, enabling the development of devices that have revolutionized communication, computation, energy, and sensing. Semiconductors, materials with electrical properties that fall between conductors and insulators, have unique characteristics that make them indispensable in modern engineering and technology.
- The study of semiconductor physics begins with understanding the Band Theory of Solids, which explains how electrons are distributed in energy bands within a material. This theory provides the framework for distinguishing conductors, insulators, and semiconductors based on their band structures and energy gaps. Semiconductors, with their tunable electrical conductivity, offer a versatile platform for applications ranging from diodes and transistors to photovoltaic cells.
- A critical aspect of semiconductor behavior is its electrical conductivity, which depends on charge carrier concentration, mobility, and temperature. Unlike conductors, semiconductors exhibit a significant change in conductivity with variations in temperature or doping, making them highly adaptable for use in electronic devices.
- The Hall Effect, another vital concept, demonstrates the response of charge carriers to an applied magnetic field, offering insights into the type, density, and mobility of carriers in a material. This phenomenon has practical applications in sensors and characterization techniques for semiconductors.
- The role of the Fermi Level and the Fermi-Dirac Probability Distribution Function is central to understanding the behavior of electrons in semiconductors, especially at varying temperatures and doping levels. These concepts provide a quantitative understanding of how semiconductors can be engineered to achieve desired electrical properties. Semiconductor physics also underpins the operation of solar cells, devices that convert light into electrical energy. The I-V characteristics of solar cells reveal the mechanisms of energy conversion and efficiency, paving the way for advancements in renewable energy technologies.
- The chapter further explores the fundamentals of sensors, which rely on semiconductors for their functionality. Sensors are classified into active and passive types, with their performance characterized by parameters like sensitivity, range, resolution, accuracy, and repeatability. Their applications span numerous fields, including healthcare, automation, and environmental monitoring. Through a detailed exploration of these topics, semiconductor physics provides the foundation for understanding the principles and applications of modern electronics and optoelectronics. This introduction aims to build a strong conceptual base, enabling students to analyze, innovate, and contribute to this rapidly evolving field.

2. Band Theory of solids

		IIIA		IVA		VA		VIA		VIIA		VIIIA	
		B		C		N		O		F		Ne	
		Al		Si		P		S		Cl		Ar	
		Ga		Ge		As		Se		Br		Kr	
		In		Sn		Sb		Te		I		Xe	
		Tl		Pb		Bi		Po		At		Rn	

A section from the periodic table, more common semiconductor materials are shown. Semiconductors are unique materials whose electrical properties can be controlled and tailored, making them the backbone of modern electronic devices. They can be categorized into different types based on their elemental composition, and their behavior is explained effectively by the band theory of solids.

Fig. 1: A section from the periodic table

**- Types of Semiconductor Materials****- Elemental Semiconductors**

- These are semiconductors composed of a single element from the periodic table, primarily from Group IV. Silicon (Si) and Germanium (Ge) are the most common elemental semiconductors.
- Silicon is widely used due to its abundance, stable chemical properties, and a band gap of 1.12 eV, which makes it ideal for electronic devices like diodes and transistors.
- Germanium has a smaller band gap (0.69 eV), making it more sensitive to temperature variations, and is used in applications like infrared sensors.

- Compound Semiconductors

- These are formed by combining two or more elements, typically from Groups III-V or II-VI in the periodic table.
- Gallium Arsenide (GaAs): Known for its high electron mobility and a direct band gap of 1.43 eV, making it ideal for high-frequency and optoelectronic applications like LEDs and lasers.
- Indium Phosphide (InP): Used in high-speed communication systems and solar cells due to its direct band gap and high efficiency.
- Cadmium Telluride (CdTe): Widely used in thin-film solar cells because of its near-ideal band gap of 1.45 eV for solar energy absorption.

- Doped Semiconductors

- Alloy semiconductors are formed by mixing two or more semiconductors in varying proportions.
- The properties of these alloys can be tuned by changing the composition.
- Silicon-Germanium ($\text{Si}_{1-x}\text{Ge}_x$): By varying the fraction 'x', the band gap and lattice constants can be tailored for specific applications like high-speed integrated circuits.
- Aluminum Gallium Arsenide ($\text{Al}_x\text{Ga}_{1-x}\text{As}$): Commonly used in optoelectronic devices such as laser diodes, where the band gap can be adjusted by changing the value of 'x'.

- Origin of energy bands formation in solids

- The origin of energy bands in solids arises from the interaction of atomic orbitals when a large number (N) of identical atoms come together to form a solid, such as a crystal lattice.
- In an isolated atom, electrons occupy discrete energy levels within atomic orbitals.
- However, when these atoms are closely packed in a solid, their atomic orbitals overlap due to the proximity of neighbouring atoms.
- This overlap causes the discrete energy levels of individual atoms to split into (N) closely spaced energy levels for each atomic energy state.
- These closely spaced levels merge to form continuous ranges of allowed energies, known as bands of allowed energies.
- Between these allowed energy bands, there exist regions where no electron energy states can exist, referred to as forbidden bands or energy gaps.
- This formation of energy bands and gaps is fundamental to the electronic properties of solids and determines whether a material behaves as a conductor, semiconductor, or insulator.

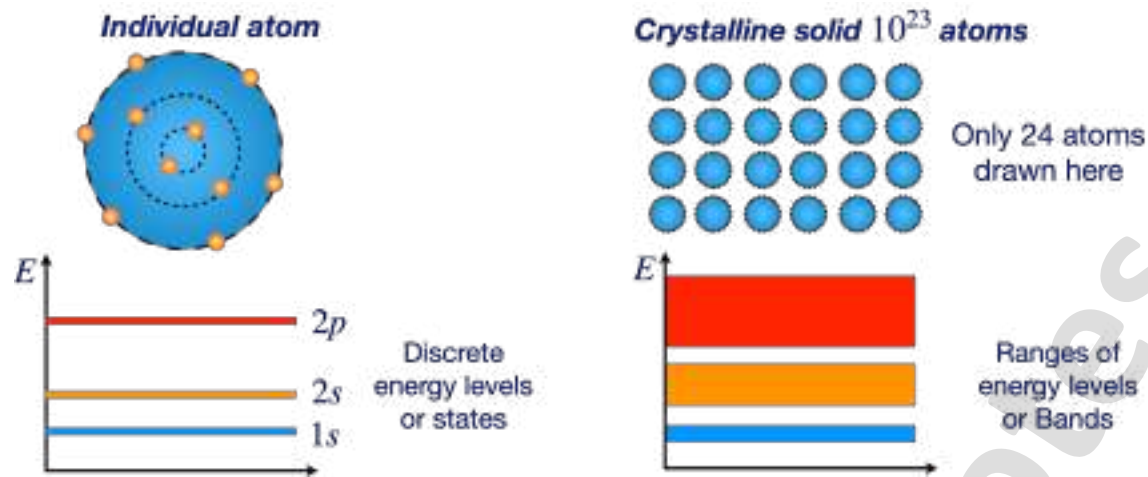


Fig. 2: Band Structure in individual atom and N number of atoms

- In an individual atom, electrons occupy discrete energy levels corresponding to atomic orbitals, such as 1s, 2s, 2p, and so on. These energy levels are well-separated and unique to the atom, arising from quantum mechanical principles. However, when N identical atoms come together to form a solid, such as in a crystal lattice, their atomic orbitals overlap due to the close proximity of atoms. This overlap causes the discrete energy levels of each atom to split into N closely spaced energy levels for every orbital. These numerous closely spaced levels combine to form continuous ranges of energy called bands. The bands that result are classified as allowed energy bands (where electrons can exist), while the regions between them, where no energy levels are available, are known as forbidden energy gaps or band gaps. This transformation of energy levels into a band structure is fundamental to understanding the electrical and optical properties of materials, as it determines whether the material is a conductor, semiconductor, or insulator.
- In an isolated atom, electrons occupy well-defined regions around the nucleus known as atomic orbitals, each associated with specific discrete energy levels. These energy levels arise from the quantized nature of electron motion in an atom, as described by quantum mechanics. Each orbital is characterized by a unique set of quantum numbers, which determine the electron's energy and spatial distribution. The energy levels are discrete because the electrons in an isolated atom cannot possess arbitrary amounts of energy; they can only occupy specific states.
- For example, in a hydrogen atom, the electron occupies quantized energy levels labeled $n = 1, 2, 3$, where n is the principal quantum number. The energy difference between these levels determines how much energy is absorbed or emitted when electrons transition between them. These discrete energy levels are the foundation for phenomena like atomic spectra and provide the basis for understanding how energy bands form when atoms interact to create solids.

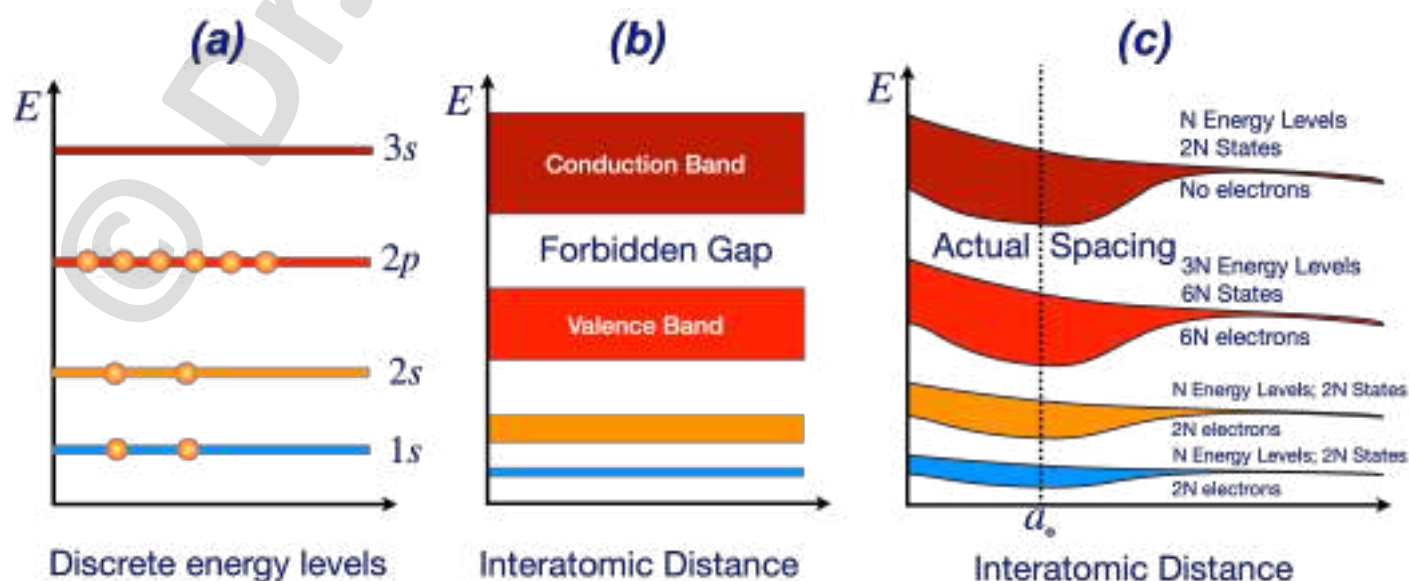


Fig. 3: Energy level of an isolated atom



- The energy band structure in solids arises from the interaction of atomic orbitals when a large number of atoms come together to form a crystal lattice. In an isolated atom, electrons occupy discrete energy levels, but in a solid, the close proximity of atoms causes their orbitals to overlap. This overlap results in the splitting of discrete energy levels into closely spaced energy states, forming continuous energy bands. The two primary bands in a solid are the valence band, which is filled with electrons bound to the atoms, and the conduction band, which is typically empty but can accommodate free electrons that contribute to electrical conductivity. The region between these two bands, where no energy levels exist, is called the band gap or forbidden energy gap. The size of the band gap determines the material's electrical properties: conductors have overlapping bands, semiconductors have a small band gap, and insulators have a large band gap. This band structure is crucial for understanding and designing materials for electronic, optical, and energy applications.
- **Energy Bands**
 - Energy bands are a fundamental concept in solid-state physics, describing the allowed ranges of energy that electrons can occupy in a solid. These bands emerge from the interaction of atomic orbitals when a large number of atoms come together to form a solid, such as in a crystal lattice.
 - In an isolated atom, electrons occupy discrete energy levels. However, in a solid, the close proximity of atoms causes the overlap of their atomic orbitals, leading to the splitting of discrete energy levels into a large number of closely spaced energy states. These states combine to form continuous energy bands. The two most significant energy bands in a solid are:
- **Valence Band (VB):**
 - The valence band is the energy band formed by grouping the energy levels of valence electrons that participate in covalent bonding within a solid. These electrons are tightly bound to their respective atoms and are not free to move under normal conditions.
 - The valence band represents the highest range of electron energies that are fully or partially occupied in the ground state of the solid. Electrons in this band are responsible for the bonding structure of the material but do not contribute to electrical conductivity unless they gain sufficient energy to leave the valence band.
- **Conduction Band (CB):**
 - The conduction band corresponds to the energy levels of free electrons that have broken away from their covalent bonds, gaining sufficient energy to become free and mobile within the solid. These free electrons contribute to electrical conductivity.
 - The conduction band is formed by grouping the range of energy levels that these free electrons can occupy. In conductors, this band overlaps with the valence band, while in semiconductors and insulators, it is separated from the valence band by a band gap.
- **Forbidden Energy Gap:**
 - The forbidden energy gap is the region between the valence band and the conduction band where no energy levels exist for electrons. Electrons cannot occupy states in this region. The energy required for an electron to transition from the valence band to the conduction band is called the band gap energy (E_g).
 - The size of the band gap determines the electrical properties of a material:
 - In conductors, the valence band and conduction band overlap, resulting in no band gap.
 - In semiconductors, the band gap is small, typically around 1 eV, allowing electrons to jump with minimal energy input.
 - In insulators, the band gap is large (greater than 3 eV), making it difficult for electrons to move from the valence band to the conduction band.

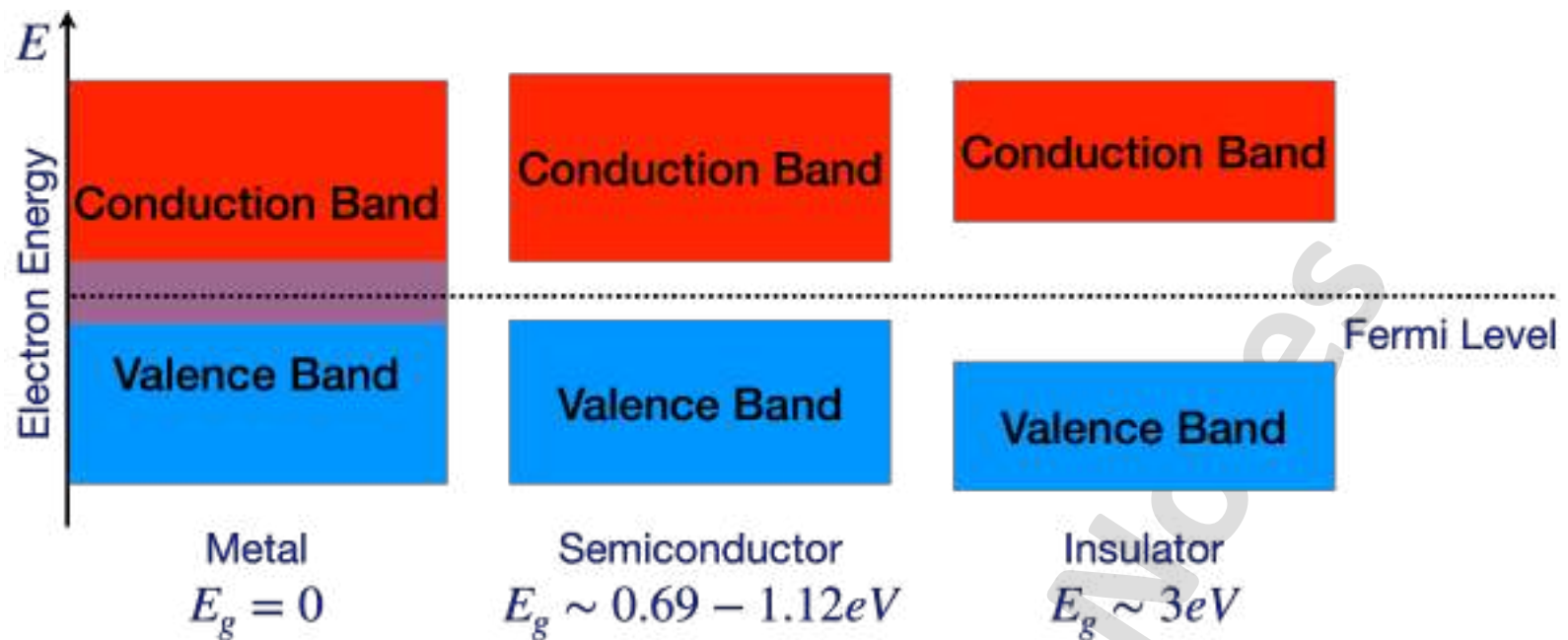


Fig. 4: Classification of solids on the basis of band theory

- Metals / Conductors

- Metals or conductors are materials in which a large number of free electrons are present and can move freely throughout the solid. These free electrons reside in the conduction band (CB) and are responsible for the high electrical conductivity of metals.
- In conductors, the valence band (VB) and conduction band overlap, resulting in a zero band gap energy ($E_g = 0$). This overlap allows electrons to move freely between the bands without requiring additional energy, enabling efficient electron flow under an applied electric field.
- Examples of conductors include metals such as copper, aluminum, silver, and gold, which are widely used in electrical and electronic applications due to their excellent conductivity. The concentration of free electrons in conductors is approximately 10^{28} electrons/ m^3 , making them highly efficient in conducting electricity.
- The resistivity of conductors typically lies in the range of $10^{-8} \Omega \cdot \text{m}$ to $10^{-6} \Omega \cdot \text{m}$, indicating very low resistance to the flow of current. Correspondingly, the conductivity of these materials is high, often in the order of 10^7 mho/m. These properties make metals essential for applications in power transmission, electrical wiring, and electronic circuitry.

- Semiconductors

- Semiconductors are materials in which the energy band gap between the valence band (VB) and the conduction band (CB) is narrow, typically 2 eV or less. Due to this small band gap, a moderate amount of energy such as thermal energy, light, or an applied potential can excite electrons from the VB to the CB. Once in the conduction band, these electrons contribute to electrical conductivity. The modest flow of current in semiconductors makes them distinct from conductors and insulators.
- Examples of semiconductors include silicon and germanium, which are widely used in electronic devices such as transistors, diodes, and solar cells. The concentration of free electrons in semiconductors is much lower than that in metals, typically around 10^{14} electrons/ m^3 , making their conductivity significantly lower. The resistivity of semiconductors varies from 10^{-4} to $10 \Omega \cdot \text{m}$, depending on factors such as temperature and doping.
- Similarly, the conductivity of semiconductors ranges from 10^{-6} to 10^4 mho/m, which is intermediate between that of insulators and metals. These tunable electrical properties, combined with their sensitivity to external stimuli, make semiconductors essential for modern electronics and optoelectronics.

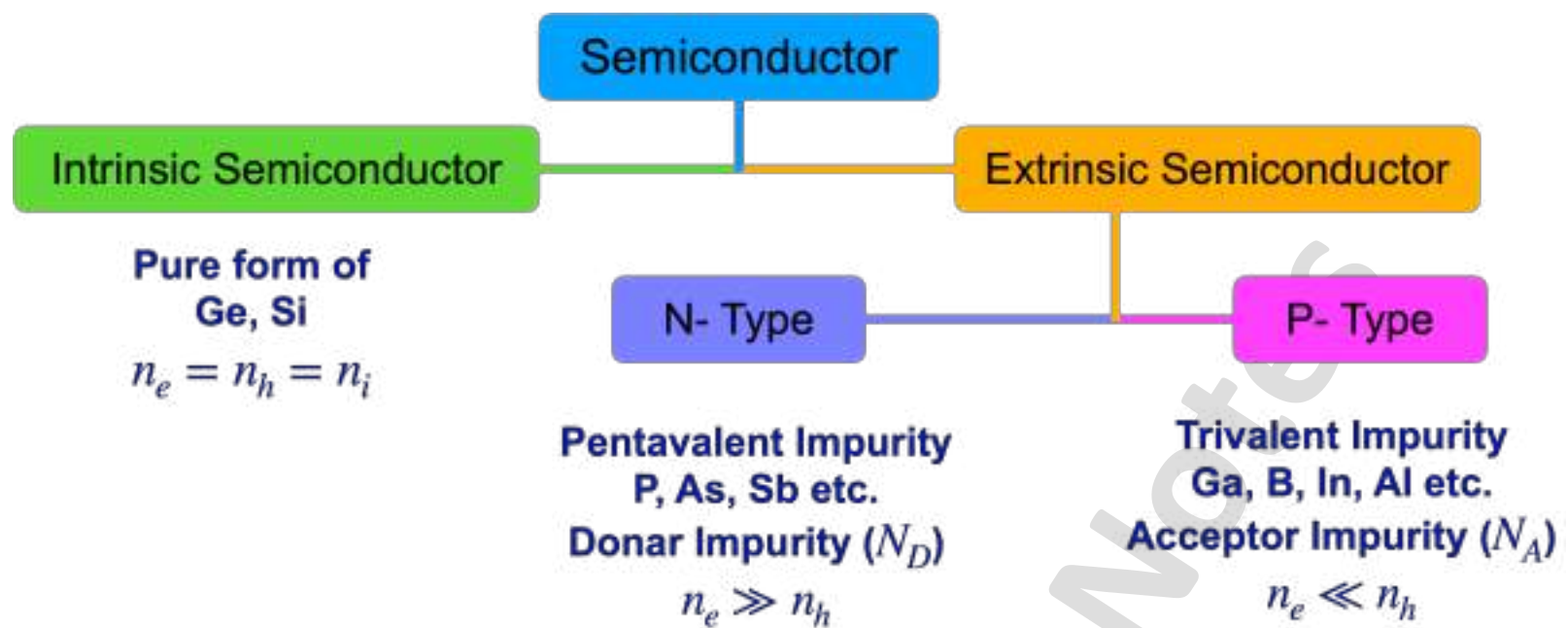


Fig. 5: Types of Semiconductors

- **Types of Semiconductors**
- Semiconductors can be classified based on their intrinsic properties and the way their electrical conductivity is modified.
- There are primarily two types of semiconductors:
- **Intrinsic Semiconductors:**

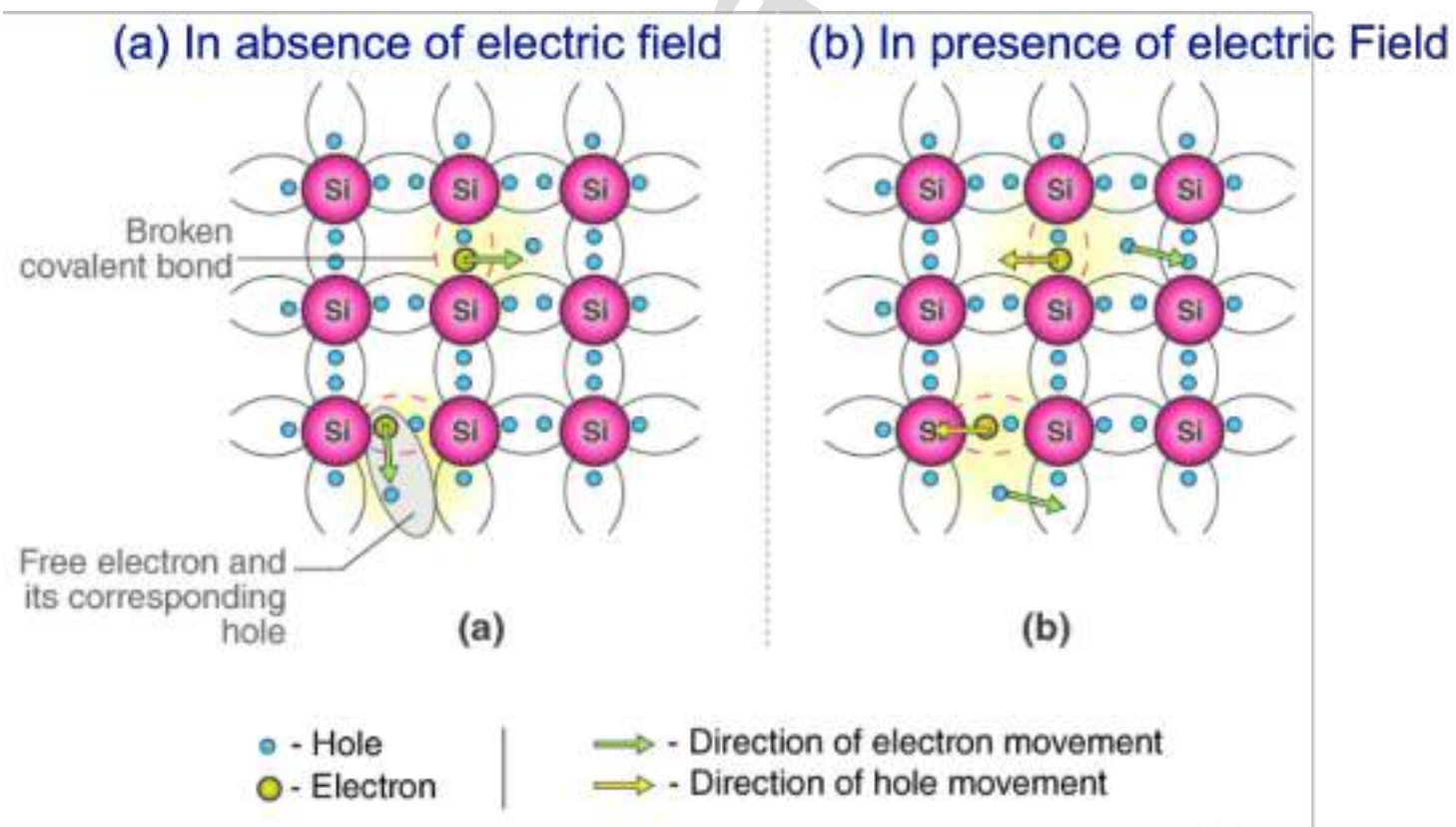


Fig. 6: Conduction mechanism in case of intrinsic semiconductors

- These are pure semiconductors that are not doped with any impurities. The electrical properties of intrinsic semiconductors are governed by the material's own crystal structure and temperature.
- In intrinsic semiconductors, the number of free electrons in the conduction band is determined by the thermal excitation of electrons from the valence band to the conduction band.
- At absolute zero, these semiconductors act as insulators, but as temperature increases, electrons gain enough energy to jump across the narrow band gap and become free to conduct electricity.
- Examples: Silicon (Si), Germanium (Ge), and Gallium Arsenide (GaAs) in their pure form.

- Extrinsic Semiconductors:

- These semiconductors are intentionally doped with small amounts of other elements (impurities) to enhance their electrical conductivity. The doping process introduces either excess free electrons or "holes" (the absence of electrons in the valence band), which contribute to electrical conductivity.

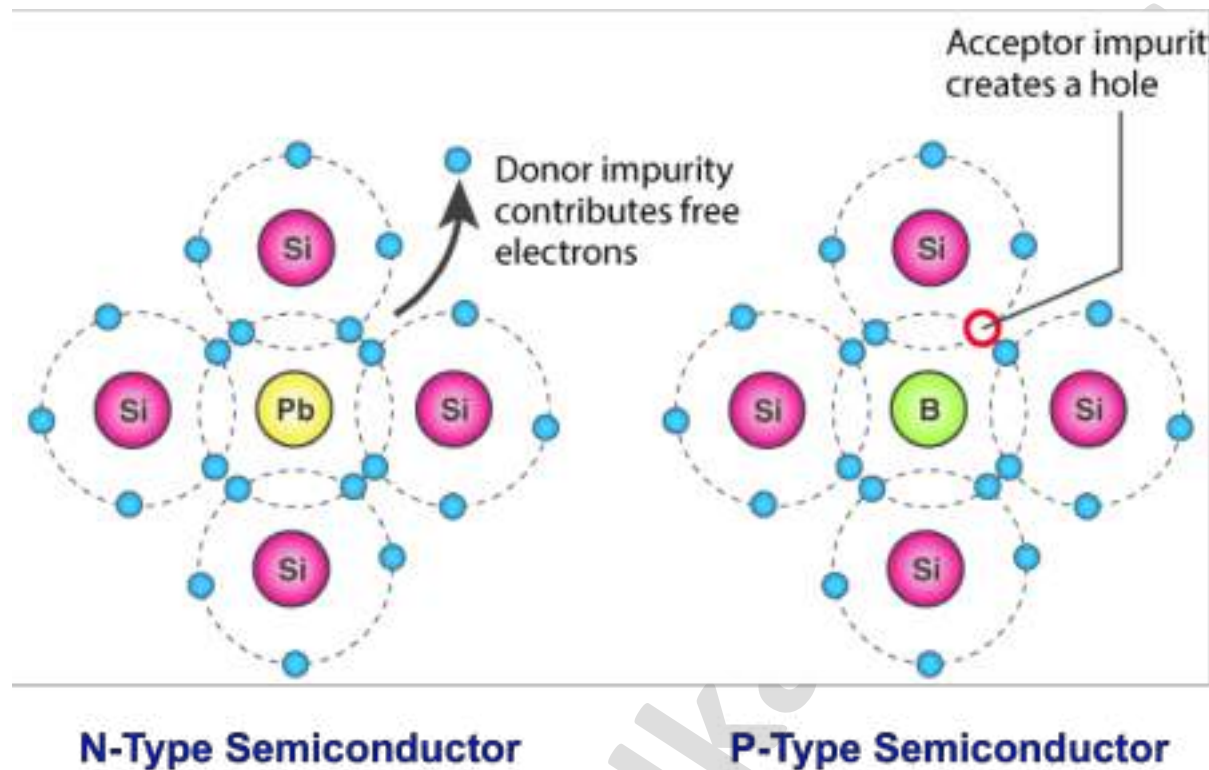


Fig. 7: Extrinsic Semiconductor

- There are two main types of extrinsic semiconductors based on the type of impurity added:

a) N-Type Semiconductor (Negative Type):

- N-type semiconductors are doped with elements that have more valence electrons than the host semiconductor. For example, silicon (which has 4 valence electrons) can be doped with phosphorus (which has 5 valence electrons).
- The extra electron from the phosphorus atom becomes a free electron in the conduction band, increasing the material's conductivity.
- In N-type semiconductors, the majority charge carriers are free electrons, while the minority carriers are holes.
- Example: Silicon doped with Lead or Arsenic.

b) P-Type Semiconductor (Positive Type):

- P-type semiconductors are doped with elements that have fewer valence electrons than the host material. For example, doping silicon with boron (which has 3 valence electrons) creates "holes" in the crystal lattice, which can move through the material like positive charge carriers.
- In P-type semiconductors, the majority charge carriers are holes, while the minority carriers are free electrons.
- Example: Silicon doped with boron.
- These two types of semiconductors—N-type and P-type—are often used together in electronic devices such as diodes and transistors to form PN junctions, which have unique electrical characteristics essential for controlling current flow.

c) Insulators:

- Insulators are materials in which the band gap between the valence band (VB) and the conduction band (CB) is very wide, typically greater than 5 eV. In these materials, electrons are tightly bound to their atoms, and a substantial amount of energy is required to move an electron from the valence band to the conduction band.



- As a result, the number of free electrons available for conduction is extremely low, and the material does not allow significant electrical current to flow even when a potential difference is applied across it.
- In insulators, because of the large band gap, electrons in the valence band cannot easily gain enough energy to jump to the conduction band under normal conditions.
- Therefore, when a potential difference is applied, only a negligible current flows, and the material exhibits very low electrical conductivity.
- The electrical resistivity of insulators is very high, ranging from $10^{12} \Omega\cdot m$ to $10^{16} \Omega\cdot m$, and their conductivity is typically around 10^{-12} mho/m .
- Examples of insulators include materials such as glass, wood, mica, and rubber, which are commonly used for electrical insulation purposes.
- Their high resistivity and inability to conduct electricity make them essential for protecting electrical circuits and ensuring safety in various applications.

4. Electrical conductivity in conductors (qualitative)

- Electrical conductivity in conductors refers to their ability to allow electric current to flow through them. It is primarily determined by the ease with which electrons can move within the material.
- Conductors, like metals (e.g., copper, silver, aluminum), have free electrons in their outermost shell that are not tightly bound to the atoms.
- These free electrons can move easily under the influence of an electric field, enabling current flow. When a conductor is connected to a power source, an electric field is established.
- This field pushes the free electrons, causing them to flow, which is the electric current.
- **Resistivity** is commonly represented by the Greek letter ρ (rho). The SI unit of electrical resistivity is the **ohm-meter** ($\Omega \cdot m$).
- **Electrical conductivity** represents a material's ability to conduct electric current. It is commonly signified by the Greek letter σ (sigma). The SI unit of electrical conductivity is **Siemens per metre** (S/m).
- Electrical conductivity (σ) is the reciprocal of resistivity (ρ)

$$\sigma = \frac{1}{\rho} \quad \dots(1)$$

σ : Conductivity (Siemens per meter, S/m)

ρ : Resistivity (Ohm meters, $\Omega \cdot m$)

- Factors Affecting Conductivity:

- **Material:** Metals like silver and copper are excellent conductors due to high free-electron density.
- **Temperature:** In most conductors, increasing temperature increases resistance, reducing conductivity.
- **Impurities:** Adding impurities (like in alloys) disrupts the electron flow, lowering conductivity.
- **Example:** Copper, one of the best conductors, has a high density of free electrons and a low resistivity ($1.68 \times 10^{-8} \Omega \cdot m$) at room temperature.

- Electrical conductivity in metals

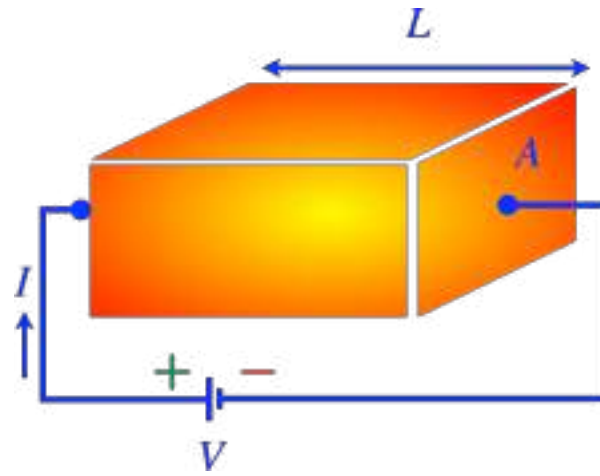


Fig. 8: Electrical conductivity in metals

- Let us consider a rectangular block of **length** L and **cross-sectional area** A . Let n be the **concentration of free electrons** available in it. If a **potential difference** V is applied across a solid, it creates an **electric field** E in the solid is given by;

$$E = \frac{V}{L} \quad \dots (2)$$

where L is the length along which charge carriers move in the solid.

- **The current** I passing across an area A is defined as the net charge Q transported through the area per unit time i.e.

$$I = \frac{Q}{t} \quad \dots (3)$$

- The magnitude of the current flowing through the material is governed by **Ohm's law** i.e

$$I = \frac{V}{R} \quad \dots (4)$$

- The **resistance** R is given by,

$$R = \rho \frac{L}{A} \quad \dots (5)$$

- The reciprocal of resistivity is known as **conductivity** i.e

$$\sigma = \frac{1}{\rho} = \frac{L}{RA} \quad \text{where } \rho \text{ is known as resistivity.} \quad \dots (6)$$

- **Total number of electrons in solids** (N) = (Electron concentration) \times (Volume)

$$\text{Hence; } N = nAL \quad \dots (7)$$

- **Total charge present in the solid** (Q) = (Total number of electrons) \times (Charge)

$$Q = Ne = neAL \quad \dots (8)$$

- **The current through the solid**, $I = \frac{Q}{t} = \frac{neAL}{t}$... (9)

$$\text{Hence; } I = neAv_d \quad \dots (10)$$

Where, v_d is the average drift velocity of electrons.



- **The current density** is given by $J = \frac{I}{A}$... (11)

$$\text{Hence; } J = \frac{neAv_d}{A} = nev_d \quad \dots (12)$$

$$\text{Now; Ohm's law } I = \frac{V}{R} \text{ but } R = \rho \frac{L}{A} \quad \text{Hence } I = \frac{VA}{\rho L} = \frac{1}{\rho} \frac{V}{L} A \quad \text{as } E = \frac{V}{L};$$

$$\text{Hence; } I = \sigma EA \quad \dots (13)$$

$$\text{Now; } J = \frac{I}{A} = \frac{\sigma EA}{A} \quad \text{Hence; } J = \sigma E \quad \dots (14)$$

This equation is known as **point form** or **microscopic form** of Ohm's law. From equations (12) and (14)

$$J = nev_d = \sigma E$$

$$\text{The conductivity can be written as; } \sigma = \frac{nev_d}{E} \quad \therefore \sigma = ne\mu \quad \dots (15)$$

where, $\mu = \frac{v_d}{E}$ The quantity μ is known as **mobility of electrons**.

- **Mobility of electrons:**

- Mobility of Electrons is a measure of how easily electrons can move through a material when subjected to an electric field. It quantifies the efficiency of electron movement in response to an applied force. The mobility (μ) of electrons is defined as the drift velocity per unit electric field:

$$\mu = \frac{v_d}{E}$$

- μ : Mobility of electrons (unit: $\text{m}^2\text{V}^{-1}\text{s}^{-1}$)

v_d : Drift velocity of electrons (m/s)

E : Electric field strength (V/m)

- **Drift Velocity:** When an electric field is applied, electrons gain a small average velocity in the direction opposite to the field. This average velocity is called drift velocity.
- **Mobility Interpretation:** Mobility indicates how quickly an electron responds to the electric field. Higher mobility means electrons can travel faster and with less resistance. Units:
- The unit of electron mobility is derived from its formula:

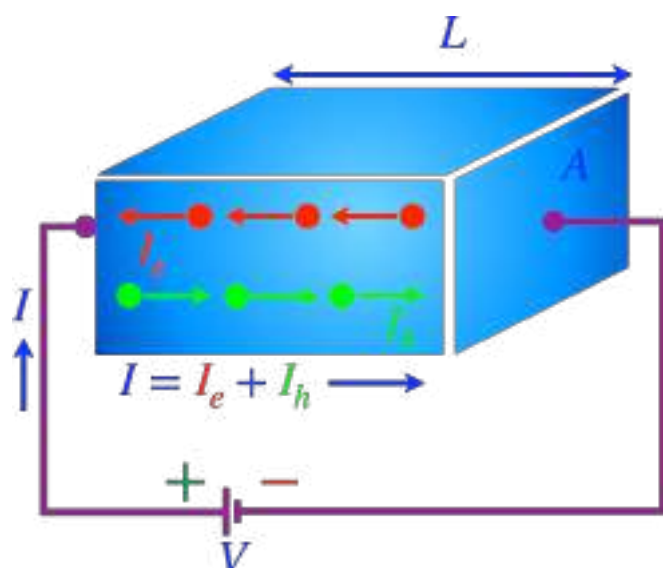
$$\mu = \frac{\text{m/s}}{\text{V/m}} = \text{m}^2\text{V}^{-1}\text{s}^{-1}.$$

- **Typical values of mobility:**

- **Metals:** Mobility in metals is relatively low (around $10^{-2} \text{ m}^2\text{V}^{-1}\text{s}^{-1}$) because electron scattering from ions and impurities is significant, despite a high density of free electrons.
- **Semiconductors:** Mobility in semiconductors is higher (order of $10^{-1} \text{ m}^2\text{V}^{-1}\text{s}^{-1}$ to $1 \text{ m}^2\text{V}^{-1}\text{s}^{-1}$) due to a reduced number of scattering events compared to metals.

- Electrical conductivity of semiconductors (Derivation)

- The electrical conductivity of a semiconductor is derived based on the contribution of both electrons and holes as charge carriers. It is determined by their concentrations, charges, and mobilities.



L – length;

A – cross sectional area

V – applied potential difference

E – electrical field generated

I – total current

I_n – current due electrons drifting in the CB

I_p – current due holes drifting in the VB

v_{d_n} – drift velocities of electrons

v_{d_p} – drift velocities of holes

n – concentrations of electrons

p – concentration of holes

Fig. 9: Electrical conductivity in semiconductor

- Derivation:

- Current Density:

When an electric field E is applied to a semiconductor, the current density J is the sum of contributions from electrons and holes:

$$J = J_n + J_p \quad \dots(16)$$

$$J_n = qn v_{d_n} : \text{Current density due to electrons.}$$

$$J_p = qp v_{d_p} : \text{Current density due to holes.}$$

Here, v_{d_n} and v_{d_p} are the drift velocities of electrons and holes, respectively.

- Drift Velocity:

The drift velocity is proportional to the applied electric field:

$$v_{d_n} = \mu_n E \quad \text{and} \quad v_{d_p} = \mu_p E \quad \dots(17)$$

- Substitute Drift Velocities into Current Density

$$J = qn\mu_n E + qp\mu_p E \quad \dots(18)$$

- Relating Current Density and Conductivity:

By Ohm's law, the current density is related to the electric field through conductivity:

$$J = \sigma E \quad \dots(19)$$

Comparing the two expressions for J

$$\sigma E = qn\mu_n E + qp\mu_p E \quad \dots(20)$$

- Solve for Conductivity:

Divide through by E (assuming $E \neq 0$):

$$\sigma = q(n\mu_n + p\mu_p) \quad \dots(21)$$

Where:

q : Elementary charge ($1.6 \times 10^{-19} \text{ C}$)

n : Concentration of electrons in the conduction band (in m^{-3})

μ_n : Mobility of electrons ($\text{m}^2 \text{V}^{-1} \text{s}^{-1}$)

p : Concentration of holes in the valence band (in m^{-3})

μ_p : Mobility of holes ($\text{m}^2 \text{V}^{-1} \text{s}^{-1}$)

This formula accounts for the contributions of both types of charge carriers (electrons and holes) to the conductivity.

- Special Cases:

- Intrinsic Semiconductors:

In intrinsic semiconductors, the electron and hole concentrations are equal ($n = p = n_i$),

where n_i is the intrinsic carrier concentration.

The conductivity becomes: $\sigma = qn_i(\mu_n + \mu_p)$...(22)

- Extrinsic Semiconductors:

For extrinsic semiconductors:

In n-type, the concentration of electrons is much greater than the concentration of holes i.e. $n \gg p$,

The majority charge carriers are electrons and the contribution of holes is neglected due to very small value.

hence $\sigma \approx qn\mu_n$...(23)

In p-type, the concentration of holes is much greater than the concentration of electrons i.e. $p \gg n$,

The majority charge carriers are holes and the contribution of electrons is neglected due to very small value.

hence $\sigma \approx qp\mu_p$...(24)

5. Hall effect and Hall coefficient (with derivation)

- Definition:

- The **Hall Effect** is the production of a voltage difference (Hall voltage) across a conductor or semiconductor when it carries an electric current and is placed in a magnetic field perpendicular to the current.

- The **Hall coefficient** is defined as the ratio of the induced electric field to the product of the current density and the applied magnetic field.

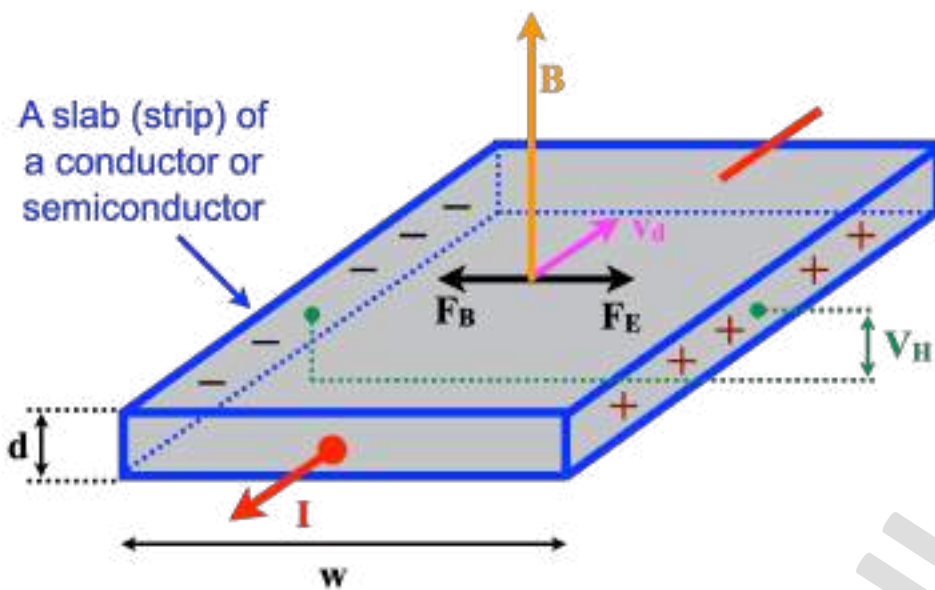
- Principle:

- When a magnetic field (B) is applied perpendicular to a current-carrying conductor or semiconductor, the moving charge carriers experience a force (Lorentz force) that pushes them to one side of the material. This accumulation of charges creates a potential difference (Hall voltage, V_H) across the conductor.

- The Hall effect is due to the nature of the current in a conductor or semiconductor. Current consists of the movement of many small charge carriers, typically electrons, holes, ions or all three. When a magnetic field is present, these charges experience a force, called the Lorentz force. When such a magnetic field is absent, the

charges follow approximately straight, line of sight paths between collisions with impurities, phonons, etc. when a magnetic field with a perpendicular component is applied, their paths between collisions are curved, thus moving charges accumulate on one face of the material. This leaves equal and opposite charges exposed on the other face, where there is a shortage of mobile charges.

- The Hall Effect is typically visualized using a rectangular slab of a conductor or semiconductor placed in a magnetic field as shown in fig. 10. Below are the key components and parameters in the context of the Hall Effect:



Cross sectional area of the semiconductor $A = wd$

w - width of the slab

d - thickness of the slab

I - current flowing through the slab

n - charge concentration

q - charge on the carriers

v_d - drift velocity of charge carriers

A - cross-sectional area of the slab

F_B - Force due to magnetic field

F_E - Force due to electric field

V_H - Hall Voltage

Fig. 10: Hall effect

- **Width of the Slab (w):** The distance between the two sides of the slab where the Hall voltage develops. It is perpendicular to the direction of the current and the magnetic field.
- **Thickness of the Slab (d):** The distance between the top and bottom surfaces of the slab. The magnetic field is applied perpendicular to this thickness.
- **Current Flowing Through the Slab (I):** Current flows longitudinally through the slab, along the length of the material. This current is responsible for moving the charge carriers.
- **Charge Concentration (n):** The number of charge carriers (electrons in n-type or holes in p-type semiconductors) per unit volume (m^{-3}). It determines the density of carriers available for conduction.
- **Charge on the Carriers (q):** The elementary charge of the carriers.
- For electrons, $q = -1.6 \times 10^{-19} \text{ C}$;
- For holes, $q = +1.6 \times 10^{-19} \text{ C}$
- **Drift Velocity of Charge Carriers (v_d):** The average velocity of charge carriers due to the applied electric field.

Related to current density (J) by: $J = \frac{I}{A}$ hence $v_d = \frac{I}{nqA}$ or $v_d = \frac{J}{nq}$

- **Cross-Sectional Area of the Slab (A):** The area through which the current flows, given by: $A = w \times d$
- **Force Due to Magnetic Field (F_B):** When a charge carrier moves in the presence of a magnetic field (B), it experiences a magnetic force due to the Lorentz force: $F_B = qv_dB$. This force pushes the carriers to one side of the slab, creating the Hall voltage.



- **Force Due to Electric Field (F_E):** As charges accumulate on one side, an electric field (E_H) is generated, creating a force that opposes the magnetic force: $F_E = qE_H$
- **Hall Voltage (V_H):** The voltage generated due to charge separation across the width of the slab.
- **Derivation of Hall Voltage and Coefficient:**

- **Lorentz Force:**

- Charge carriers moving with velocity v_d (drift velocity) in the presence of a magnetic field experience a force: $F_B = q(v_d \times B)$... (25)

This force pushes the carriers to one side, creating an electric field E_H that opposes further accumulation of charges.

- Force due to electric field on the charge carriers is; $F_E = qE_H$... (26)

- **Equilibrium:**

- At equilibrium, the electric force equals the magnetic force: If magnitude of both forces is equal and net force on charge carrier is zero.

$$F_B = F_E$$

hence from equation (25) and (26)

$$qE_H = qv_d B$$

Therefore:

$$E_H = v_d B \quad \dots (27)$$

- **Drift Velocity:**

- The drift velocity is related to the current density:

$$v_d = \frac{J}{nq} \quad \dots (28)$$

Substituting v_d equation (28) into E_H equation (27):

$$E_H = \frac{J}{nq} B \quad \therefore \frac{1}{nq} = \frac{E_H}{JB} \quad \dots (29)$$

- **Hall Coefficient:**

$$R_H = \frac{E_H}{JB} = \frac{\frac{JB}{qn}}{JB} \quad \therefore R_H = \frac{1}{nq} \quad \dots (30)$$

where,

q : Charge of an electron (C)

n : Carrier concentration (m^{-3})

Unit of R_H :

$$R_H = \frac{\text{m}^3}{\text{C}} \quad \text{or } \text{m}^3\text{C}^{-1}$$



- Hall Voltage:

- If V_H is **potential difference** generated along the width of the slab due to the **electric field** E_H , then, $E_H = \frac{V_H}{w}$.

Using equation (27) $E_H = v_d B$

We can write,

$$v_d B = \frac{V_H}{w} \quad \therefore V_H = B v_d w$$

$$\text{as, } v_d = \frac{I}{n q w d} \quad \therefore V_H = B \frac{I}{n q w d} w \quad \text{hence } V_H = \frac{B I}{n q d}$$

$$\therefore V_H = \frac{1}{n q} \frac{B I}{d} \quad \text{as } R_H = \frac{1}{n q} \quad \text{hence } V_H = R_H \frac{B I}{d} \quad \dots(31)$$

Unit of V_H : Volt

- Applications of Hall effect

(a) Determination of type of semiconductor

- The Hall voltage is; $V_H = R_H \frac{B I}{d}$ and Hall coefficient; $R_H = V_H \frac{d}{B I}$
- If value of R_H is **positive** then type of **semiconductor is P-type**.
- If R_H is **negative** the type of **semiconductor is N-type**.

(b) Determination of charge carrier concentration

- This value of Hall coefficient is also equal to; $R_H = \frac{1}{n q}$
- Hence, charge carrier concentration; $n = \frac{1}{R_H q}$...(32)
- Thus, if value of R_H is known, the charge carrier concentration can be found.

(c) Determination of charge carrier mobility

- The electrical conductivity is given by; $\sigma = n q \mu$ where μ is mobility of charge carriers.
- Thus; $\mu = \frac{\sigma}{n q}$ as $R_H = \frac{1}{n q}$; $\mu = \sigma R_H$...(33)
- Thus, the **charge mobility** can be determined using Hall coefficient.

6. Fermi energy, Fermi Level, Fermi Dirac probability distribution function, Fermi level (Definition)

- **Fermi energy (E_F):**
- Fermi energy is the energy of the highest occupied quantum state in a system of fermions (such as electrons) at absolute zero temperature (0 K). At 0 K, all energy states below the Fermi energy are fully occupied, and all states above it are empty.
- It represents the maximum energy level that electrons can occupy in a material at absolute zero. Fermi energy is a fundamental property in metals, semiconductors, and insulators that determines their electrical and thermal behavior. Used in quantum mechanics and solid-state physics.

- Fermi Level:

- The Fermi level is the energy level at which the probability of an electron being present is 50% at a given temperature. Plays a crucial role in determining carrier concentrations in semiconductors. Shifts depending on doping in semiconductors (n-type or p-type). It represents the measure of the energy of the least tightly bound electrons in a solid.
- **In intrinsic semiconductors:** Fermi level lies approximately at the center of the energy gap.
- **In extrinsic semiconductors:**
 - **n-type:** Fermi level shifts closer to the conduction band.
 - **p-type:** Fermi level shifts closer to the valence band.

- Fermi-Dirac Probability Distribution Function:

- **Definition:** The Fermi-Dirac distribution function describes the probability $f(E)$ of an electron occupying a particular energy state E at a given temperature (T). This function takes into account the Pauli Exclusion Principle, which states that no two electrons can occupy the same quantum state simultaneously and the indistinguishable nature of electrons.

- The Formula:

$$f(E) = \frac{1}{e^{\frac{(E - E_F)}{k_B T}} + 1} \quad \dots(34)$$

Where:

E : Energy of the electron state

E_F : Fermi energy (the energy at which the probability of occupation is 50%)

k_B : Boltzmann constant (1.38×10^{-23} J/K)

T : Absolute temperature in Kelvin

$$\text{At } T = 0K: \quad f(E) = \begin{cases} 1 & \text{if } E < E_F \\ 0 & \text{if } E > E_F \end{cases}$$

At $T > 0K$: The probability decreases smoothly as energy increases above E_F .

The graph of $f(E)$ versus energy E provides valuable insights into how electron occupancy changes with energy and temperature.

X-Axis: Represents the energy levels (E) of electrons.

The Fermi energy (E_F) is marked on this axis as the reference point.

Y-Axis: Represents the probability $f(E)$ of an electron occupying an energy level $f(E)$ ranges from 0 to 1.

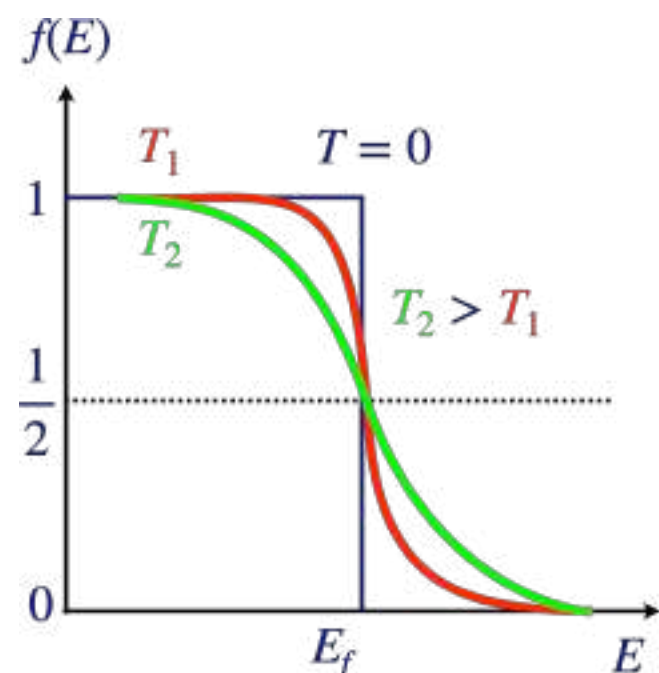


Fig. 11: The Fermi function



- **Behaviour at different temperatures:**

- **At Absolute Zero Temperature ($T = 0K$):**

i) For $E < E_F$:

$$f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} = \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0} = 1$$

$f(E) = 1$ (all states below E_F are fully occupied).

...(35)

ii) For $E > E_F$:

$$f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} = \frac{1}{1 + e^{+\infty}} = \frac{1}{1 + \infty} = 0$$

$f(E) = 0$ (all states above E_F are unoccupied).

...(36)

The distribution becomes a step function at $T = 0K$.

iii) For $E = E_F$

$$f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} = \frac{1}{1 + e^{0/0}} = \text{Indeterminate}$$

...(37)

- **At Non-Zero Temperatures ($T > 0K$):**

The distribution $f(E)$ becomes smooth due to thermal excitation. Some electrons occupy states above E_F , and some states below E_F become unoccupied.

i) For $E = E_F$

$$f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} = \frac{1}{1 + e^0} = \frac{1}{1 + 1} = \frac{1}{2} = 0.5. \text{ The probability is 50\%.}$$

...(38)

ii) For very high energies ($E \gg E_F$):

$$f(E) \approx e^{-\frac{(E-E_F)}{k_B T}}, \text{ similar to the Maxwell-Boltzmann distribution.}$$

...(39)

- **Position of Fermi level:**

- The Fermi level in an intrinsic semiconductor is located near the middle of the energy gap between the conduction band minimum (E_C) and the valence band maximum (E_V). Its position is determined by the effective densities of states in the conduction band and valence band.

a) In intrinsic semiconductor

Let, N_C : Number of electrons in conduction band

N_V : Number of electrons in valence band

N : Total number of electrons in both conduction and valence bands

$$N = N_C + N_V \quad \dots(40)$$

The probability that there are N_C electrons occupy energy state E_C is;

$$P(E_C) = \frac{N_C}{N} \quad \dots(41)$$

According to Fermi-Dirac distribution function, the probability of electron in conduction band occupying energy level will be given by;

$$f(E_C) = \frac{1}{1 + e^{\frac{(E_C - E_F)}{kT}}} \quad \dots(42)$$

As equations (41) and (42) represents the same probability i.e.

$$P(E_C) = f(E_C)$$

$$\frac{N_C}{N} = \frac{1}{1 + e^{\frac{(E_C - E_F)}{kT}}} \quad \text{hence} \quad N_C = \frac{N}{1 + e^{\frac{(E_C - E_F)}{kT}}} \quad \dots(43)$$

$$\text{Similarly for valence band} \quad N_V = \frac{N}{1 + e^{\frac{(E_V - E_F)}{kT}}} \quad \dots(44)$$

From equations (40) substituting values of and from (43) and (44)

$$N = \frac{N}{1 + e^{\frac{(E_C - E_F)}{kT}}} + \frac{N}{1 + e^{\frac{(E_V - E_F)}{kT}}} \quad \therefore 1 = \frac{1}{1 + e^{\frac{(E_C - E_F)}{kT}}} + \frac{1}{1 + e^{\frac{(E_V - E_F)}{kT}}}$$

$$\left[1 + e^{\frac{E_C - E_F}{kT}}\right] \left[1 + e^{\frac{E_V - E_F}{kT}}\right] = \left[1 + e^{\frac{E_C - E_F}{kT}}\right] + \left[1 + e^{\frac{E_V - E_F}{kT}}\right] \quad \text{Solving this we get}$$

$$\exp\left[\frac{E_C + E_V - 2E_F}{kT}\right] = 1 \quad \text{Taking the logarithm of both sides} \quad \frac{E_C + E_V - 2E_F}{kT} = 0$$

$$E_C + E_V - 2E_F = 0 \quad \text{hence} \quad 2E_F = E_C + E_V$$

$$E_F = \frac{E_C + E_V}{2} \quad \dots(45)$$

The Fermi level lies at the center of the bandgap in an intrinsic semiconductor, $E_F = \frac{E_g}{2}$

Its exact position depends on the relative effective masses of electrons and holes, as these determine N_C and N_V . At higher temperatures, the carrier concentration increases, but the position of the Fermi level remains unchanged for intrinsic semiconductors.

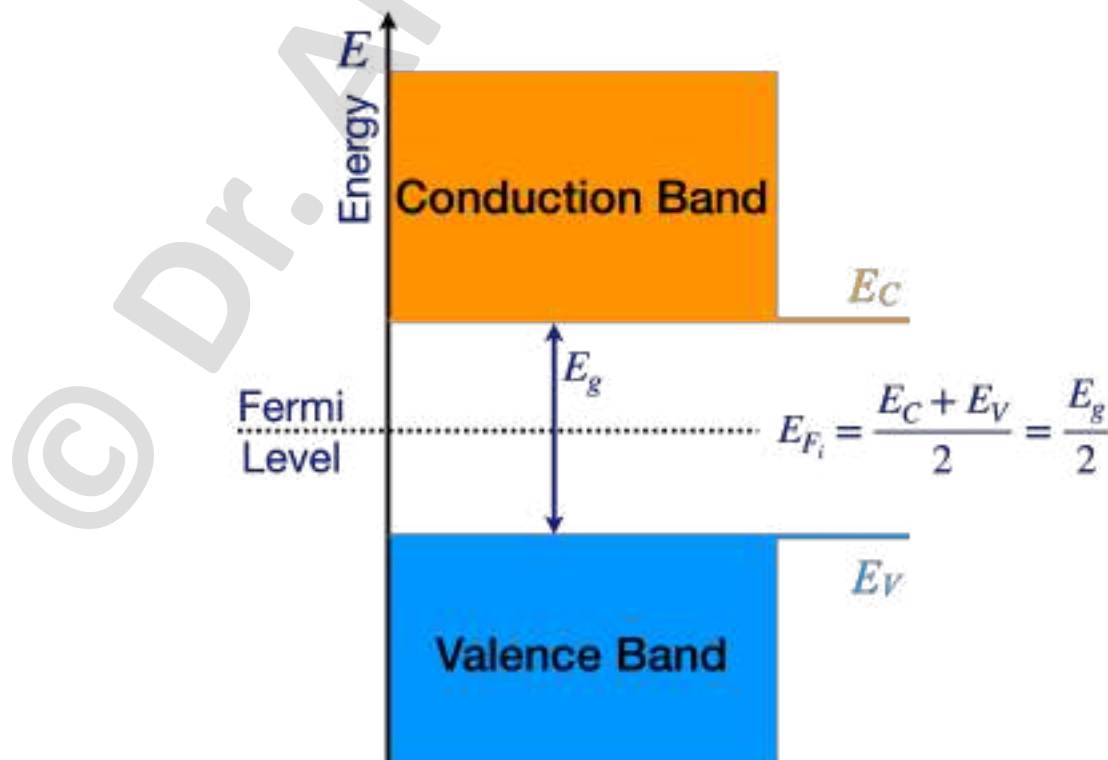


Fig. 11: Position of Fermi level in intrinsic semiconductor at $T = 0K$

b) In extrinsic semiconductor

i) Position of Fermi level in n-Type

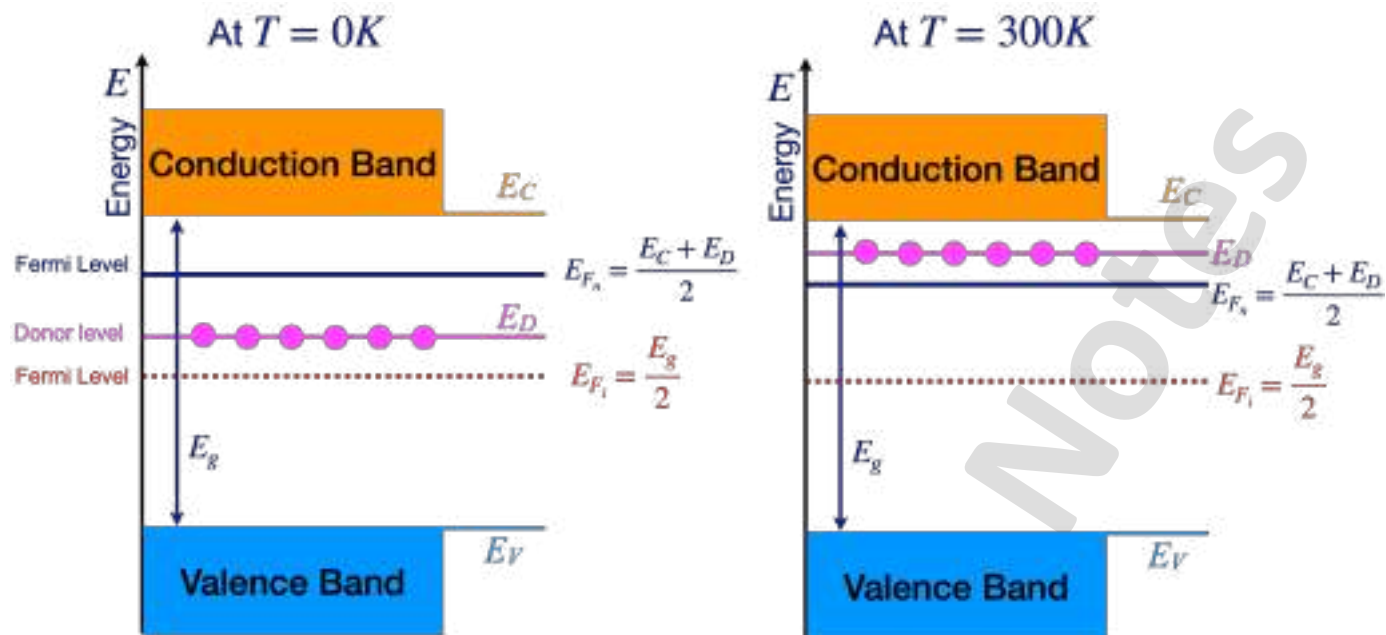


Fig. 12: Position of Fermi level in n-Type at $T = 0K$ and $T = 300K$

- In an n-type semiconductor, the addition of donor impurities (e.g., phosphorus in silicon) introduces energy levels just below the conduction band. These donor levels donate electrons to the conduction band, making electrons the majority carriers. The position of the Fermi level depends on temperature (T) and the doping concentration.
- **At Absolute Zero Temperature (At $T = 0K$)**
 - At $T = 0K$, all donor levels are fully occupied by electrons since there is no thermal excitation. The conduction band is empty, and the valence band is fully occupied. The Fermi level lies just below the conduction band, near the donor energy levels, as the electrons are tightly bound to the donor atoms at this temperature.
- **At Room Temperature (At $T > 0K$):**
 - As the temperature increases, electrons from the donor levels are thermally excited into the conduction band, contributing to electrical conductivity. The Fermi level moves upward toward the conduction band, reflecting the increased population of electrons in the conduction band. The exact position of the Fermi level depends on the doping concentration: Low Doping: The Fermi level is closer to the middle of the bandgap but still above the intrinsic Fermi level. High Doping: The Fermi level moves closer to or even enters the conduction band, especially in heavily doped (degenerate) semiconductors.
- **Variation of Fermi Level with Temperature in an n-type Semiconductor**
 - In the n-type semiconductor at low temperatures, some donor atoms are ionized and provide electrons to the conduction band while others remain neutral. As electrons in the conduction band are only due to the transitions from the donor levels, the Fermi level must lie between the impurity donor levels and the bottom of the conduction band. When $T = 0K$, E_{F_n} lies midway between the donor levels and the bottom of the conduction band. It is thus, $E_{F_n} = \frac{E_C + E_D}{2}$ at $T = 0K$(46)
 - As the temperature increases the donor levels gradually get depleted and the Fermi level moves downward.
 - At the temperature of complete depletion of donor levels, T_d , the Fermi level coincides with the donor level E_D . Thus, $E_{F_n} = E_D$ at $T = T_d$.

- As the temperature grows further above T_d , the Fermi level shifts downward in an approximately linear fashion.
- At a temperature T_i , the intrinsic process contributes to electron concentration significantly.
- At higher temperatures, the n-type semiconductor loses its extrinsic character and behaves as an intrinsic semiconductor. In the intrinsic region, the electron concentration in conduction band increases exponentially and the Fermi level approaches the intrinsic value.

Thus,

$$E_{F_n} = E_{F_i} = \frac{E_g}{2} \text{ at } T \geq T_i$$

$$\text{At } T = 0K; \quad E_{F_n} = \frac{E_C + E_D}{2}$$

$$\text{At } T = T_d; \quad E_{F_n} = E_D$$

$$\text{At } T \geq T_i; \quad E_{F_n} = E_{F_i} = \frac{E_g}{2}$$

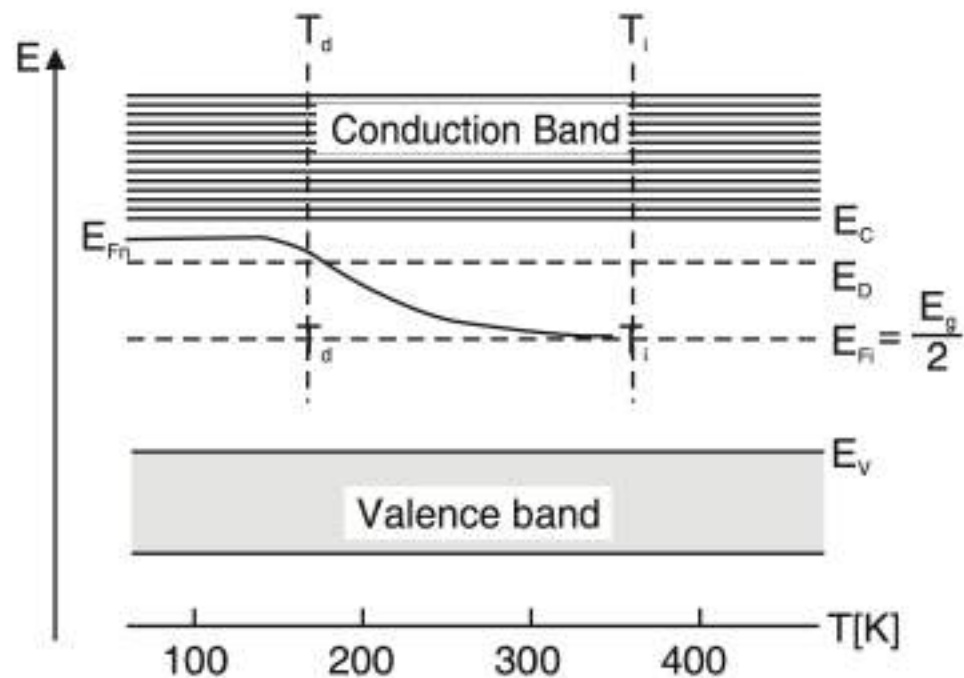


Fig. 13: Qualitative dependence of Fermi level on temperature in an n-type semiconductor

- Variation of Fermi Level with doping concentration in an n-type Semiconductor

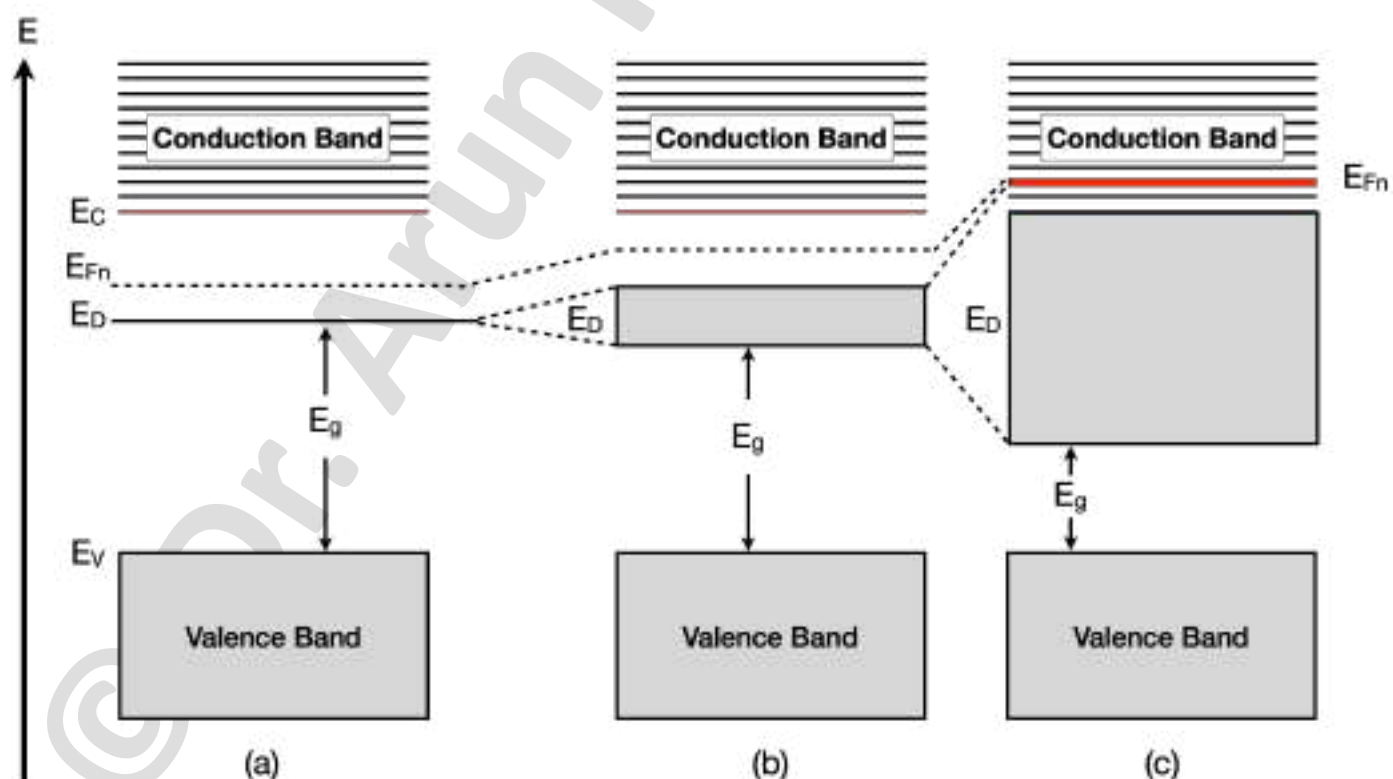


Fig. 14: Energy band diagrams of an n-type semiconductor at three different levels of doping;
(a) low level doping; (b) medium doping; (c) heavy doping.

- The addition of donor impurity to an intrinsic semiconductor leads to the formation of discrete donor levels below the bottom edge of the conduction band.

- At Low Doping Concentration:

- At low donor impurity concentrations, the donor atoms are far apart, and their energy levels remain discrete. The Fermi level shifts upward from its intrinsic position toward the conduction band but does not enter the conduction band. The shift is because the donor electrons contribute additional free electrons to the conduction band.

- At Moderate Doping Concentration:

- As the doping concentration increases, the distance between donor atoms decreases. The discrete donor energy levels begin to interact and form a donor energy band just below the conduction band. The Fermi level moves closer to the conduction band as the donor band becomes more prominent.

- At High Doping Concentration (Degenerate Semiconductor):

- With further increase in doping concentration, the donor band broadens and overlaps with the conduction band. At this point the Fermi level moves into the conduction band, indicating that the material behaves like a degenerate semiconductor (similar to a metal). The material has a very high carrier concentration, and the bandgap effectively narrows.

ii) Position of Fermi level in P-Type

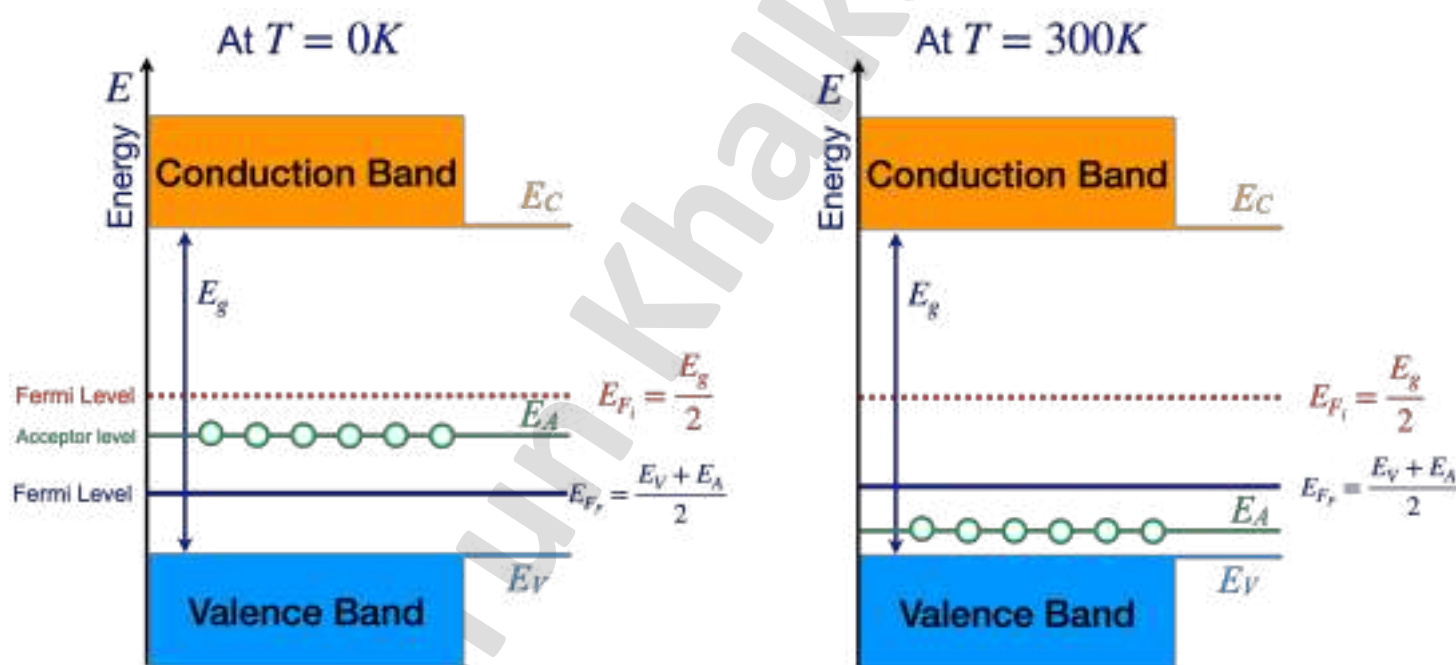


Fig. 15: Position of Fermi level in p-Type at $T = 0K$ and $T = 300K$

- In a p-type semiconductor, the addition of acceptor impurities (e.g., boron in silicon) creates energy levels just above the valence band. These acceptor levels accept electrons from the valence band, leaving behind holes, which act as the majority carriers. The position of the Fermi level depends on temperature (T) and the doping concentration.

- At Absolute Zero Temperature (At $T = 0K$):

- At $T = 0K$, all acceptor levels are unoccupied by electrons, and there are no thermally generated carriers. The valence band is fully occupied, and the conduction band is completely empty. The Fermi level lies just above the valence band, close to the acceptor energy levels, because there are no free electrons or holes at this temperature.

- **At Room Temperature (At $T > 0K$):**

- As the temperature increases, electrons from the valence band are thermally excited into the acceptor levels, leaving behind holes in the valence band. The creation of holes increases the conductivity of the material, with holes acting as the majority carriers.
- The Fermi level shifts downward toward the valence band, reflecting the higher concentration of holes in the valence band compared to electrons in the conduction band. The exact position of the Fermi level is determined by the acceptor doping concentration and temperature. For higher doping concentrations, the Fermi level moves closer to the valence band.

- **Variation of Fermi Level with Temperature in a p-type Semiconductor**

- In case of p-type semiconductor, in the low temperature region, holes in the valence band are only due to the transitions of electrons from the valence band to the acceptor levels. As the valence band is the source of electrons and the acceptor levels are the recipients for them, the Fermi level must lie between the top of the valence band and the impurity acceptor levels.
- When $T = 0K$, Fermi level lies midway between the acceptor levels and the top of the valence band.
- Thus,

$$E_{F_p} = \frac{E_V + E_A}{2} \text{ at } T = 0K. \quad \dots(47)$$

- As the temperature increases the acceptor levels gradually get filled and the Fermi level moves upward. At the temperature of saturation T_s , the Fermi level coincides with the acceptor level E_A .

$$\text{Thus, } E_{F_p} = E_A \text{ at } T = T_s. \quad \dots(48)$$

- As the temperature grows above T_s , the Fermi level shifts upward in an approximately linear fashion.
- At a temperature T_i intrinsic behaviour sets in. At higher temperatures, the p-type semiconductor loses its extrinsic character and behaves as an intrinsic semiconductor. In the intrinsic region, the hole concentration in the valence band increases exponentially and the Fermi level approaches the intrinsic value.

$$\text{Thus, } E_{F_p} = E_{F_i} = \frac{E_g}{2} \text{ at } T = T_i \quad \dots(49)$$

$$\text{At } T = 0K; \quad E_{F_p} = \frac{E_V + E_A}{2}$$

$$\text{At } T = T_s; \quad E_{F_p} = E_A.$$

$$\text{At } T = T_i; \quad E_{F_p} = E_{F_i} = \frac{E_g}{2}$$

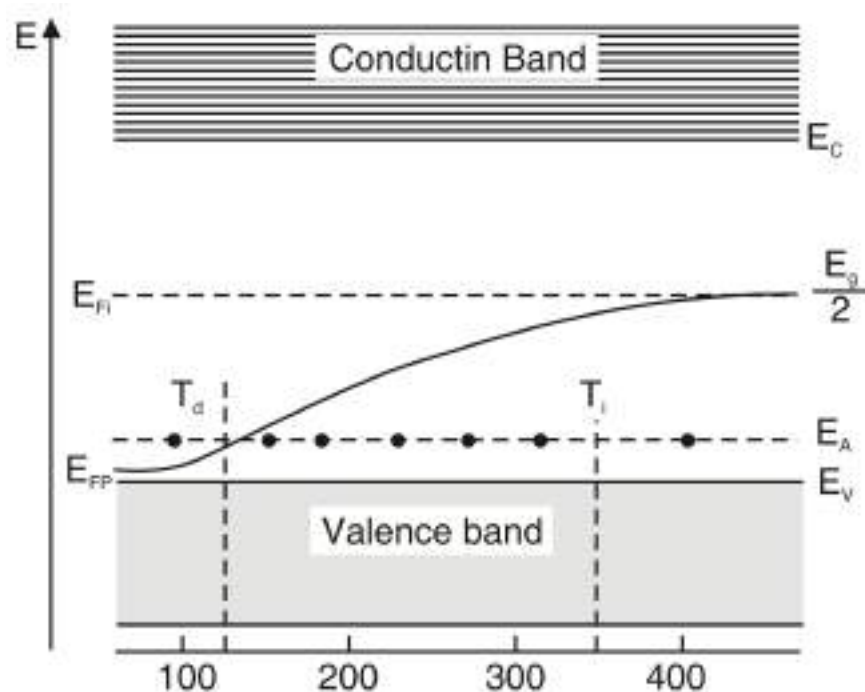
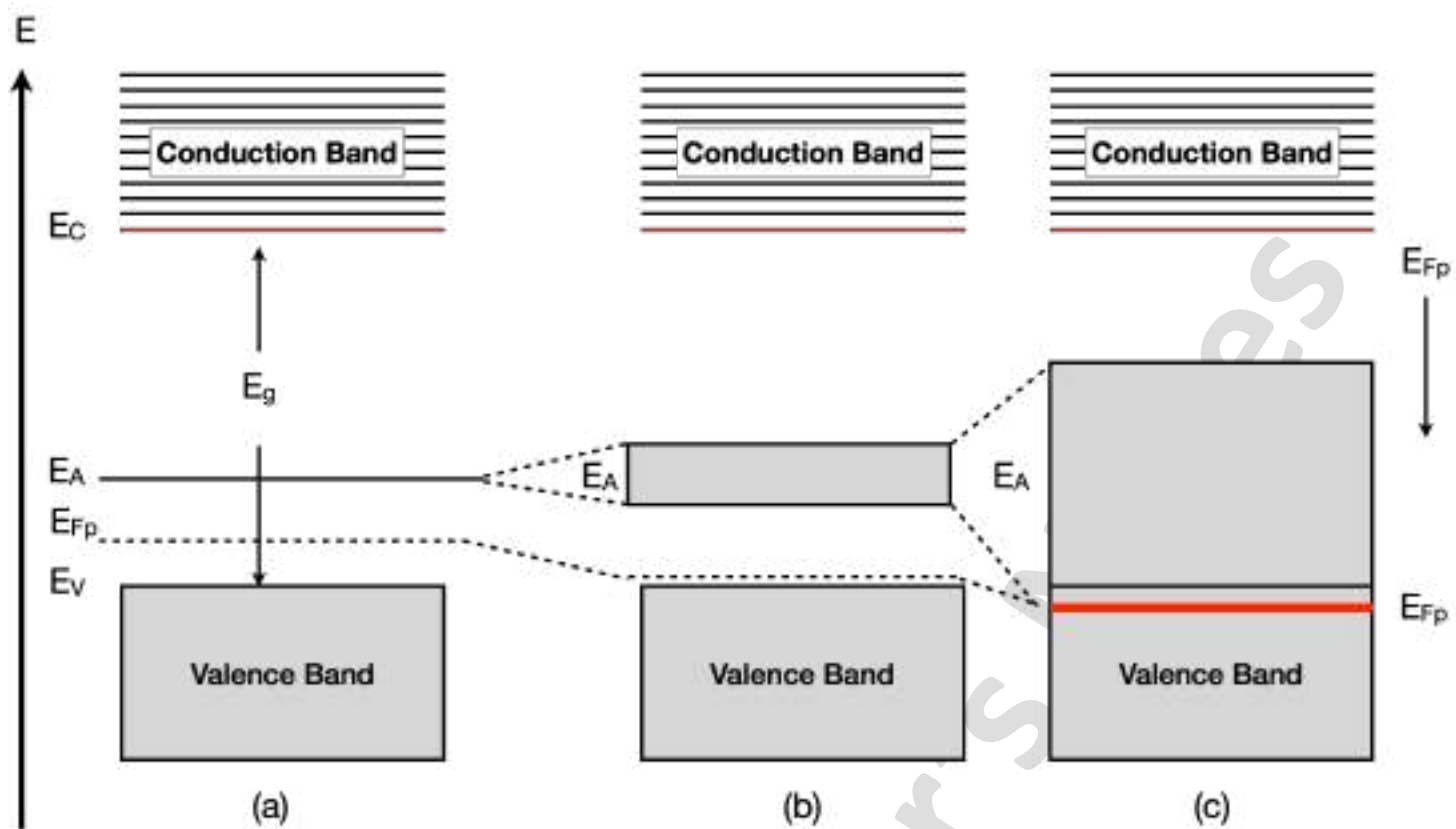


Fig. 16: Qualitative dependence of Fermi level on temperature in a p-type semiconductor



**Fig. 17: Energy band diagrams of an p-type semiconductor at three different levels of doping;
(a) low level doping; (b) medium doping; (c) heavy doping.**

- The diagram depicting the variation of the Fermi level (E_F) with doping concentration in a p-type semiconductor shows the progressive shift of E_F toward and into the valence band (E_V) as the acceptor impurity concentration increases.
- In an intrinsic semiconductor, the Fermi level is positioned near the middle of the energy bandgap, equidistant between the conduction band (E_C) and valence band (E_V), since the electron and hole concentrations are equal.
- **Low Doping (Lightly Doped p-Type):**
 - When a small concentration of acceptor impurities (such as boron) is added, they create acceptor energy levels just above E_V .
 - The Fermi level shifts downward from its intrinsic position toward E_V because the acceptor atoms introduce holes (majority carriers) in the valence band.
- **High Doping (Heavily Doped p-Type):**
 - As the doping concentration increases further, the acceptor levels start to interact and form a continuous acceptor band just above E_V . The Fermi level moves even closer to E_V , reflecting the increase in hole density.
- **Degenerate p-Type Semiconductor:**
 - At very high impurity concentrations, the acceptor band overlaps with the valence band, and the Fermi level moves into the valence band itself.
 - This signifies that the material has become degenerate, exhibiting metallic-like behavior with a high hole concentration in the valence band.

7. P-N junction

- A PN junction is a fundamental structure in semiconductor physics, formed by joining P-type and N-type semiconductor materials. It is the building block of many electronic devices, such as diodes, transistors, and solar cells.

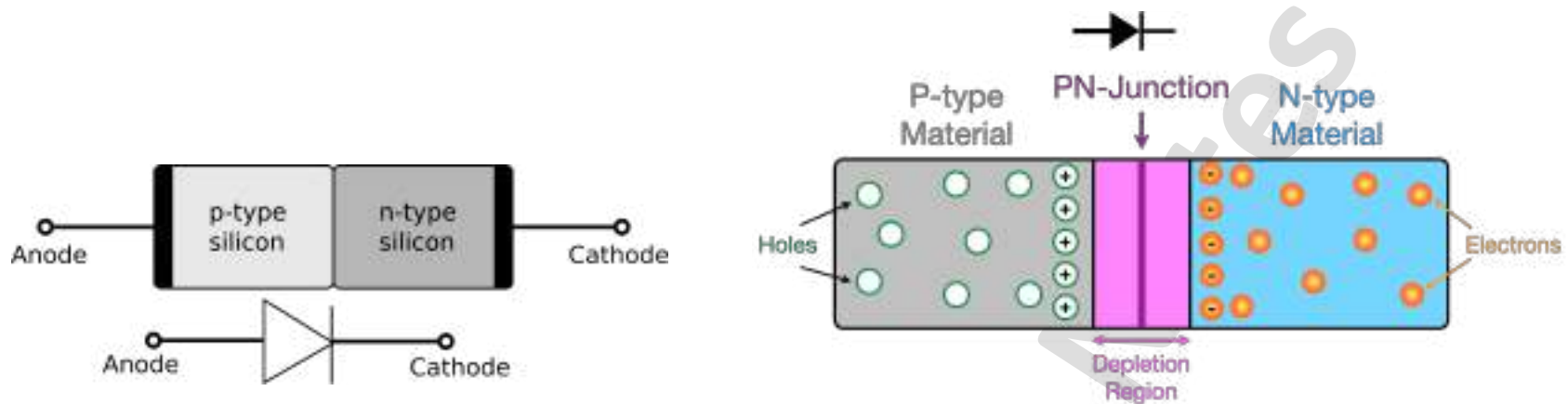


Fig. 18: A P–N junction. The circuit symbol is shown: the triangle corresponds to the P side.

- P-type Semiconductor:

- Doped with acceptor impurities (e.g., boron or gallium). Has an abundance of holes (positive charge carriers)

- N-type Semiconductor:

- Doped with donor impurities (e.g., phosphorus or arsenic). Has an abundance of electrons (negative charge carriers).

- Formation of the PN Junction:

- When p-type and n-type materials are joined to form a p-n junction, electrons from the n-side, which has a high concentration of free electrons, diffuse into the p-side, where holes dominate as majority carriers. Similarly, holes from the p-side diffuse into the n-side.
- As these charge carriers move across the junction, they recombine with their counterparts, leaving behind immobile positive ions in the n-region and immobile negative ions in the p-region. This creates a region near the junction known as the depletion region, which is devoid of free charge carriers.
- The accumulation of immobile ions generates an electric field across the junction. This electric field produces a built-in potential (or barrier potential) that opposes further diffusion of electrons and holes, maintaining equilibrium in the junction. The depletion region and built-in potential are fundamental to the operation of semiconductor devices like diodes and transistors.

- Depletion Region:

- A region near the junction where mobile charge carriers (electrons and holes) are depleted. Contains immobile ions (positive on the N-side and negative on the P-side). Acts as an insulating barrier.

8. A PN junction diode:

- A p-n junction diode is a two-terminal semiconductor device formed by joining p-type and n-type materials. It allows current to flow primarily in one direction, making it a key component in rectification and switching applications.
- At the junction, electrons from the n-side and holes from the p-side diffuse and recombine, creating a depletion region with an internal electric field.
- This electric field determines the behavior of the diode under different biasing conditions.

- Zero Bias (Unbiased PN Junction)

In a zero-bias condition, no external voltage is applied across the p-n junction. The behavior of the junction in this state is determined by the natural properties of the materials and the interaction of charge carriers at the junction. electrons from the n-region diffuse into the p-region, and holes from the p-region diffuse into the n-region due to the concentration gradient. This diffusion leads to recombination near the junction. The recombination of free electrons and holes near the junction leaves behind immobile ions: Positive donor ions in the n-region. Negative acceptor ions in the p-region. These ions form a depletion region near the junction, devoid of free charge carriers. The electric field created by the immobile ions opposes further diffusion of charge carriers. This results in a built-in potential across the junction, typically 0.7 V for silicon and 0.3 V for germanium. At equilibrium, the diffusion of carriers is balanced by the drift caused by the electric field. In the zero-bias condition, the diffusion current (due to carrier movement from high to low concentration) and the drift current (due to the electric field) are equal and opposite. As a result, no net current flows across the junction. When P and N type semiconductors are in isolated from each other they are said to be in non-equilibrium state. Fermi level of P-type semiconductor is located close to be top of the valence band. Fermi level of N-type semiconductor is located close to the bottom of the conduction band. The Fermi level in N region shifts down by an energy eV_o whereas Fermi level in P region shifts upward by the same energy eV_o , where V_o is the potential barrier across the junction.

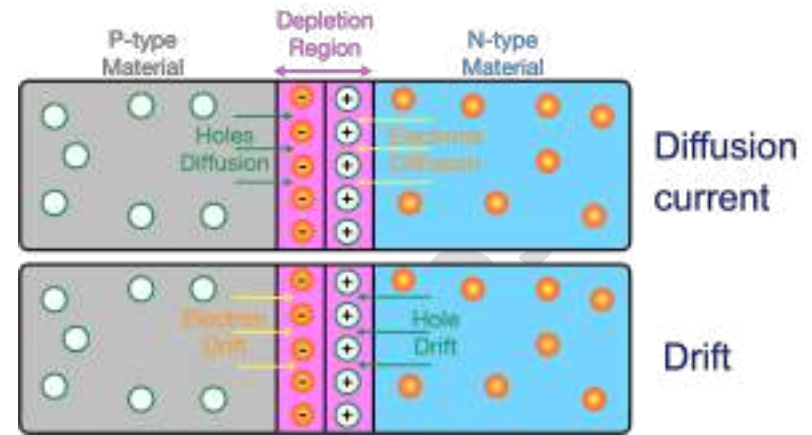


Fig. 19: Current flow through an ideal PN junction

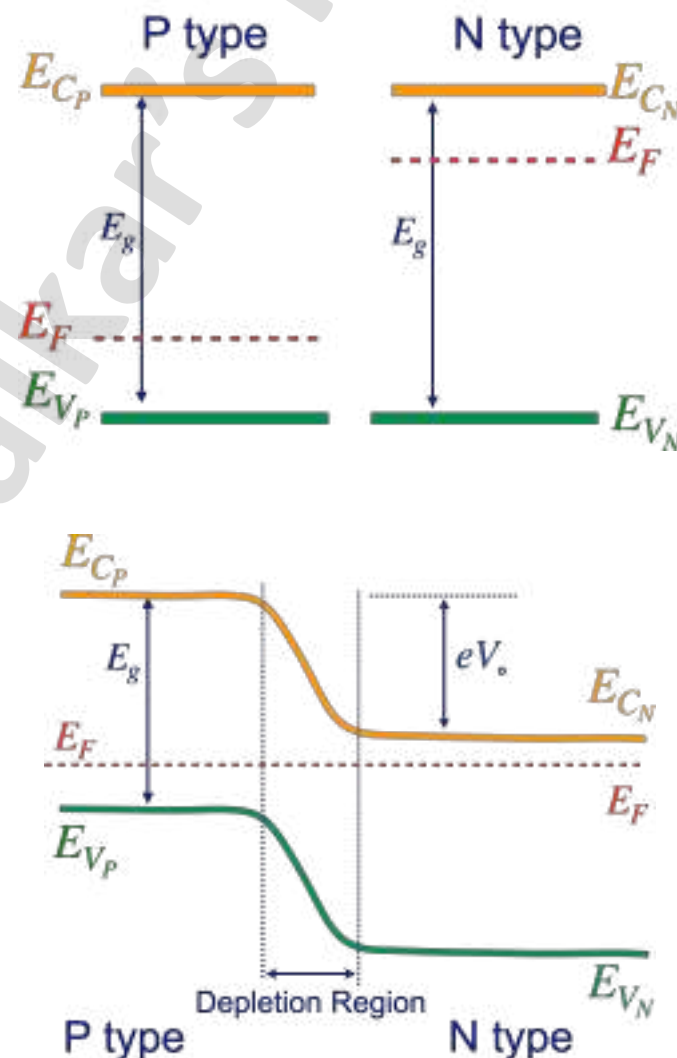


Fig. 20: Energy band diagram for zero bias

- Forward Bias:

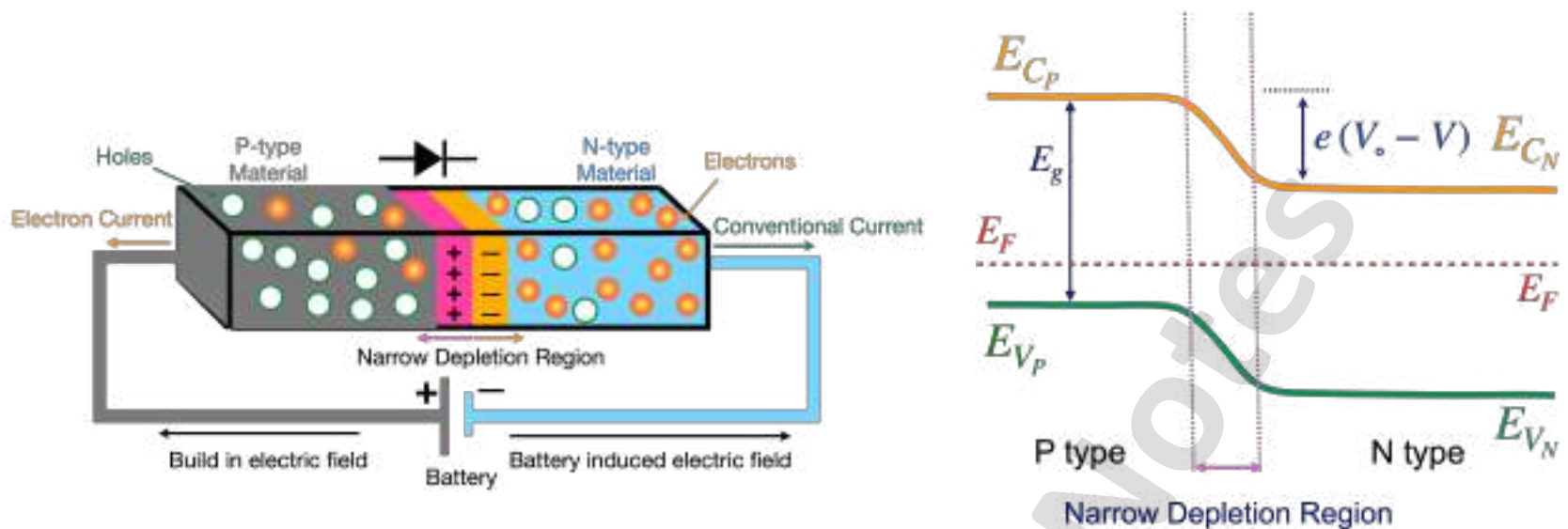


Fig. 21: PN Junction diode in forward biased mode and band formation

- In forward bias, a positive voltage is applied to the p-side of the p-n junction and a negative voltage to the n-side. This reduces the width of the depletion region by counteracting the built-in electric field, allowing charge carriers to move more freely across the junction. Electrons from the n-side are pushed toward the junction, while holes from the p-side are similarly driven toward the junction.
- When these charge carriers meet, they recombine, resulting in a flow of current through the diode. The forward bias significantly lowers the barrier potential, enabling an exponential increase in current as the applied voltage increases. The potential difference V should be greater than potential barrier of V_o . Potential in N region rises by $e(V_o - V)$. The Fermi level of P region goes down. Electrons in N region now face a lower potential barrier. The width of potential barrier is reduced.

- Reverse Bias:

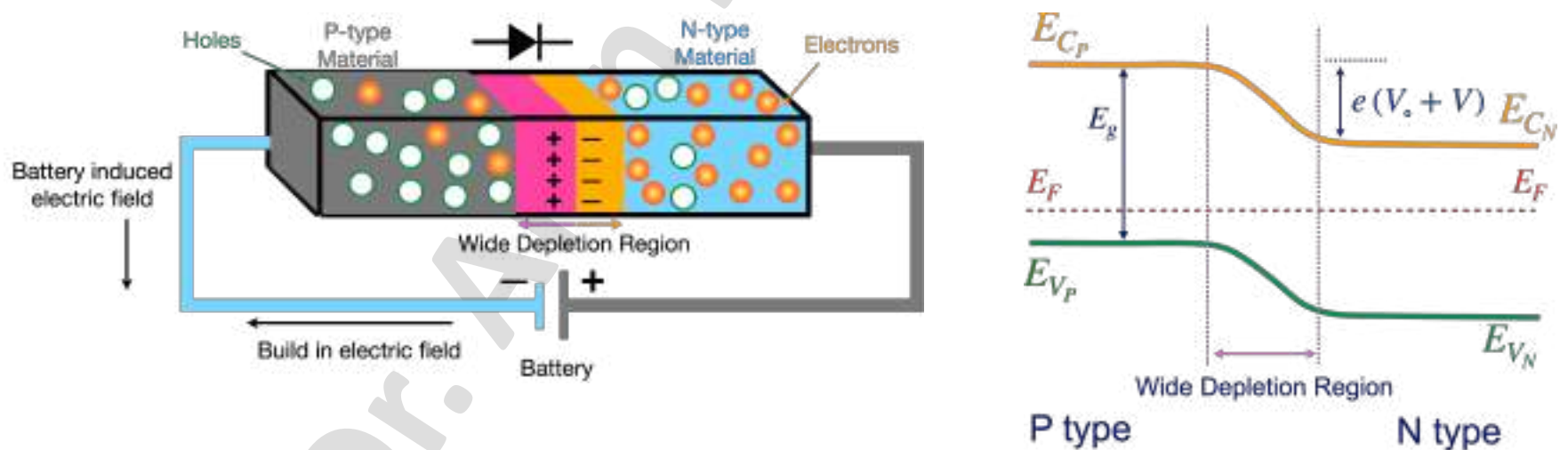


Fig. 22: PN Junction diode in reverse biased mode and band formation

- In reverse bias, a positive voltage is applied to the n-side of the p-n junction and a negative voltage to the p-side. This increases the width of the depletion region as the external voltage enhances the built-in electric field, pulling electrons and holes further away from the junction. The widened depletion region acts as a strong insulating barrier, effectively blocking the flow of current.
- However, a small leakage current, caused by the thermal generation of minority carriers, may still flow across the junction. This leakage current is typically negligible under normal conditions. Potential difference V is applied to diode in reverse bias. Due to this electrons are removed from N region. Potential in N region decreases by $e(V_o + V)$. Electrons enter into P region and hence potential in this region rises. The width of potential barrier is increased.

- I-V Characteristics of PN junction diode:

The I-V characteristics of a p-n junction diode describe the relationship between the voltage applied across the diode and the resulting current. In the forward bias region, when a positive voltage is applied to the p-side and a negative voltage to the n-side, the current remains negligible for small voltages. Once the applied voltage exceeds the threshold voltage (typically 0.7V for silicon and 0.3V for germanium), the depletion region narrows, and current increases exponentially with voltage. In the reverse bias region, where the p-side is connected to a negative voltage and the n-side to a positive voltage, the current is extremely small due to minority carriers and is almost constant, called the leakage current. However, when the reverse voltage exceeds the breakdown voltage, a significant reverse current flows, which can damage the diode unless it's designed for breakdown operation (e.g., Zener diodes). These characteristics make the p-n junction diode an essential component for rectification and current control in circuits.

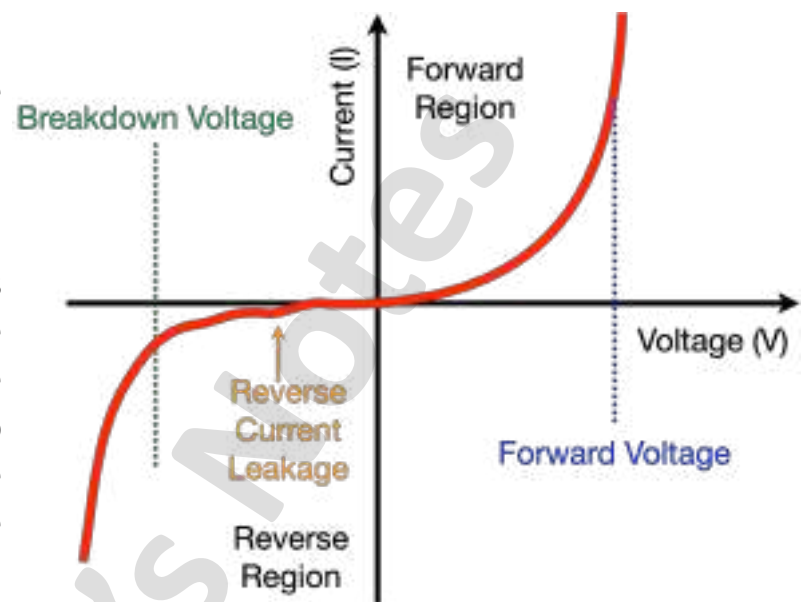


Fig. 23: I-V Characteristics of PN junction diode

- Applications of PN Junctions:

- Diodes: Allow current to flow in one direction only.
- Transistors: Used as switches or amplifiers in electronic circuits.
- Solar Cells: Convert light energy into electrical energy.
- LEDs (Light-Emitting Diodes): Emit light when forward-biased.

9. Solar cell

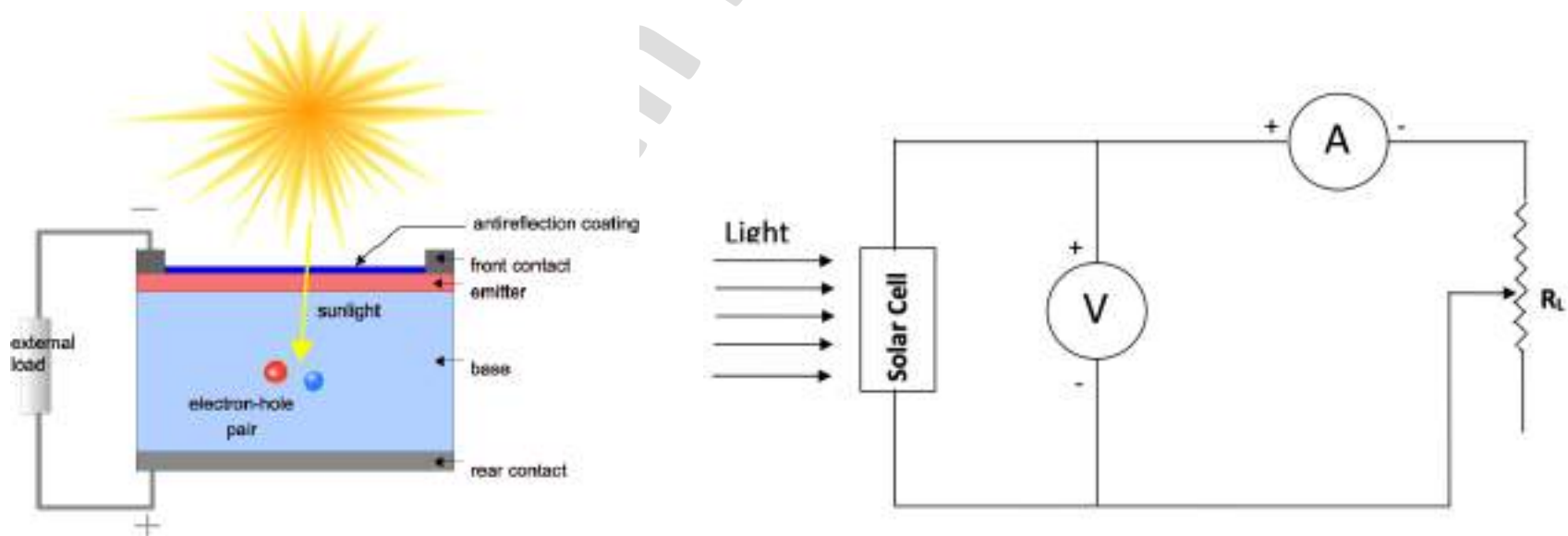


Fig. 24 a) Cross section of solar cell. b) Circuit diagram for solar cell.

- A solar cell is a semiconductor device that converts light energy directly into electrical energy through the photovoltaic effect. The photovoltaic effect is the generation of voltage and electric current in a material upon exposure to light. The voltage induced by the PV cell depends on the intensity of light incident on it. The name photovoltaic is because of their voltage producing capability. The energised electron is known as the photoelectrons. The working of the Photovoltaic cell depends on the photoelectric effect. The photovoltaic effect is closely related to the photoelectric effect. Solar cells are the fundamental building blocks of solar panels and are used to harness solar energy for various applications, from powering small devices to large-scale electricity generation.

- Basic Principle:

- The basic principle behind a solar cell is the photovoltaic effect, where light (photons) strikes a semiconductor material, exciting electrons and creating electron-hole pairs. These free carriers are then separated by the built-in electric field at the p-n junction, generating a flow of electric current when the circuit is closed.

- Working Mechanism:

- Absorption of Photons: When sunlight strikes the surface of the solar cell, photons are absorbed by the semiconductor material (typically silicon), which excites electrons in the material.
- Generation of Electron-Hole Pairs: The absorbed photons provide energy that causes electrons to move from the valence band to the conduction band, creating electron-hole pairs.
- Separation of Charge Carriers: The p-n junction within the solar cell creates an internal electric field that separates the electrons and holes. Electrons move toward the n-side (negative), and holes move toward the p-side (positive).
- Electric Current Generation: The movement of charge carriers creates a potential difference (voltage) across the junction. When an external circuit is connected, electrons flow from the n-side to the p-side through the external circuit, generating current and thus electrical power.

- Energy band diagram and I-V curve:

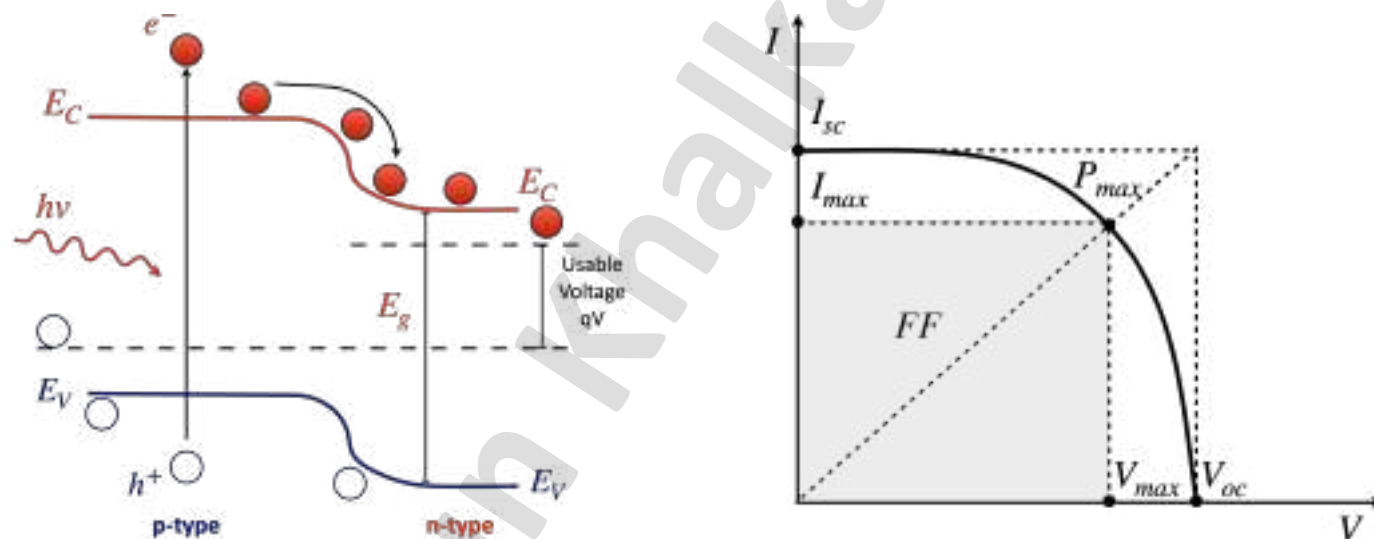


Fig. 25: Energy band diagram and I-V curve for solar cell

- When the sunlight falls on the upper P-region, it generates the electron-hole pairs in both P and N regions. At the junction, barrier potential attracts electrons from P-region into N-region and holes from N-region into P-region. The accumulation of charges on the two sides of the junction produces a voltage. If an external circuit is connected across the solar cell terminals, a current flows through the circuit.

- Key Parameters of a Solar Cell:

- I_{sc} (Short-Circuit Current):

- The current that flows when the terminals of the solar cell are shorted (i.e., zero voltage across the cell). It is a measure of the maximum current that the cell can produce under light exposure. Initially when load resistance R_L is kept minimum, the maximum current flows in the circuit. When the load is zero ($R_L \rightarrow 0$), maximum current is known as short circuit current.

- V_{oc} (Open-Circuit Voltage):

- The voltage across the solar cell when no external load is connected (i.e., the circuit is open). It represents the maximum voltage the solar cell can generate under illumination. As load resistance is increased, the voltage across the load resistance R_L increases and current starts decreasing. When the load is maximum ($R_L \rightarrow \infty$), the current is very small and the voltage across the load is maximum.



- **I_{max} (Maximum Current):**

- The current at which the solar cell produces its maximum power output, typically when the cell is operating at its optimal voltage.

- **V_{max} (Maximum Voltage):**

- The voltage at which the solar cell produces its maximum power output, typically under the conditions where the current is at I_{max} .

- **Fill Factor (FF):**

- A measure of the efficiency of the solar cell in converting the maximum available power. It is the ratio of the maximum power output (P_{max}) to the product of I_{sc} and V_{oc} .

- A higher fill factor indicates better performance:
$$FF = \frac{I_{max} \times V_{max}}{I_{sc} \times V_{oc}} = \frac{P_{max}}{I_{sc} \times V_{oc}} \quad \dots(50)$$

- **Efficiency (η):**

- The efficiency of a solar cell is the ratio of the electrical power output to the total power input from the sunlight. It is given by:

$$\eta \% = \frac{P_{max}}{P_{in}} \times 100 \% \quad \dots(51)$$

- P_{in} is the power from the sunlight incident on the cell, and P_{max} is the maximum power the cell can deliver.

- **Factors to Improve Efficiency:**

- **Material Quality:** Using high-quality semiconductor materials with fewer defects (e.g., monocrystalline silicon) can improve the absorption of light and the generation of electron-hole pairs.
- **Light Absorption:** Incorporating anti-reflective coatings and surface texturing can increase the amount of light absorbed by the cell.
- **Optimal P-N Junction:** The design of the p-n junction, including the doping concentration, can be adjusted to optimize the separation of charge carriers and reduce recombination losses.
- **Temperature Control:** Keeping the solar cell cool can help maintain efficiency, as high temperatures can reduce the cell's voltage and performance.
- **Multi-junction Cells:** Using multiple semiconductor materials with different bandgaps stacked on top of each other can capture a wider range of the solar spectrum, increasing efficiency.

- **Limitations of Solar Cells:**

- **Efficiency Limits:** Even under ideal conditions, the maximum theoretical efficiency of a solar cell is limited by factors such as the bandgap of the material, recombination losses, and thermal losses.
- **High Cost:** The production cost of high-efficiency solar cells (e.g., monocrystalline silicon) remains relatively high, though costs have been decreasing over time.
- **Energy Conversion Efficiency:** Solar cells typically have efficiency rates between 15% and 25%, which means a significant amount of sunlight is not converted into electricity.
- **Weather and Location Dependent:** Solar cell efficiency is affected by environmental factors like cloud cover, shading, dust, and geographic location, limiting their output.
- **Energy Storage:** Solar energy generation is intermittent, so efficient energy storage solutions (such as batteries) are required for reliable power supply during non-sunny hours.

**- Advantages of solar cell**

- Renewable Energy Source: Solar energy is abundant and renewable, meaning it can be harnessed as long as the sun shines, providing a sustainable solution for electricity generation.
- Environmentally Friendly: Solar cells produce clean energy without emitting greenhouse gases or pollutants, helping to reduce air pollution and mitigate climate change.
- Low Operating Costs: After installation, the operating and maintenance costs of solar power systems are low. Solar cells require minimal maintenance and have long lifespans, typically around 25-30 years.
- Reduces Electricity Bills: By generating your own electricity, solar cells can significantly reduce electricity bills. In some regions, excess energy can be fed back into the grid, further lowering costs through net metering.
- Energy Independence: Solar cells enable individuals, businesses, and even countries to reduce their dependence on fossil fuels and the electrical grid, leading to greater energy security.
- Scalable and Flexible: Solar power systems can be tailored to fit a wide range of applications, from small rooftop installations to large-scale solar farms. They can also be integrated into existing infrastructure like solar windows or roof tiles.
- Low Maintenance Requirements: Solar cells have no moving parts, making them reliable and requiring very little maintenance. Regular cleaning and occasional checks are sufficient to keep them functioning efficiently.
- Quiet Operation: Solar power generation is silent, unlike other power generation systems like wind turbines or generators, making it ideal for residential areas and noise-sensitive locations.
- Off-Grid Capability: Solar cells are an ideal solution for remote or off-grid locations, where extending electrical infrastructure would be costly or impractical. They provide power where traditional grids are unavailable.
- Job Creation: The solar industry has seen significant growth, creating jobs in manufacturing, installation, and maintenance, contributing to economic development in many regions.
- These advantages make solar cells a highly attractive and viable option for clean, sustainable, and cost-effective energy production.

- Applications of Solar Cells:

- Solar Power Generation: Solar cells are used in solar panels to generate electricity for residential, commercial, and industrial applications. They form the backbone of solar power plants.
- Space Satellites: Solar cells power spacecraft and satellites, providing energy in space where traditional power sources are unavailable.
- Consumer Electronics: Solar cells are used to power small devices like calculators, lights, and watches.
- Remote and Off-Grid Areas: Solar cells provide power to remote locations that do not have access to the electrical grid, offering sustainable energy solutions.
- Solar Vehicles: Some electric vehicles use solar cells integrated into their surface to supplement battery charging.

10. Basics of sensors:

- **Definition:** Sensors are specialized devices designed to detect and respond to changes in their surroundings or within a specific system. These changes can be physical, such as temperature, pressure, or light; chemical, such as the presence of specific substances; or biological, such as detecting microorganisms or biomolecules. Once a sensor identifies a change, it converts this information into an electrical signal or another readable format, allowing electronic systems or devices to process and respond accordingly.

- **Example:**

In humans, sensory organs function as natural sensors. The nose and mouth detect chemicals in the air and food, helping us perceive smells and tastes. Eyes act as light sensors, allowing us to see. Skin senses pressure and temperature, enabling touch perception. Ears detect sound waves, allowing us to hear. These biological sensors continuously gather information, helping us interact with and respond to our environment.



Fig. 26: Human Sensors

- A sensor is a device that receives a stimulus (measurand) and responds with an electrical signal. A sensor may have several energy conversion steps before it produces and outputs an electrical signal since most stimuli are not electrical. Any sensor is an energy converter. In a sensor system, different types of stimuli (S1, S2, and S3) interact with various transducers and sensors to produce an electrical signal output (e). Here's how the process works step by step as shown in Fig. 27

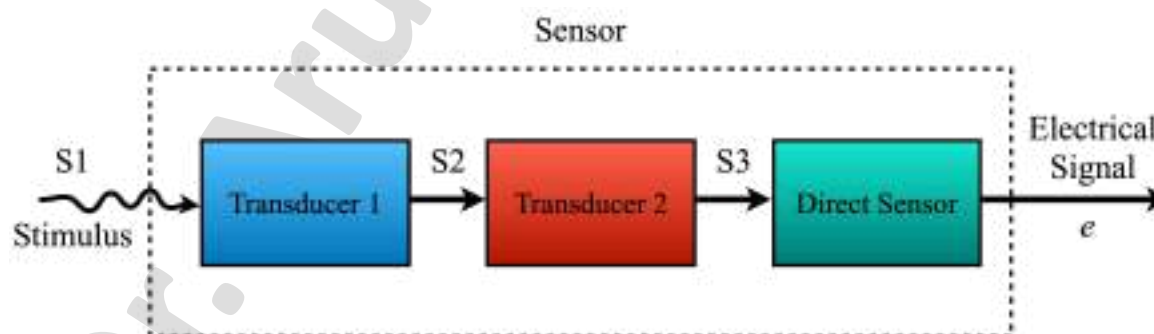


Fig. 27: Block diagram of sensor

- S1 represents a physical, chemical, or biological change in the environment. Transducer 1 detects this stimulus and converts it into another form of energy, typically an intermediate mechanical or electrical signal.
- Similar to S1, S2 is another environmental change. Transducer 2 processes S2 and transforms it into a usable intermediate signal.
- Unlike S1 and S2, S3 directly interacts with a sensor that does not require an intermediate transducer. This sensor directly converts S3 into an electrical signal.
- The signals from Transducer 1, Transducer 2, and the direct sensor are processed and combined into a final electrical signal (e). This electrical signal can be interpreted by other electronic systems for further processing, display, or control applications.

- **Components:**

- Sensor: Detects the physical parameters (e.g., temperature, pressure).
- Signal Conditioning: Amplifies and filters the signal to make it suitable for further processing.
- Analog-to-Digital Converter (ADC): Converts the analogue signal into a digital signal.
- Microcontroller: Processes the digital signal and makes decisions based on the input.
- Output/Display: Shows the processed data or triggers an action based on the sensor input.



Fig. 29: Components of sensor

- **Basic Functionality:**

- Detection: The sensor detects a physical property from the environment.
- Conversion: The detected input is converted into an electrical signal.
- Transmission: The electrical signal is transmitted for processing or display.
- Processing: The signal is processed to interpret the information.
- Output: The processed information is output in a readable form.

- **Types of sensors:**

Sr. No.	Passive sensor	Active sensor
1	Does not require external power	It requires power
2	It can only be used to detect energy when the naturally occurring energy is available	Provides its own energy source for illumination
3	No interference problem in the environment can operate in the same environment condition	Less interference problem can operate in different environment conditions
4	Sensitive to weather condition	Not sensitive
5	Not well suited for darkness conditions	Works well in darkness conditions
6	Difficulties in interpreting the output signals	Easy to interpret
7	Less control of noise	Better control of noise
8	Low price	High price
9	Examples: Thermocouples, Photodiodes, Photovoltaic Cells, Radiometers, Pyrometers, Microphones, Barometers, Galvanometers, Seismometers, Accelerometers, Magnetometers, Hygrometers, Hydrophones, Radiant Energy Detectors etc.	Examples: Radar Sensors, Lidar (Light Detection and Ranging), Ultrasonic Sensors, Laser Rangefinders, Infrared Sensors, Sonar (Sound Navigation and Ranging), RFID (Radio Frequency Identification) Tags, Optical Proximity Sensors, Microwave Sensors, Capacitive Sensors, Piezoelectric Sensors etc.

- **Sensors based on their detection properties.**

- There are many sensors commonly used in various applications. All these sensors are categorized as per their physical properties like temperature, resistance, pressure, heat flow etc. The following is a brief discussion on different types of sensors.
- Temperature sensors:Thermostat, Thermistor, Resistive temperature detector, Thermocouple, Position sensors, Light sensors, Sound sensor, Proximity sensor, Accelerometer, Infrared sensor, Pressure sensor, Ultrasonic sensors, Touch sensor, Humidity sensor, Colour sensor, Chemical sensor , Seismic sensor, Magnetic sensor.

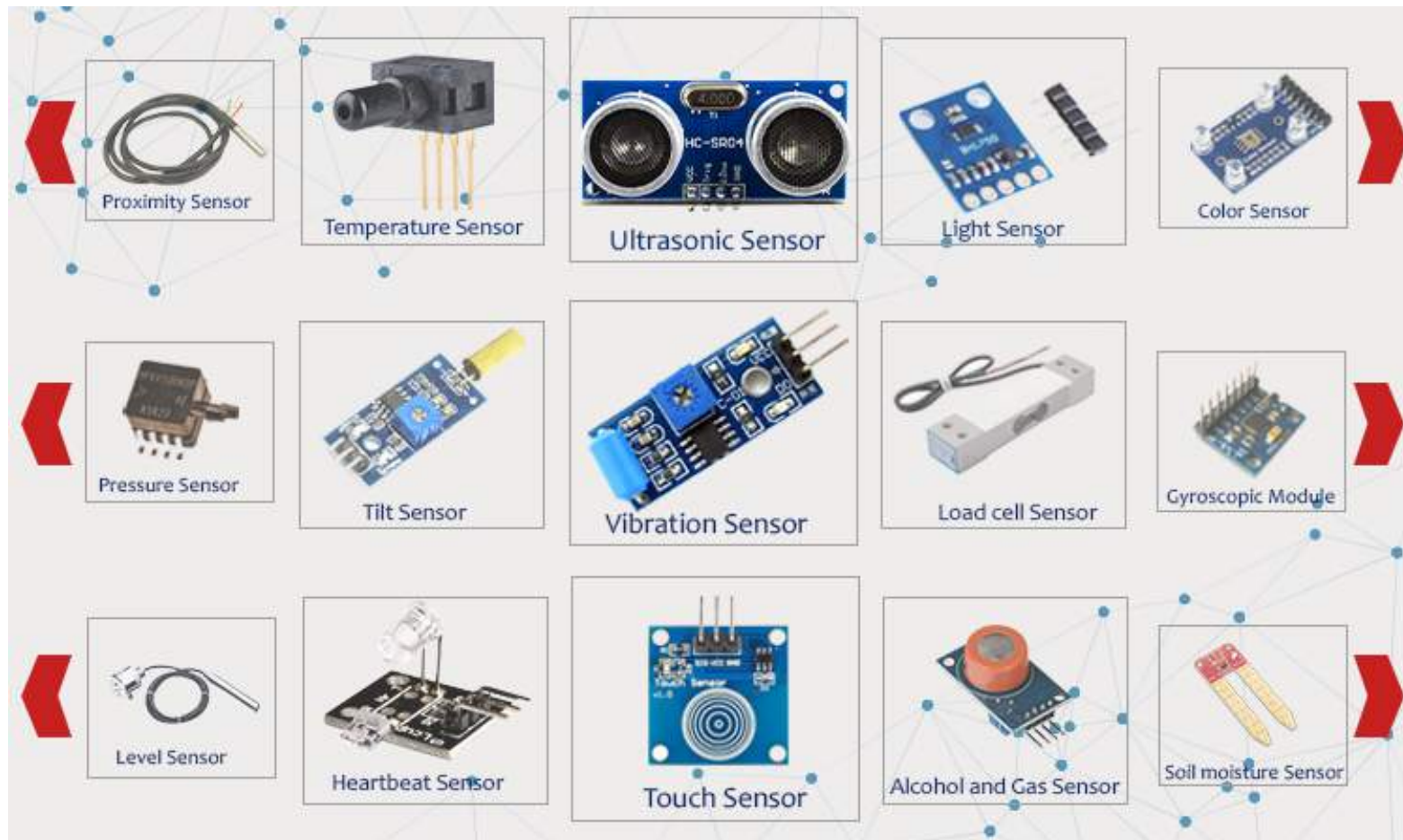


Fig. 30: Examples of sensors

- **Piezoelectric Sensor:**
- **Piezoelectric Effect**
- Piezoelectricity (also called the piezoelectric effect) is the presence of an electrical potential across the sides of a crystal when mechanical stress is applied by squeezing it.
- In a working system, the crystal acts like a tiny battery with a positive charge on one face and a negative charge on the opposite face.
- Examples: Mechanical stress analyzer, Lighters

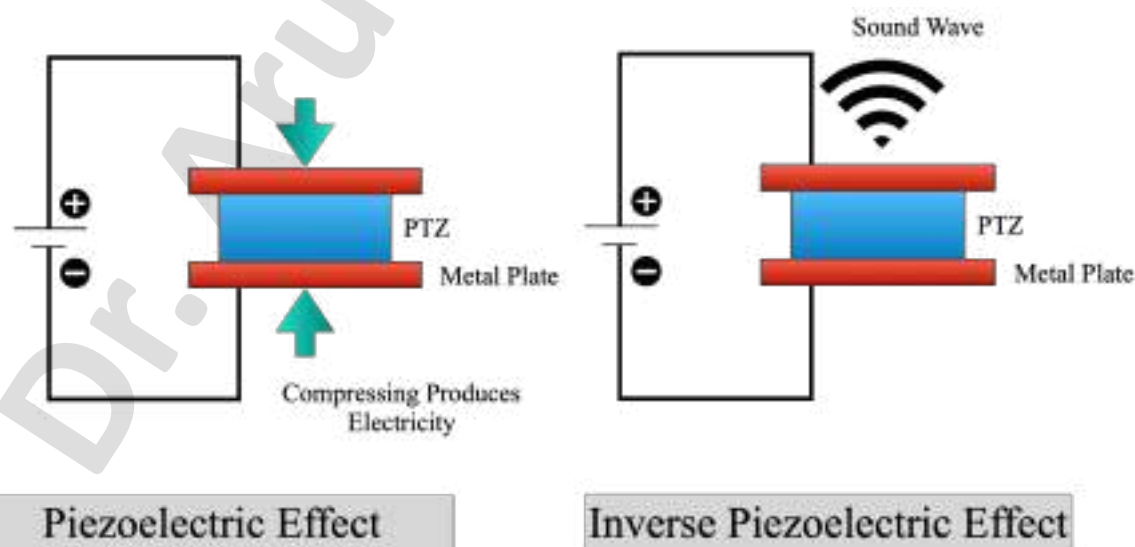


Fig. 31: Photoelectric sensor

- **Inverse Piezoelectric Effect**
- The effect is reversible. Whenever an electric field is applied to crystal terminals, it undergoes mechanical stress and results in shape change. This is known as the Inverse Piezoelectric Effect.
- Examples: Quartz Watch, Piezo Buzzers.

- Piezoelectric Sensor:

- A piezoelectric sensor works based on the principle of piezoelectricity, where certain materials produce an electric charge in response to mechanical stress or pressure.
- The term "piezoelectric" is derived from the Greek word "piezein," meaning to press or squeeze, and refers to the ability of certain materials to generate electric charges when subjected to mechanical deformation.

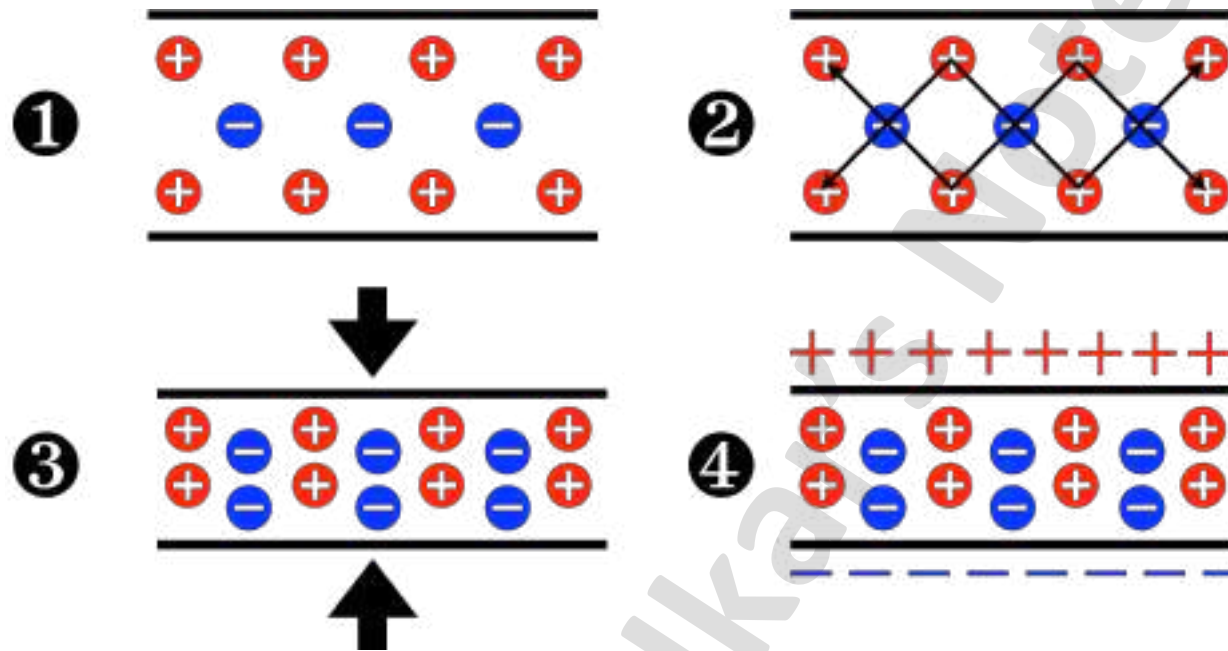


Fig. 32: Principle of piezoelectricity

- Piezoelectric Sensor Circuit:

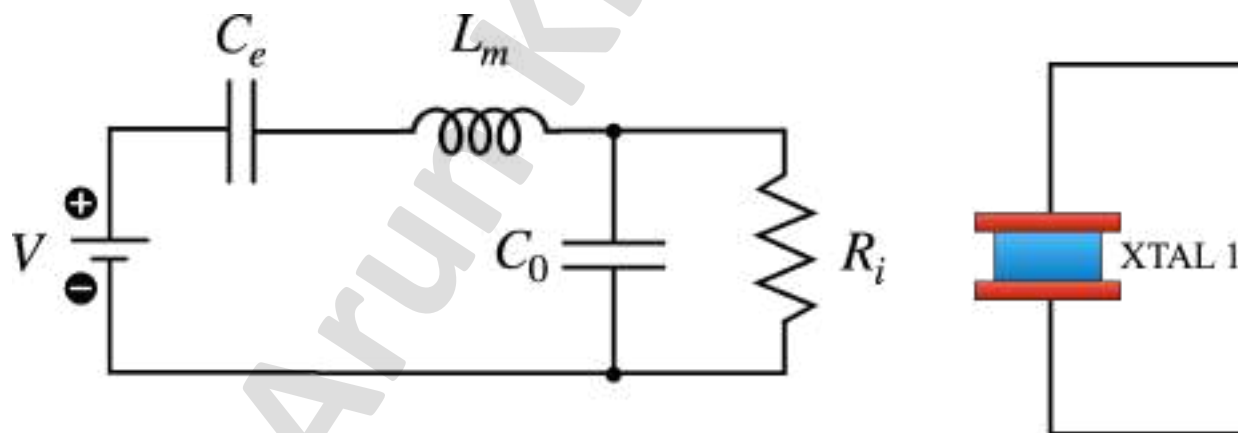


Fig. 33: Piezoelectric Sensor Circuit

- It consists of internal Resistance R_i which is also known as insulator resistance. An inductor L_m is connected which produces inductance due to the inertia of the sensor. The value of capacitance C_e is inversely proportional to the elasticity of the sensor material. To obtain the complete response of the sensor, load and leakage resistance should be larger enough such that low frequency is maintained.
- Internal Resistance (Insulator Resistance): The internal resistance, also known as insulator resistance, represents the resistance of the piezoelectric material itself to the flow of electrical charge. It can affect the overall sensitivity and response time of the sensor. A higher internal resistance may reduce the leakage of charge, but excessive resistance can slow down the response time of the sensor, making it less effective for high-frequency applications.
- Inductance: The sensor is typically connected to an inductor, which produces inductance due to the inertia of the sensor material. This inertia refers to the sensor's resistance to changes in its state of motion when subjected to mechanical stress. The inductance acts as a damping element, affecting the dynamic response of

the sensor and helping to smooth out rapid fluctuations in the signal caused by high-frequency mechanical vibrations. The inductance, along with the internal resistance, determines the frequency response of the piezoelectric sensor.

- **Capacitance:** The capacitance of the sensor is related to the elasticity of the material. The elasticity refers to the material's ability to deform and return to its original shape when mechanical stress is removed. The value of capacitance is inversely proportional to the elasticity of the sensor material; in other words, stiffer (less elastic) materials result in lower capacitance, while more elastic materials result in higher capacitance. The capacitance plays a crucial role in determining the voltage output of the sensor for a given applied force.
- **Load and Leakage Resistance:** To ensure a complete response from the piezoelectric sensor, it is important that the load resistance and leakage resistance are large enough. The larger these resistances, the less leakage current will flow through the system, ensuring that the sensor's output signal remains stable. These resistances help maintain the sensor's operation at low frequencies, which is especially important for accurately measuring slow or constant forces. If the load and leakage resistances are too low, the output signal may decay too quickly or be too noisy for accurate measurements.
- **Working Mechanism:**
 - **Piezoelectric Material:** The sensor consists of a piezoelectric material, typically a crystal (like quartz) or a ceramic (such as lead zirconate titanate, PZT), which has a unique crystalline structure that lacks a center of symmetry.
 - **Application of Mechanical Stress:** When external force or pressure (such as vibration, force, or acceleration) is applied to the piezoelectric material, it causes a deformation in the crystal lattice. This mechanical deformation shifts the positions of the charged particles within the crystal structure.
 - **Generation of Electric Charge:** The deformation results in the separation of positive and negative charges within the material, creating an electric dipole. This leads to the generation of an electric charge on the surface of the material. The amount of generated charge is directly proportional to the magnitude of the applied force or pressure.
 - **Signal Output:** The generated electric charge can be collected by attaching electrodes to the surface of the piezoelectric material. This charge is then converted into a measurable voltage or current output. The signal is proportional to the amount of mechanical stress applied.
 - **Response to Changes in Pressure or Force:** Piezoelectric sensors are particularly sensitive to dynamic changes in pressure, force, or vibration. They are widely used in applications that require monitoring of forces, vibrations, or accelerations, such as in pressure sensors, accelerometers, and microphones.
 - **Decay of Charge:** A characteristic feature of piezoelectric sensors is that they primarily respond to dynamic changes in force or pressure. Once the applied force is removed, the generated charge gradually decays, meaning the sensor is not suitable for detecting static or constant pressures. However, for continuous monitoring of dynamic forces, the output is often passed through a charge amplifier to maintain a steady reading.
- **Applications:**
 - Piezoelectric sensors are used in various fields, including:
 - **Vibration sensing:** In machines, motors, and structures to detect vibrations.
 - **Pressure measurement:** In applications like engine monitoring and pressure transducers.
 - **Force/Load sensing:** In applications like weighing scales, accelerometers, and impact sensors.
 - **Medical Devices:** Such as ultrasound imaging and monitoring devices.
 - **Microphones:** To convert sound into an electrical signal.

- Photodiode Sensor:

- A photodiode is a semiconductor device that converts light energy into electrical energy. Essentially, it functions as a light sensor that generates an electric current when exposed to light.
- Photodiodes are commonly referred to as light detectors, light sensors, or photo sensors. The conversion of light into electrical energy in a photodiode occurs through the photovoltaic effect.

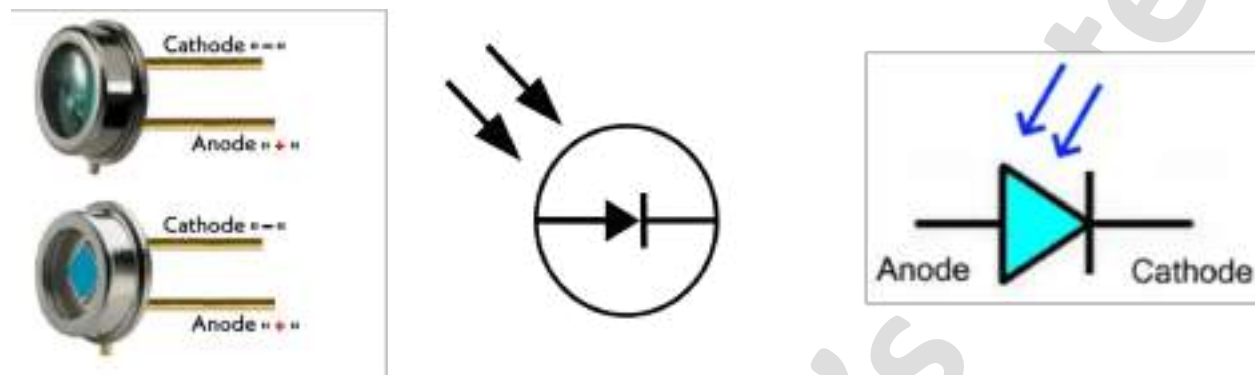


Fig. 34: Photodiode and its symbol

- Working Principle:

- The basic principle behind the operation of a photodiode is the photovoltaic effect, where photons (light particles) striking the photodiode's junction cause the release of electron-hole pairs. When light is incident on the photodiode, the energy from the photons excites electrons in the semiconductor material.
- This causes electrons to be displaced, creating a photocurrent. The magnitude of the photocurrent is directly proportional to the intensity of the incoming light.
- The photodiode, when connected to an external circuit, produces a current or voltage that corresponds to the amount of light absorbed.

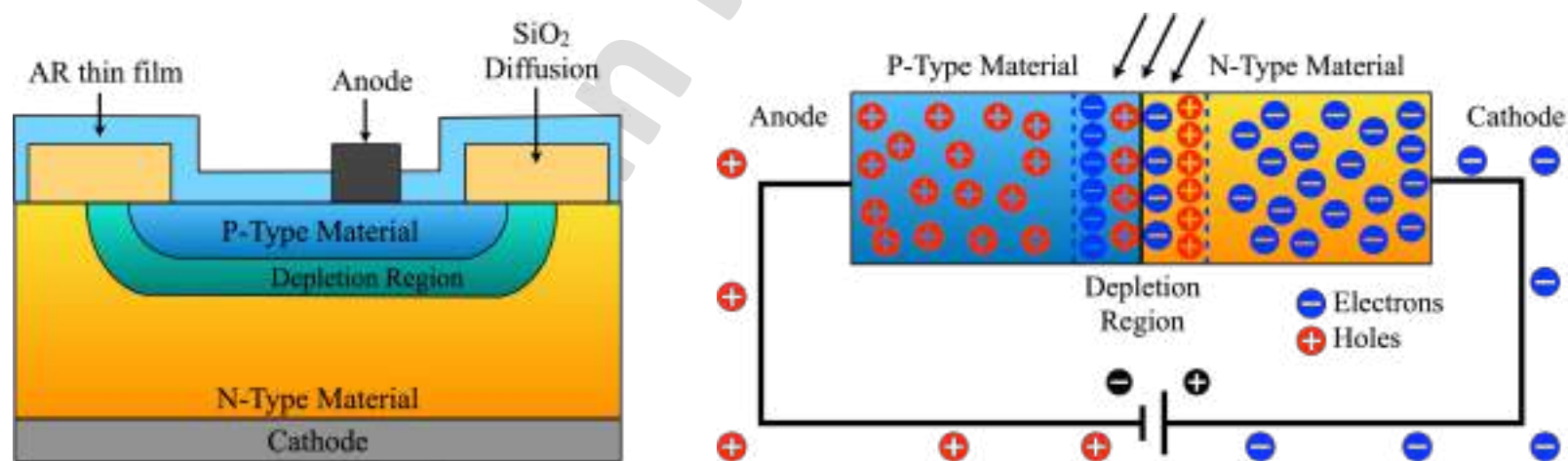


Fig. 35: Schematic and junction diagram of Photodiode Sensor

- Construction:

- A typical photodiode consists of two layers of semiconductor materials: P-type and N-type, which are joined together to form a PN junction. The junction area is where the light absorption occurs, generating the photocurrent.
- P-Type and N-Type Semiconductors: The P-type semiconductor has an excess of holes (positive charge carriers), while the N-type semiconductor has an excess of electrons (negative charge carriers). When the two materials are joined, they form a PN junction, which is the key functional area of the photodiode.
- Exposure to Light: To detect light effectively, the junction is exposed to light rays. The photodiode is usually covered with a glass or optical lens. The lens serves multiple purposes: it protects the semiconductor material

and increases the surface area of the photodiode to gather more light, thus enhancing its sensitivity. The lens allows more light to enter the junction, improving the efficiency of light absorption.

- **Black Layer or Metalized Coating:** The remainder of the photodiode is typically covered with a black layer or a metalized coating, which helps in minimizing unwanted reflections or stray light. This ensures that only the light intended for detection is absorbed, improving the accuracy of the sensor.

- Photodiode: I-V Characteristics

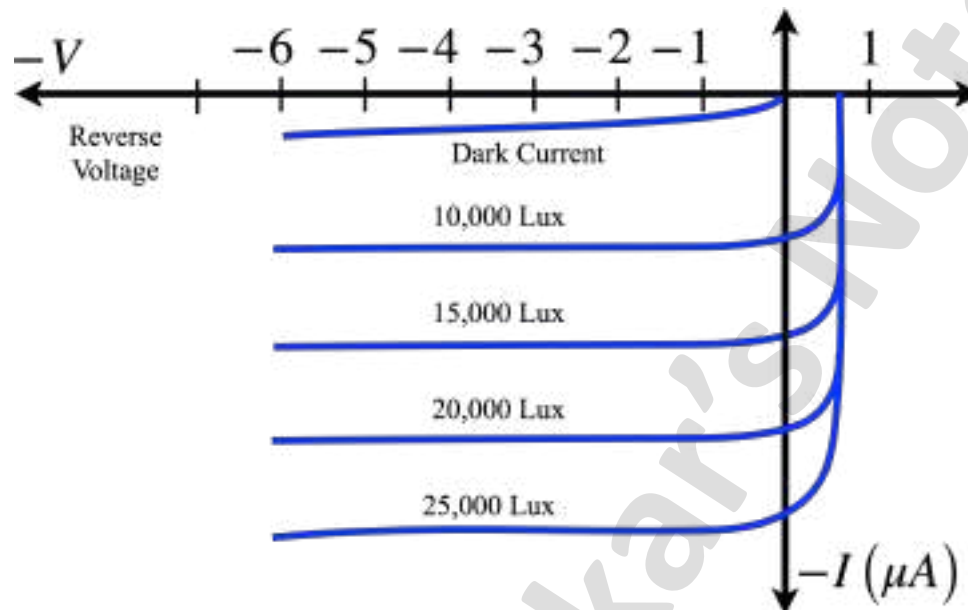


Fig. 36: I-V Characteristics of Photodiode

- The I-V characteristics of a photodiode under varying light intensities such as 10K Lux, 15K Lux, 20K Lux, and 25K Lux show how the photocurrent increases as the intensity of the incident light increases.
- The I-V curve under dark conditions will be at the baseline with very small reverse current and a sharp rise in forward bias.
- Under 10K Lux, the curve shifts slightly upwards, indicating a small increase in photocurrent.
- At 15K Lux, 20K Lux, and 25K Lux, the curve progressively shifts further upward, reflecting larger photocurrents.
- The slope of the curve in reverse bias will be steeper, and the total current in forward bias will increase.

- Types of Photodiodes:

- **Photovoltaic Mode:** In this mode, the photodiode generates a voltage or current when illuminated. It operates without the need for an external bias.
- **Photoconductive Mode:** Here, the photodiode is reverse-biased, and the current increases when light is incident on the device. This mode is used for higher speed applications.
- **Avalanche Photodiodes (APD):** These are designed for higher sensitivity and are operated in a reverse bias with an avalanche effect to increase gain.

- Applications:

- Photodiodes have a wide range of applications due to their ability to detect light and convert it into electrical signals. Common uses include:
 - **Light Sensing:** In devices such as cameras, light meters, and automatic lighting systems.
 - **Fiber Optic Communication:** Used for detecting light signals in optical fiber systems.
 - **Solar Cells:** Photodiodes are employed in solar energy systems to convert sunlight into electrical power.
 - **Medical Devices:** In applications such as pulse oximeters, where light absorption is measured in tissues.
 - **Laser Systems:** For measuring the intensity of laser beams in various scientific experiments.
 - **Environmental Sensing:** In applications where light intensity or changes in light conditions need to be monitored, such as weather stations or plant growth monitoring.



- Advantages and Disadvantages of Photodiode:

Sr. No.	Advantages	Disadvantages
1	High Speed of Response: Photodiodes respond quickly to changes in light intensity, making them suitable for high-speed applications like optical communication.	Limited Current Output: Photodiodes generate a small amount of current, requiring amplification for some applications.
2	High Sensitivity: They are highly sensitive to light, even in low-light conditions, allowing for precise detection of light signals.	Temperature Sensitivity: Their performance can vary with temperature changes, requiring compensation in certain environments.
3	Compact Size: Photodiodes are small, lightweight, and easy to integrate into electronic circuits.	Directional Sensitivity: Photodiodes are sensitive to the angle of incident light, which may limit their use in applications requiring omnidirectional light detection.
4	Wide Wavelength Range: They can detect a broad spectrum of light, from ultraviolet to infrared, depending on the material used.	Reverse Bias Requirement: In some cases, reverse biasing is needed to enhance response time, adding complexity to the circuit.
5	Low Noise: Photodiodes have low internal noise, enhancing their performance in detecting weak signals.	Limited Dynamic Range: Their ability to detect extremely high or low light intensities may be limited.
6	Cost-Effective: They are relatively inexpensive and widely available, making them accessible for various applications.	Dark Current: A small leakage current (dark current) flows even in the absence of light, which can affect accuracy in sensitive applications.
7	Low Power Consumption: Photodiodes require minimal power to operate, making them energy-efficient.	Vulnerability to Damage: Photodiodes can be damaged by exposure to excessive light or high reverse voltage.
8	Longevity: They have a long operational lifespan with consistent performance over time.	Non-Ideal for High-Light Intensity: They may saturate or perform less effectively under extremely high light intensity.
9	Linear Response: Photodiodes provide a linear response to light intensity, allowing accurate measurements.	Material Limitations: The material used for photodiodes determines their wavelength range, limiting their effectiveness for certain applications.
10	Wide Application Range: They are versatile and used in fields like telecommunications, medical devices, and consumer electronics.	Noise at High Frequencies: When operated at high frequencies, photodiodes may introduce noise, reducing performance.

**- Characteristics of Sensors**

- Range: Defines the minimum and maximum values that a sensor can accurately measure. Example: A temperature sensor might measure from 20°C to 100°C.
- Sensitivity: Indicates how much the sensor's output changes in response to a change in the measured quantity. Example: A highly sensitive light sensor can detect small variations in light intensity.
- Resolution: The smallest detectable increment of the quantity being measured. Example: A pressure sensor with a resolution of 0.1 psi can distinguish changes as small as 0.1 psi.
- Accuracy: Describes how close the measured value is to the true value of the quantity being measured. Example: An accurate pH sensor provides pH readings within ± 0.1 pH units of the actual value.
- Repeatability: Indicates the sensor's ability to produce the same output for repeated measurements under the same conditions. Example: A highly repeatable sensor consistently measures distance with minimal variation.

- Applications of Sensors

- Environmental Monitoring: Measure temperature, humidity, air quality, etc., for weather forecasting and pollution control.
- Industrial Automation: Monitor parameters like pressure, flow rate, level, and position in manufacturing processes for quality control and efficiency.
- Medical and Healthcare: Used in patient monitoring systems to measure vital signs such as heart rate, blood pressure, and oxygen levels.
- Automotive Industry: Sensors for vehicle speed, proximity detection, parking assistance, and engine monitoring.
- Consumer Electronics: Touch sensors, motion sensors, ambient light sensors in smartphones, tablets, and smart home devices.
- Agriculture: Soil moisture sensors, weather sensors for precision farming and irrigation control.



11. Solved Problems

Problems on conductivity

Problem 1: Calculate the energy gap of Germanium, given that it is transparent to radiation of wavelength greater than 17760\AA .

Solution:

Formula: $E_g = h\nu$

$$E_g = h \frac{c}{\lambda} = \frac{6.626 \times 10^{-34} \times 2.99 \times 10^8}{17760 \times 10^{-10}} = 1.12 \times 10^{-19} \text{ J} = \frac{1.12 \times 10^{-19} \text{ J}}{1.6 \times 10^{-19} \text{ C}} \quad \text{Hence } E_g = 0.7 \text{ eV}$$

Problem 2: Calculate the energy gap of silicon (in eV), given that it is transparent to radiation of wavelength greater than 11000\AA .

Solution:

Formula: $E_g = h\nu$

$$E_g = h \frac{c}{\lambda} = \frac{6.626 \times 10^{-34} \times 2.99 \times 10^8}{11000 \times 10^{-10}} = 1.80 \times 10^{-19} \text{ J} = \frac{1.80 \times 10^{-19} \text{ J}}{1.6 \times 10^{-19} \text{ C}} \quad \text{Hence } E_g = 1.12 \text{ eV}$$

Problem 3: Calculate the number of acceptors to be added to a germanium sample to obtain the resistivity of $8\text{ }\Omega \cdot \text{cm}$

[Given $\mu = 1600 \text{ cm}^2/\text{V} \cdot \text{s}$]

Solution:

$$\text{The resistivity equation is } \rho = \frac{1}{n_a e \mu_h} \text{ hence } n_a = \frac{1}{\rho e \mu_h} = \frac{1}{8 \times 1.6 \times 10^{-19} \times 1600}$$

Hence, $n_a = 4.876 \times 10^{14}/\text{cc}$

Problem 4: A germanium sample has 4.56×10^{22} atoms/cc and a donor impurity in the ratio of one part per 10^{10} is added to create an N type semiconductor. If the mobility of charge carriers is $3900 \text{ cm}^2/\text{V} \cdot \text{s}$, find the conductivity of silicon.

Solution:

Density of atoms in germanium = 4.56×10^{22} atoms/cc, Donor impurity = 1 atom / 10^{10} Si atoms,

Mobility of charge carriers = $3900 \text{ cm}^2/\text{V} \cdot \text{s}$.

$$\text{Charge carrier density; } n = \frac{4.56 \times 10^{22}}{10^{10}} = 4.56 \times 10^{12}/\text{cc}$$

Thus, the conductivity equation; $\sigma = n e \mu_e$

$$\sigma = 4.56 \times 10^{12} \times 1.6 \times 10^{-19} \times 3900 \quad \sigma = 2.849 \times 10^{-3} \text{ }\Omega/\text{cm}.$$

Problem 5: Calculate the conductivity of pure silicon at room temperature when concentration of carriers is 1.6×10^{10} per cc [$\mu_e = 1500 \text{ cm}^2/\text{V} \cdot \text{s}$, $\mu_h = 500 \text{ cm}^2/\text{V} \cdot \text{s}$].

Solution:

The intrinsic conductivity equation; $\sigma_i = e n_i (\mu_e + \mu_h)$

$$\sigma_i = 1.6 \times 10^{-19} \times 1.6 \times 10^{10} (1500 + 500) \quad \sigma_i = 5.126 \times 10^{-6} \text{ }\Omega/\text{cm}$$



Problem 6: Calculate the conductivity of germanium sample if a donor impurity is added to the extent of one part in 10^9 germanium atoms at room temperature.

[Given: Atomic weight of germanium: 72.6, Density of Ge: 5.32 gm/cc, Avogadro Number: $6.022 \times 10^{23} \text{ mol}^{-1}$, Mobility: $\mu = 3800 \text{ cm}^2/\text{V.s}$].

Solution:

The conductivity equation; $\sigma = ne\mu_e$

$$\text{Number of Ge atoms} = \frac{\text{Avogadro number} \times \text{Density of Ge}}{\text{Atomic weight of Ge}} = \frac{6.022 \times 10^{23} \times 5.32}{72.6} = 4.412 \times 10^{22} / \text{cc}$$

There is one donor atom per 10^9 atoms of Ge atoms.

$$\text{Hence; } n = \frac{4.412 \times 10^{22}}{10^9} = 4.41 \times 10^{13} / \text{cc}$$

The conductivity, therefore is; $\sigma = ne\mu_e$

$$\sigma = 4.41 \times 10^{13} \times 1.6 \times 10^{-19} \times 3800 \quad \sigma = 0.0268 \text{ } \Omega/\text{cm}.$$

Problem 7: The resistivity of intrinsic silicon at room temperature is $3000 \text{ } \Omega\text{m}$. Calculate the intrinsic carrier density.

[Given: $\mu_e = 0.17 \text{ m}^2/\text{V.s}$, $\mu_h = 0.035 \text{ m}^2/\text{V.s}$, $e = 1.6 \times 10^{-19} \text{ C}$.]

Solution: The resistivity is; $\rho_i = \frac{1}{n_i \cdot e (\mu_e + \mu_h)}$

$$\text{Hence, } n_i = \frac{1}{\rho_i \cdot e (\mu_e + \mu_h)} = \frac{1}{3000 \times 1.6 \times 10^{-19} (0.17 + 0.035)} = 1.01626 \times 10^{16} / \text{m}^3.$$

Problem 8: Calculate the number of acceptor atoms must be added to an intrinsic semiconductor to obtain resistivity as $10 \text{ } \Omega \cdot \text{cm}$. Given: $\mu_e = 1700 \text{ cm}^2/\text{V.s}$, $e = 1.6 \times 10^{-19} \text{ C}$

Solution:

$$\mu_e = 1700 \text{ cm}^2/\text{V.s}, e = 1.6 \times 10^{-19} \text{ C}, \rho = 10 \text{ } \Omega\text{cm}$$

For acceptors i.e. for p-type semiconductor, the conductivity is $\sigma_p = n_h e \mu_h$

$$\text{Hence; } n_h = \frac{\sigma_p}{e \cdot \mu_h} = \frac{1}{\rho \cdot e \cdot \mu_h} = \frac{1}{10 \times 1.6 \times 10^{-19} \times 1700} = 3.676 \times 10^{14} / \text{cm}^3.$$

Problem 9: A sample of intrinsic silicon at room temperature has a carrier concentration of $1.5 \times 10^{16} / \text{m}^3$.

A donor impurity is added to the extent of 1 donor atom per 10^8 atoms of silicon. If the concentration of silicon atoms is $5 \times 10^{28} \text{ atoms/m}^3$, determine the resistivity of the material.

(Given $\mu_e = 0.135 \text{ m}^2/\text{V.s}$ and $\mu_h = 0.048 \text{ m}^2/\text{V.s}$)

Solution:

$$\text{Donor atom density is given as } N_D = \frac{N}{10^8} = \frac{5 \times 10^{28} / \text{m}^3}{10^8} = 5 \times 10^{20} / \text{m}^3$$

Free electron concentration is given by $n_n = N_D = 5 \times 10^{20} / \text{m}^3$



Hole concentration is given by $p_n = \frac{n_i^2}{n_n} = \frac{(1.5 \times 10^{16}/m^3)^2}{5 \times 10^{20}/m^3} = 4.5 \times 10^{11}/m^3$.

Resistivity of the material $\rho = \frac{1}{\sigma} = \frac{1}{e(n_n \mu_e + p_n \mu_h)}$

$$\rho = \frac{1}{1.602 \times 10^{-19} C (5 \times 10^{20} \times 0.135 m^2/V.s + 4.5 \times 10^{11} \times 0.048 m^2/V.s)} = 0.092 \Omega m$$

Problems on Hall effect

Problem 10: The Hall coefficient of a specimen of a doped silicon is found to be $3.66 \times 10^{-3} m^3/C$. The resistivity of specimen is $8.93 \Omega m$. Determine the mobility of the charge carriers.

Solution:

$$R_H = 3.66 \times 10^{-3} m^3/C, \rho = 8.93 \Omega m \quad \text{hence } \sigma = \frac{1}{\rho} = \frac{1}{8.93}$$

$$\text{Mobility } \mu = \sigma R_H \text{ therefore, } \mu = \frac{1}{8.93} \times 3.66 \times 10^{-3} \quad \text{hence } \mu = 0.4098 \times 10^{-3} cm^2/V.s.$$

Problem 11: A slab of silicon, 2 cm in length, 1.5 cm wide, and 2 mm thick, is subjected to a magnetic field of 0.5T along its thickness. When a current of 0.5A flows along the length, the voltage measured across its width is 3.64mV. Calculate the concentration of mobile electrons in silicon.

Solution: Length of silicon slab: $L = 2 \times 10^{-2} m$, Width of silicon slab: $w = 1.5 \times 10^{-2} m$, Thickness of silicon slab: $d = 2 \times 10^{-3} m$, Magnetic field: $B = 0.5T$, Current: $I = 0.5A$,

Hall voltage: $V_H = 3.648 mV = 3.648 \times 10^{-3}$, Charge of an electron: $e = 1.602 \times 10^{-19}$

The Hall voltage is given by:

$$V_H = \frac{IB}{ned} \quad \therefore n = \frac{IB}{edV_H} \quad \text{Substituting Values} \quad n = \frac{(0.5)(0.5)}{(1.602 \times 10^{-19})(2 \times 10^{-3})(3.648 \times 10^{-3})}$$

$$n = \frac{0.25}{1.1681 \times 10^{-24}} = 2.14 \times 10^{23} \text{ electrons}/m^3 \quad \text{This is the concentration of mobile electrons in silicon.}$$

Problem 12: A copper specimen having length 1 m, width 1 cm and thickness 1 mm is conducting a current of 1 ampere along its length. The specimen is kept in magnetic field of 1 Tesla along its thickness. It experiences Hall effect and Hall voltage $0.074 \mu V$ appears along its width. If conductivity of copper is $5.8 \times 10^7 \Omega/m$, find the hall coefficient and mobility of electrons in the specimen.

Solution: $l=1m$, $d=1cm = 10^{-2}m$, $t = 1mm = 10^{-3} m$, $B = 1 \text{ Tesla}$, $I = 1 \text{ amp}$, $V_H = 0.074 \times 10^{-6} \text{ Volts}$, $\sigma =$

$5.8 \times 10^7 \Omega/m$. The Hall Voltage equation is; $V_H = R_H \frac{BId}{A}$ hence, $R_H = V_H \frac{A}{BId}$

$$R_H = \frac{0.074 \times 10^{-6} \times 10^{-2} \times 10^{-3}}{1 \times 1 \times 10^{-2}} \text{ hence } R_H = 0.074 \times 10^{-9} m^3/C.$$

$$\text{Now, } \sigma = \frac{\mu}{R_H} \text{ hence } \mu = \sigma \times R_H = 5.8 \times 10^7 \times 0.074 \times 10^{-9}$$

$$\text{Hence Mobility of electrons in the specimen is; } \mu = 0.4292 \times 10^{-2} \frac{m^2}{V.s}$$



Problem 13: An n-type germanium sample has a donor density of $10^{21}/\text{m}^3$. It is arranged in a Hall experiment having magnetic field of 0.5 T and the current density is 500 A/m^2 . Find the Hall voltage if the sample is 3 mm wide.

Solution:

Given: Current density $J = 500 \text{ A/m}^2$, $B = 0.5 \text{ T}$, $N_D = 10^{21}/\text{m}^3$, $w = 3 \text{ mm} = 3 \times 10^{-3} \text{ m}$

The Hall Voltage equation is;

$$V_H = R_H \frac{BI}{t} = \frac{1}{ne} \cdot \frac{BI}{t} = \frac{1}{ne} \cdot \frac{B}{t} \cdot \frac{I \cdot A}{A} = \frac{1}{ne} \cdot \frac{B \cdot J \cdot A}{t} = \frac{1}{ne} \cdot \frac{B \cdot J \cdot w \cdot t}{t} = \frac{B \cdot J \cdot w}{ne}$$

$$V_H = \frac{B \cdot J \cdot w}{ne} \text{ But } n = N_D \text{ hence } V_H = \frac{B \cdot J \cdot w}{N_D \cdot e}$$

$$V_H = \frac{B \cdot J \cdot w}{N_D \cdot e} = \frac{0.5 \text{ T} \times 500 \text{ A/m}^2 \times 3 \times 10^{-3} \text{ m}}{10^{21}/\text{m}^3 \times 1.602 \times 10^{-19} \text{ C}} = 4.7 \times 10^{-3} \text{ V} = \mathbf{4.7 \text{ mV}}$$

$$\text{Unit:} = 1 \frac{\text{TAm}^2}{\text{C}} = 1 \frac{\text{N}}{\text{Am}} \cdot \frac{\text{Am}^2}{\text{C}} = 1 \frac{\text{N} \cdot \text{m}}{\text{C}} = 1 \frac{\text{J}}{\text{C}} = 1 \text{ V}$$

Problem 14: A copper strip 2.0cm wide and 1.0mm thick is placed in a magnetic field with $B=1.5 \text{ wb/m}^2$.

If a current of 200 A is set up in the strip, calculate Hall voltage that appears across the thickness.

Assume $R_H = 6 \times 10^{-7} \text{ m}^3/\text{C}$.

Solution:

$$V_H = R_H \cdot \frac{IB}{t} = 6 \times 10^{-7} \text{ m}^3/\text{C} \cdot \frac{200 \text{ A} \times 1.5 \text{ wb/m}^2}{10^{-3} \text{ m}} = 0.18 \text{ V}$$

Problem 15: An electric field of 100 V/m is applied to a sample of n-type semiconductor whose Hall coefficient is $-0.0125 \text{ m}^3/\text{C}$. Determine the current density in the sample, Given $m_e = 0.6 \text{ m}^2/\text{V} \cdot \text{s}$.

Solution:

$$\text{Current density } J = \frac{\mu_e E}{R_H} J = \frac{\mu_e E}{R_H} = \frac{0.36 \text{ m}^2/\text{V} \cdot \text{s} \times 100 \text{ V/m}}{-0.0125 \text{ m}^3/\text{C}} = -2880 \text{ C/s} \cdot \text{m}^2 \text{ hence } \mathbf{J = -2880 \text{ A/m}^2}$$

Problem 16: In a Hall coefficient experiment, a current of 0.25 A is sent through a metal strip having thickness 0.2 mm and width 5 mm. The Hall voltage is found to be 0.15 mV when a magnetic field of 2000 gauss is used.

(a) What is the carrier concentration?

(b) What is the drift velocity of the carriers?

Solution:

(a) The carrier concentration,

$$n = \frac{IB}{V_H \cdot e \cdot t} = \frac{0.25 \text{ A} \times 0.2 \text{ T}}{0.15 \times 10^{-3} \text{ V} \times 1.602 \times 10^{-19} \text{ C} \times 0.2 \times 10^{-3} \text{ m}} = \mathbf{1.04 \times 10^{25} \text{ carriers/m}^3}$$

(b) Drift velocity of the carriers, 2000 gauss = 0.2 T

$$v_d = \frac{V_H}{wB} = \frac{0.15 \times 10^{-3} \text{ V}}{5 \times 10^{-3} \text{ m} \times 0.2 \text{ T}} = 0.15 \frac{\text{V}}{\text{mT}} = \mathbf{0.15 \text{ m/s}}$$



Problems on Fermi Function

Problem 17: Find the temperature at which there is 1% probability that a state with energy 2 eV is occupied. Given that Fermi energy is 1.5 eV.

Solution:

The Fermi-Dirac probability distribution function gives the probability of an energy state E being occupied by an

$$\text{electron is given by } f(E) = \frac{1}{1 + e^{\frac{(E - E_f)}{kT}}}$$

Hence, $E - E_f = 2\text{eV} - 1.5\text{eV} = 0.5\text{eV}$ and $f(E) = 1\%$ hence,

$$f(E) = \frac{1}{1 + e^{\frac{(E - E_f)}{kT}}} \Rightarrow \frac{1}{100} = \frac{1}{1 + e^{0.5/kT}}$$

Hence $e^{0.5/kT} = \frac{0.99}{0.01} = 99$, Taking logarithms on both sides, we get, $\frac{0.5\text{eV}}{kT} = 2.303 \log(99)$

$$T = \frac{0.5\text{eV}}{2.303 \log 99 \times 8.61 \times 10^{-5} \text{eV}} = 1262\text{K} \quad \mathbf{T = 1262K.}$$

Problem 18: Evaluate the Fermi function for energy kT above the Fermi energy.

Solution:

Given: $E - E_f = kT$

$$\text{Using } f(E) = \frac{1}{1 + e^{\frac{(E - E_f)}{kT}}} = \frac{1}{1 + e^{\frac{kT}{kT}}} = \frac{1}{1 + e^1} = \frac{1}{1 + 2.78} = \frac{1}{3.78} = \mathbf{0.269}$$

Problem 19: In a solid, consider the energy level lying 0.01 eV below Fermi level. What is the probability of this level not being occupied by an electron?

Solution:

Let $E = E_f - 0.01\text{eV}$

Hence $E - E_f = -0.01\text{eV}$ and

kT at $T = 300\text{K}$ is

$$kT = 8.617 \times 10^{-5} \text{eV K}^{-1} \times 300\text{K} = 0.026\text{eV}$$

$$\text{Hence using } f(E) = \frac{1}{1 + e^{\frac{(E - E_f)}{kT}}}$$

$$f(E) = \frac{1}{1 + e^{\frac{-0.01\text{eV}}{0.026\text{eV}}}} = \frac{1}{1 + e^{-0.387}} = \frac{1}{1 + 0.679} = \frac{1}{1.679} = 0.596$$

The probability of an energy level E not being occupied by an electron is given by $[1 - f(E)]$.

$$[1 - f(E)] = 1 - 0.596 = \mathbf{0.404.}$$



Sr. No.	Question statement	Marks
1	Give a brief of formation of bands in solids	4
2	Draw a neat, labelled diagram to illustrate Hall effect. State and explain Hall effect.	4
3	Draw a neat, labelled diagram to illustrate Hall effect. State Hall effect. What does the Hall effect's equilibrium condition mean?	4
4	State Hall effect. Give an expression for Hall voltage and Hall coefficient. Explain terms involved in it.	4
5	State Hall effect. Give its applications.	4
6	Derive an expression for Hall voltage and Hall coefficient	4
7	Obtain an expression for conductivity of an intrinsic as well as extrinsic semiconductor.	4
8	What is the Fermi-Dirac function? Describe its behaviour at $T=0$ and $T>0K$	4
9	What is the Fermi-Dirac function? For any positive temperature what is probability of occupancy of Fermi energy level? Hence define Fermi energy level.	4
10	Define Fermi level for a semiconductor. With a neat and labelled diagram, show the position of Fermi level for an intrinsic semiconductor. Interpret the diagram.	4
11	With a neat and labelled diagram, show the variation of position of Fermi level for P type extrinsic semiconductor with temperature. Interpret the diagram.	4
12	With a neat and labelled diagram, show the variation of position of Fermi level for N type extrinsic semiconductor with temperature. Interpret the diagram.	4
13	With a neat and labelled diagram, show the variation of position of Fermi level for P type extrinsic semiconductor with doping concentration. Interpret the diagram.	4
14	With a neat and labelled diagram, show the variation of position of Fermi level for N type extrinsic semiconductor with doping concentration. Interpret the diagram.	4
15	Interpret the flow of majority carriers in a forward biased diode, with the help of a neat labelled energy band diagram.	4
16	Draw energy band picture of a diode when it is (i) unbiased (ii) forward biased (iii) reverse biased	4
17	Draw IV characteristics of a solar cell. Explain terms-(i) Short circuit current (ii) Open circuit voltage (ii) Fill factor	4
18	What is a sensor? Define Active and passive sensors.	4
19	What is a Photodiode? State, 2 diverse applications of a photodiode.	4
20	State working principle of Active and Passive Sensor. Give Examples of Active and Passive Sensors	4



Sr. No.	Question statement	Marks
21	Calculate the conductivity of Germanium specimen, if the donor impurity is added to the extent of 1 part in 10^8 Ge atoms at room temperature. Avogadro No. is 6.02×10^{23} atoms / mole. At. Wt of $Ge = 72.6$. Density of $Ge = 5.32 \text{ gm/cm}^3$ Mobility of electron is $\mu_e = 3800 \text{ cm}^2/\text{V.s}$	4
22	Calculate the conductivity of pure silicon at room temperature when the concentration of carriers is $1.5 \times 10^{16} / \text{m}^3$ and motilities are $\mu_e = 0.12 \text{ m}^2/\text{V.s}$ $\mu_p = 0.05 \text{ m}^2/\text{V.s}$ $n_e = n_p = n_i = 1.5 \times 10^{16} / \text{m}^3$.	4
23	The resistivity of n type semiconductor is $10^{-6} \Omega . \text{cm}$. Calculate the number of donor atoms added to obtain this resistivity. ($\mu_e = 1000 \text{ cm}^2/\text{V.s}$)	4
24	Calculate the conductivity of extrinsic silicon at room temperature if the donor impurity added is 1 in 10^8 silicon atoms. No of silicon atoms / unit volume = $5 \times 10^{22} \text{ atoms /cm}^3$ Mobility of electron is $\mu_e = 1300 \text{ cm}^2/\text{V.s}$	4
25	Find resistivity of copper if each atom of copper contributes one free electron At. Wt. of copper is 63.5. Density of copper 8.96 gm/cc $\mu_e = 43.28 \text{ cm}^2/\text{V.s}$ Avogadro number: 6.02×10^{23} atoms / mole	4
26	Calculate the conductivity of pure silicon at room temperature when the concentration of charge carriers is $1.6 \times 10^{10} / \text{cm}^3$.	4
27	A copper specimen with length 1 meter, width 1cm and thickness 1mm is conducting current of 1 Amp along its length and is applied with a magnetic field of 1 Tesla along its thickness. It experiences Hall effect and a Hall voltage of $0.074 \mu\text{V}$ appears along its width. Calculate Hall coefficient and the mobility of electrons in copper. Conductivity of copper is $5.8 \times 10^7 \text{ mho/meter}$.	4
28	A slab of silicon 2 cm in length, 1.5 cm wide and 2mm thick is applied with magnetic field 0.4 T along its thickness. When a current of 75 A flows along the length, the voltage measured across width is 0.81 mV. Calculate the concentration of mobile electrons in silicon.	4
29	The resistivity of doped silicon is $9 \times 10^{-3} \text{ Ohm-m}$. Hall coefficient is $3.6 \times 10^{-4} \text{ m}^3/\text{C}$. Assuming single carrier concentration, find carrier concentration, mobility and density of charge.	4
30	A silver wire in the form of a ribbon 0.50 cm wide and 0.1 mm thick. When a current of 2 amperes passes through ribbon, perpendicular to 0.80 Tesla magnetic field, calculate the Hall voltage produced across width. density of silver is 10.5 gm/cc and At. wt of silver is 108.	4

UNIT 2: QUANTUM MECHANICS

1. Introduction

- Quantum physics, also known as quantum mechanics, is a fundamental branch of physics that explores the behavior of matter and energy at the smallest scales, such as atoms and subatomic particles. Unlike classical physics, which explains the motion of macroscopic objects, quantum mechanics delves into phenomena that defy intuition, including wave-particle duality, quantum superposition, and entanglement. At its core, quantum physics provides a framework to understand the nature of reality and the interactions of particles with energy in ways that classical theories cannot.
- The importance of quantum physics in engineering physics is profound. It forms the foundation for many cutting-edge technologies, such as semiconductors, lasers, quantum computing, and nanotechnology. By applying quantum principles, engineers can design innovative devices like transistors, which are the building blocks of modern electronics, and highly precise sensors for medical, defense, and industrial applications. Moreover, quantum mechanics underpins advancements in renewable energy, such as the development of more efficient solar cells and energy storage systems.

2. The domain of validity for Classical Mechanics

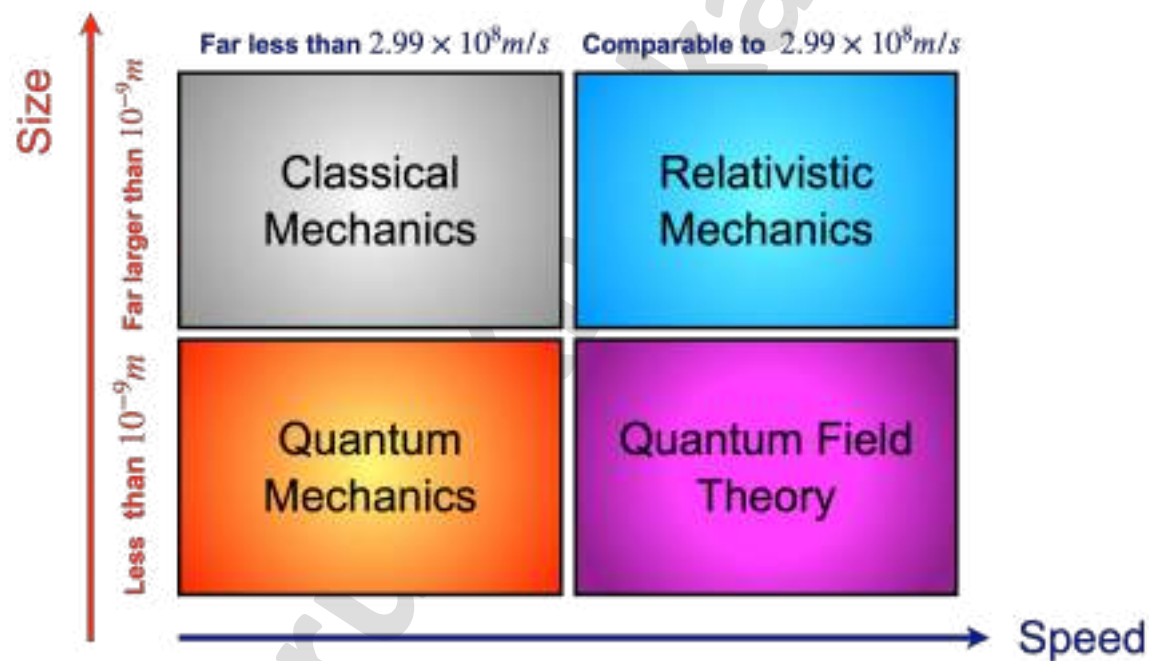


Fig. 1: The domain of validity

- The domains of validity are shown in figure which are:
 - Classical mechanics with size far larger than 10^{-9} m and with speed far less than $2.99 \times 10^8 \text{ m/s}$
 - Relativistic mechanics with size far larger than 10^{-9} m and with speed comparable to $2.99 \times 10^8 \text{ m/s}$
 - Quantum Mechanics with size less than 10^{-9} m and with speed less than $2.99 \times 10^8 \text{ m/s}$.
 - Quantum Field Theory with size less than 10^{-9} m and with speed Comparable to $2.99 \times 10^8 \text{ m/s}$
- Many branches of classical mechanics are simplifications or approximations of more accurate forms; two of the most accurate being general relativity and relativistic statistical mechanics. Geometric optics is an approximation to the quantum theory of light, and does not have a superior "classical" form.
- When both quantum mechanics and classical mechanics cannot apply, such as at the quantum level with many degrees of freedom, quantum field theory (QFT) is of use.
- QFT deals with small distances and large speeds with many degrees of freedom as well as the possibility of any change in the number of particles throughout the interaction.



- When treating large degrees of freedom at the macroscopic level, statistical mechanics becomes useful. Statistical mechanics describes the behaviour of large (but countable) numbers of particles and their interactions as a whole at the macroscopic level.
- Statistical mechanics is mainly used in thermodynamics for systems that lie outside the bounds of the assumptions of classical thermodynamics.
- In the case of high velocity objects approaching the speed of light, classical mechanics is enhanced by special relativity.
- In case that objects become extremely heavy deviations from Newtonian mechanics become apparent and can be quantified by using the parameters post-Newtonian formalism. In that case, General relativity (GR) becomes applicable.
- However, until now there is no theory of Quantum gravity unifying GR and QFT in the sense that it could be used when objects become extremely small and heavy.

3. Classical Mechanics

- Classical mechanics, often referred to as Newtonian mechanics, is a branch of physics developed by Isaac Newton and other scientists to describe the motion of macroscopic objects under the influence of forces. It is based on Newton's three laws of motion, which explain concepts such as inertia, the relationship between force and acceleration, and the principle of action and reaction.
- Classical mechanics assumes a deterministic framework, meaning the future state of a system can be precisely predicted if the initial conditions such as position, velocity, and forces acting on an object are known. It is widely used to explain the behavior of everyday objects, from the motion of planets and vehicles to the dynamics of machines and structures.
- However, classical mechanics is limited to macroscopic scales and fails to accurately describe phenomena at atomic or subatomic levels, necessitating the development of quantum mechanics to address such complexities.
- **Failure of Classical Mechanics and the Need for Quantum Mechanics**
- Classical physics, primarily based on Newton's laws of motion and gravitation, successfully describes the motion of macroscopic bodies. However, as experimental evidence accumulated in the early twentieth century, it became evident that classical mechanics had significant limitations. Newtonian mechanics failed when applied to objects moving at speeds comparable to the speed of light and to phenomena at atomic and subatomic scales.
- To address the failure at high velocities, Albert Einstein introduced the special theory of relativity in 1905, which revolutionized the concepts of absolute mass, space, and time. Relativity demonstrated that rest, motion, length, and time are not absolute but relative, depending on the observer's frame of reference. The theory invalidated the concept of motion through a hypothetical "ether" and provided a foundation for understanding phenomena in high-energy physics, quantum theory, and atomic physics.
- Classical mechanics also failed to describe atomic phenomena, such as the behavior of electrons within an atom. According to classical theory, the negatively charged electron, attracted to the positively charged nucleus, should either spiral into the nucleus due to electrostatic forces or radiate energy as it accelerates in orbit, eventually collapsing into the nucleus. This prediction, however, contradicts the observed stability of atoms. The inability of classical mechanics to explain this stability highlighted its inadequacy for phenomena at quantum scales.
- These shortcomings led to the development of quantum mechanics, a revolutionary framework to describe the behavior of particles at atomic and subatomic levels. Quantum mechanics resolved the paradoxes of classical mechanics, offering explanations for atomic stability, discrete energy levels, and various phenomena that classical theories could not address. It has since become a cornerstone of modern physics, enabling advancements in fields such as atomic theory, quantum computing, and nanotechnology.

**- Limitations of classical physics**

- Classical physics, based on theories such as Newtonian mechanics, thermodynamics, and Maxwell's equations, provides a comprehensive understanding of macroscopic phenomena in the physical world. It explains the motion of objects, heat transfer, and electromagnetic waves with remarkable accuracy in everyday scenarios. However, as scientific inquiry delved into atomic and subatomic scales, classical physics failed to account for several phenomena, revealing its limitations and paving the way for the development of quantum mechanics.
- Atomic Stability:
Classical physics could not explain why atoms are stable. According to Maxwell's electromagnetic theory, electrons orbiting the nucleus should emit electromagnetic radiation continuously, losing energy and spiraling into the nucleus. This would make atoms unstable, contradicting experimental observations.
- Blackbody Radiation:
Classical physics predicted the "ultraviolet catastrophe" for blackbody radiation, suggesting infinite energy at high frequencies, which was not observed experimentally. Planck's quantum hypothesis resolved this by introducing quantized energy levels.
- Photoelectric Effect:
The classical wave theory of light failed to explain why light below a certain frequency, regardless of its intensity, cannot eject electrons from a metal surface. Quantum mechanics resolved this through Einstein's concept of photons, or quantized packets of light energy.
- Spectral Lines of Atoms:
Classical theories could not explain the discrete spectral lines observed in atomic emission and absorption spectra. For example, the hydrogen atom's spectral series was inexplicable until quantum mechanics introduced quantized energy levels.
- Dual Nature of Light and Particles:
Classical physics treated light as a wave and matter as particles. However, experiments like Young's double-slit experiment and electron diffraction revealed that both light and particles exhibit wave-particle duality, which classical theories could not reconcile.
- Microscopic Systems:
Classical physics assumes deterministic behavior, meaning that the future state of a system can be precisely predicted given initial conditions. However, at the atomic and subatomic levels, systems exhibit probabilistic behavior, requiring a new framework.
- **Need for Quantum Mechanics**
- To address these limitations, quantum mechanics emerged as a revolutionary framework that fundamentally changed our understanding of nature. Quantum mechanics introduced new principles and concepts to explain phenomena beyond the scope of classical physics.
- Quantization of Energy:
Quantum mechanics introduced the idea that energy is not continuous but quantized. This resolved issues like blackbody radiation and the photoelectric effect, as energy transitions occur in discrete amounts.
- Wave-Particle Duality:
Quantum mechanics unified the wave and particle nature of light and matter through concepts like de Broglie's hypothesis and Schrödinger's wave equation. This explained phenomena such as interference and diffraction for particles.



- **Uncertainty Principle:**

Heisenberg's uncertainty principle introduced the idea that certain pairs of physical properties, such as position and momentum, cannot be simultaneously measured with arbitrary precision. This principle addressed the inherent limitations of measurements at microscopic scales.

- **Atomic Structure:**

Quantum mechanics, through the Bohr model and later refinements, explained the stability of atoms and the existence of discrete energy levels, leading to a better understanding of chemical bonding and molecular structures.

- **Statistical Nature of Microscopic Systems:**

Unlike classical physics, which is deterministic, quantum mechanics provides a probabilistic framework, using wave functions to describe the likelihood of finding a particle in a particular state.

- **Technological Advancements:**

Quantum mechanics is essential for understanding and designing modern technologies, including semiconductors, lasers, quantum computers, and nanotechnology, which classical physics cannot describe accurately.

4. Wave Particle duality

- Wave-particle duality is a fundamental concept in quantum mechanics that describes the dual nature of electromagnetic radiation and matter, exhibiting both wave-like and particle-like behavior depending on the experimental setup. This duality defies classical intuition, which treats waves and particles as mutually exclusive concepts.

- **Particle nature of electromagnetic radiation**

- Einstein's explanation of the photoelectric effect, Compton effect, blackbody radiation, and emission and absorption of radiation demonstrated the particle-like behavior of electromagnetic waves.

- **Photoelectric Effect:**

Einstein proposed that light consists of discrete packets of energy called photons. When light of a certain frequency strikes a metal surface, photons transfer their energy to electrons, causing them to be ejected. This particle-like interaction could not be explained by the classical wave theory of light.

- **Compton Effect:**

The scattering of X-rays by electrons demonstrated that photons behave as particles with momentum. The change in wavelength of the scattered X-rays supported the idea that light has particle-like properties.

- **Blackbody Radiation:**

Classical physics failed to explain the energy distribution of blackbody radiation. Planck's quantization of energy levels and concept of photons successfully resolved this issue, highlighting the particle nature of light.

- **Emission and Absorption of Radiation:**

Quantum theory describes how substances emit and absorb electromagnetic radiation in discrete energy packets (quanta), further supporting the idea of light as a collection of photons.

- **Wave nature of electromagnetic radiation**

- Electromagnetic radiation also exhibits wave-like properties, as seen in various macroscopic optical phenomena:

- **Interference:**

The superposition of light waves produces constructive and destructive interference patterns, demonstrating its wave-like nature.

- **Diffraction:**
When light passes through a small aperture or around obstacles, it spreads out, creating patterns characteristic of waves.
- **Polarization:**
The orientation of oscillating electric fields in light waves is evidence of its wave-like behavior, which cannot be explained by particle theory alone.
- **Dual Characteristics**
- The dual nature of electromagnetic radiation means that it exhibits wave-like or particle-like behavior depending on the experiment, but both properties cannot be observed simultaneously. For instance:
 - When performing an interference experiment, light behaves as a wave.
 - When studying the photoelectric effect, light behaves as a stream of particles.
- It is impossible to separate the wave and particle nature of electromagnetic radiation entirely. Instead, this duality is intrinsic and highlights the limitations of classical physics, requiring a quantum framework to describe such phenomena. Wave-particle duality applies not only to electromagnetic radiation but also to matter, as demonstrated by de Broglie’s hypothesis, which shows that particles like electrons exhibit wave-like behavior under certain conditions.
- Wave-particle duality is a cornerstone of quantum mechanics, offering profound insights into the behavior of light, matter, and the fundamental nature of reality.

Aspect	Wave Nature	Particle Nature
Definition	Exhibits properties of waves such as interference, diffraction, and polarization.	Exhibits discrete and localized properties like momentum and energy transfer.
Representation	Described by a wave equation (e.g., Maxwell's equations for electromagnetic waves).	Represented as a stream of particles (e.g., photons for light or electrons for matter).
Behavior	Spreads out over space and shows superposition effects.	Localized in space and interacts as discrete packets of energy.
Phenomena Explained	Explains interference, diffraction, and polarization.	Explains phenomena like the photoelectric effect, Compton effect, and blackbody
Energy Distribution	Energy is distributed continuously over the wavefront.	Energy is quantized and concentrated in packets called quanta or photons.
Momentum	Momentum is associated with the wave vector and spreads over the wave.	Momentum is discrete and can be transferred as a single unit during interaction.
Observability	Observed in macroscopic optical phenomena like interference and diffraction.	Observed in phenomena involving discrete interactions like electron ejection or scattering.
Experimental Evidence	Supported by Young’s double-slit experiment, diffraction, and polarization experiments.	Supported by Einstein’s photoelectric effect, Compton scattering, and Planck’s quantization of energy.
Mathematical Description	Uses wave functions or sinusoidal equations to describe properties.	Uses particle mechanics, energy quantization, and momentum equations.
Examples	Water waves, sound waves, electromagnetic waves (in diffraction or interference experiments).	Photons in the photoelectric effect, electrons in scattering experiments, or billiard balls in classical mechanics.



5. De Broglie hypothesis of matter waves

- The de Broglie hypothesis, proposed by Louis de Broglie in 1924, revolutionized our understanding of the dual nature of matter. De Broglie suggested that just as light exhibits both wave and particle characteristics, all moving particles, such as electrons, protons, atoms, and molecules, also have an associated wave-like nature. These waves, called de Broglie waves or matter waves, are intrinsic to the motion of particles and guide their behavior.

- **Wave-Particle Duality:**

- De Broglie extended the concept of wave-particle duality to matter, proposing that every moving particle exhibits wave-like properties in addition to its particle nature.

- **Matter Waves:**

- Matter waves are associated with moving particles like electrons, protons, and even macroscopic objects, though the wave nature becomes negligible for larger bodies due to their mass.
- Matter waves are not mechanical waves and can propagate even in a vacuum.
- Matter waves are not electromagnetic waves and are not associated with the motion of charged particles alone; they apply to neutral particles as well.

- **De Broglie Wavelength:**

The wavelength (λ) associated with a moving particle is given by the de Broglie equation:

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

where h is Planck's constant, and $p = mv$ is the momentum of the particle (mass m multiplied by velocity v).

- **Universal Applicability:**

- De Broglie's hypothesis applies to all objects in motion, but the wave effects are significant only for particles with very small mass, such as electrons. For macroscopic objects, the de Broglie wavelength is so small that it is practically undetectable.

- **Non-Mechanical and Non-Electromagnetic Waves:**

- Matter waves differ fundamentally from mechanical waves (e.g., sound waves) and electromagnetic waves (e.g., light). They represent a quantum phenomenon unique to particles in motion.

- **Experimental Confirmation:**

- The de Broglie hypothesis was experimentally confirmed through electron diffraction experiments by Davisson and Germer, which demonstrated the wave-like behavior of electrons when passed through a crystalline material.

- **Significance of De Broglie Hypothesis**

- The hypothesis established the foundation of wave mechanics, a key aspect of quantum mechanics.
- It explained the wave-like behavior of particles, such as interference and diffraction, which classical mechanics could not describe.
- The concept of matter waves guided the development of Schrödinger's wave equation, which became central to quantum theory.
- The de Broglie hypothesis thus unified the wave and particle aspects of matter, providing profound insights into the quantum behavior of particles at microscopic scales.

- Louis de Broglie used Einstein's equation $E = mc^2$ and incorporated it with Planck's equation $E = h\nu$.
- This brought together the relationship of the mass of a photon and speed of light with the photon energy.

$$mc^2 = h\nu;$$

$$mc = \frac{h\nu}{c} = p$$

where,

E : Energy; m : mass of photon;

c : speed of light, p is momentum

Since wavelength is; $\lambda = \frac{\text{Speed of light}}{\text{frequency}}; \lambda = \frac{c}{f}$

Momentum is equivalent to; $p = \frac{h\nu}{c} = \frac{h}{\lambda}$

de Broglie changed the equation to its equivalent;

$$p = \frac{h}{\lambda}; \lambda = \frac{h}{p}; \lambda = \frac{h}{mv} \quad \dots(1)$$

- where p is momentum, the product of mass of particle and velocity, wavelength (λ) and Planck's constant (h).
- This equation is also known as the **de Broglie wavelength**.

i) de Broglie wavelength of a particle in terms of its kinetic energy

- The de Broglie wavelength of a particle can also be expressed in terms of its kinetic energy (K.E.).

The de Broglie wavelength is given by: $\lambda = \frac{h}{p}$

where;

λ : de Broglie wavelength

h : Planck's constant

p : momentum of the particle ($p = mv$)

- The momentum p can be related to the kinetic energy of the particle:

$$K.E. = \frac{1}{2}mv^2 \quad \dots(2)$$

Rewriting this for

$$v = \sqrt{\frac{2K.E.}{m}} \quad \dots(3)$$

Substituting this into $p = mv$:

$$p = m \cdot \sqrt{\frac{2K.E.}{m}} = \sqrt{2m \cdot K.E.} \quad \dots(4)$$

Now, substituting $p = \sqrt{2m \cdot K.E.}$ into the de Broglie wavelength equation (1);

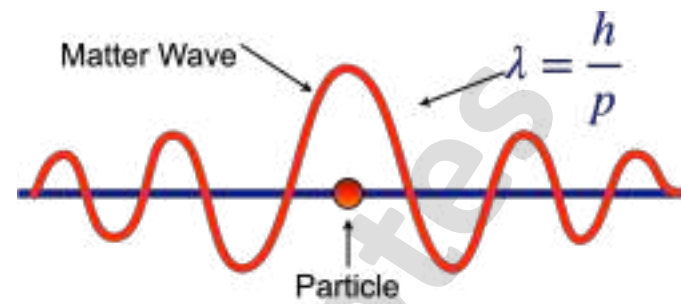


Fig. 2: Matter wave



$$\lambda = \frac{h}{\sqrt{2m \cdot K.E.}}$$

Final Formula

- The de Broglie wavelength in terms of kinetic energy is:

$$\lambda = \frac{h}{\sqrt{2m \cdot K.E.}} \text{ or } \lambda = \frac{h}{\sqrt{2m \cdot E}} \quad \dots(5)$$

Where,

h : Planck's constant (6.626×10^{-34} Js)

m : Mass of the particle (in kilograms)

E : Kinetic energy of the particle (in joules)

- This equation allows us to calculate the wavelength associated with a moving particle when its kinetic energy is known, providing a direct connection between its wave-like behavior and energy. This is particularly useful for microscopic particles like electrons, where the wave nature is significant.

ii) de Broglie wavelength of an electron/proton accelerated by Potential Difference

- When an electron or proton is accelerated by a potential difference V , its kinetic energy increases due to the work done by the electric field. The de Broglie wavelength of the particle can be calculated using this kinetic energy.

- **Kinetic Energy from Potential Difference:** When a charged particle like an electron or proton is accelerated through a potential difference V , the kinetic energy ($K.E.$) gained by the particle is given by:

$$K.E. = qV \quad \dots(6)$$

where:

q is the charge of the particle.

For an electron, $q = -e$, and for a proton, $q = +e$, where e is the elementary charge, $e = 1.602 \times 10^{-19}$ C.

V is the potential difference.

- **De Broglie Wavelength Formula:** The de Broglie wavelength (λ) is given by the formula

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

where h is Planck's constant and p is the momentum of the particle.

- **Momentum of the Particle:** The momentum of the particle can be related to its kinetic energy.

$$\text{From the classical equation } K.E. = \frac{p^2}{2m},$$

$$\text{we can solve for the momentum } p = \sqrt{2mK.E.} \quad \dots(7)$$

Substituting the expression (6) for $K.E. = qV$,

$$\text{expression (7) can be written as: } p = \sqrt{2m \cdot qV} \quad \dots(8)$$

- **Final Formula for De Broglie Wavelength:**

Now substitute (8) in equation (1).

$$p = \sqrt{2m \cdot qV} \text{ into the de Broglie wavelength equation:}$$



$$\lambda = \frac{h}{\sqrt{2m \cdot qV}}$$

- The de Broglie wavelength of an electron or proton accelerated by a potential difference V is given by:

$$\lambda = \frac{h}{\sqrt{2m \cdot qV}} \quad \text{or} \quad \lambda = \frac{h}{\sqrt{2m \cdot eV}} \quad \dots(9)$$

where:

h is Planck's constant (6.626×10^{-34} Js),

m is the mass of the particle (electron or proton),

q is the charge of the particle (elementary charge e),

V is the potential difference in volts.

$$\text{For an electron; } \lambda = \frac{12.26}{\sqrt{V}} \text{ \AA} \quad \dots(10)$$

$$\text{For a proton; } \lambda = \frac{0.286}{\sqrt{V}} \text{ \AA} \quad \dots(11)$$

where:

m is the mass of the particle (for an electron, $m_e = 9.11 \times 10^{-31}$ kg; for a proton, $m_p = 1.67 \times 10^{-27}$ kg).

- This formula allows us to calculate the wavelength associated with the particle after being accelerated by a potential difference, highlighting the wave nature of matter in motion.

6. Properties of matter waves

- Wavelength of matter wave; $\lambda = \frac{h}{mv}$
- Wavelength is inversely proportional to the mass of particle $\lambda \propto \frac{1}{m}$; As $m \downarrow$ (lighter particle) $\rightarrow \lambda \uparrow$.
- Wavelength is inversely proportional to the velocity of particle $\lambda \propto \frac{1}{v}$; As $v \downarrow$ (particle velocity) $\rightarrow \lambda \uparrow$.
- If $v = \infty$; $\lambda = 0 \rightarrow$ infinite velocity for matter waves.
- If $v = 0$; $\lambda = \infty \rightarrow$ finite velocity for matter waves.
- Matter waves are produced by the motion of the particles and are independent of the charge, hence they are neither electromagnetic nor acoustic waves.
- They can travel through vacuum and do not require any material medium for their propagation.
- The smaller the velocity of the particle, the longer is the wavelength of the matter waves associated with it.
- The lighter the particle, the longer is the wavelength of the matter wave associated with it.
- The velocity of matter waves depends on the velocity of the material particle and is not a constant quantity.
- The velocity of matter waves is greater than the velocity of light.
- They exhibit diffraction phenomenon as any other waves.

- Properties of Matter Waves (Expanded)

- Wavelength and Mass:

- Wavelength is inversely proportional to the mass of the particle:

- According to de Broglie's relation, the de Broglie wavelength (λ) is given by:

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

where: h is Planck's constant, m is the mass of the particle, v is the velocity of the particle.

- From this equation, we can see that the wavelength of matter waves is inversely proportional to the mass of the particle. For lighter particles, the wavelength is longer, while for heavier particles, the wavelength is shorter. For example, an electron (which has a very small mass) will have a much larger de Broglie wavelength than a proton or a macroscopic object moving with the same velocity.

- Wavelength and Velocity:

Wavelength is inversely proportional to the velocity of the particle:

Since, the wavelength of matter waves decreases as the velocity of the particle increases. Therefore, the faster the particle moves, the shorter the wavelength associated with its matter wave. For very fast particles (high velocities), the de Broglie wavelength becomes extremely small, making the wave-like behavior harder to observe.

- Extreme Case of Infinite Velocity:

As the velocity of the particle approaches infinity, the de Broglie wavelength approaches zero. In this case, the particle's wave-like nature becomes negligible. This suggests that at extremely high speeds, the classical particle behavior dominates over the wave behavior.

- Finite Velocity of Matter Waves:

Even though the de Broglie wavelength depends on the velocity of the particle, it is important to note that the velocity of the matter waves is not a constant quantity. The velocity of matter waves is tied to the velocity of the particle itself. Therefore, the velocity of matter waves will change as the velocity of the particle changes.

- Independence from Charge:

Matter waves are produced by the motion of all particles, regardless of whether they are charged or neutral. Unlike electromagnetic waves, which require oscillating electric and magnetic fields, matter waves are not affected by charge. Hence, matter waves are not electromagnetic waves. Also, they are not acoustic waves (mechanical waves), since they do not require a medium to propagate.

- Travel Through Vacuum:

Unlike mechanical waves, which require a material medium for propagation (like sound waves in air or water waves), matter waves can travel through a vacuum. This property makes them fundamentally different from acoustic waves and also emphasizes their quantum mechanical nature.

- Effect of Particle Velocity on Wavelength:

The smaller the velocity of the particle, the longer the wavelength: As the velocity of a particle decreases, its de Broglie wavelength increases. This means that at very low velocities, the particle's wave-like behavior becomes more significant, and phenomena such as diffraction become more pronounced.

The lighter the particle, the longer the wavelength: Since de Broglie wavelength is inversely proportional to mass, lighter particles such as electrons exhibit much longer wavelengths compared to heavier particles, such as protons or neutrons, for the same velocity.

- Velocity of Matter Waves vs. Speed of Light:

The velocity of matter waves is not constrained by the speed of light. In fact, the velocity of matter waves can exceed the speed of light. This is in line with quantum mechanics, where particles can exhibit wave-like behavior without being limited by relativistic constraints. However, this does not violate relativity, as the information or energy carried by the matter wave still cannot travel faster than the speed of light.

- Diffraction Phenomenon:

Matter waves exhibit diffraction, a fundamental property of waves. This occurs when matter waves pass through slits or around obstacles, and they spread out, forming interference patterns. This phenomenon is similar to how light waves diffract and interfere, further supporting the wave-particle duality and confirming the wave nature of matter.

- These properties illustrate the wave-particle duality of matter and are fundamental to understanding quantum mechanics, with profound implications in fields such as electron microscopy, quantum tunneling, and atomic structure.

7. Concept of Wave Packet

- In quantum mechanics, a wave packet is a superposition of several waves with different wavelengths or frequencies, creating a localized wave that can represent a particle. A wave packet is typically used to describe a particle in motion, where the center of the wave packet moves with the particle's velocity.

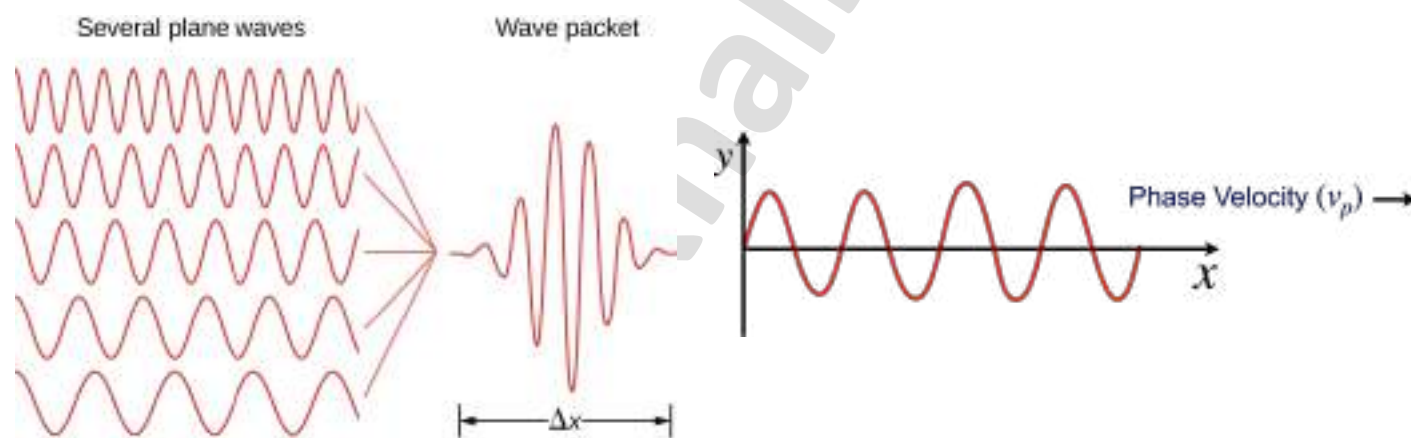


Fig. 3: Wave packet and Phase velocity

- The wave packet can be described using two important concepts: phase velocity and group velocity.

- Phase Velocity (v_p)

- The phase velocity (v_p) is the velocity at which the phase of a single wave propagates. It is defined as the velocity at which the crest (or any specific point) of a wave moves. For a single wave with a definite wavelength (λ) and frequency (f), the phase velocity is given by:

$$v_p = \frac{\omega}{k} \quad \dots(12)$$

where: v_p = phase velocity,

$$\omega = \text{angular frequency, } \omega = 2\pi f, \quad \dots(13)$$

$$k = \text{wave number, } k = \frac{2\pi}{\lambda}. \quad \dots(14)$$

- Alternatively, using the relationship between angular frequency and wave number;

$$v_p = \frac{f}{k} \quad \dots(15)$$

- Phase Velocity Interpretation:

- The phase velocity is the speed at which the phase of the wave (e.g., the crest) moves.
- For matter waves, the phase velocity does not correspond to the velocity of the particle associated with the wave packet.
- The phase velocity can be greater than the speed of light in certain situations, but this does not violate relativity because it does not carry information or energy.

- Group Velocity

- The group velocity (v_g) represents the velocity at which the overall shape of the wave packet (or the modulation) propagates. It is the velocity of the envelope of the wave packet, which can be interpreted as the velocity of the particle that the wave packet represents. The group velocity is particularly important in the context of wave packets because it determines the velocity of information and energy transfer.

The group velocity is given by:

$$v_g = \frac{d\omega}{dk} \quad \dots(16)$$

where:

v_g = group velocity,

ω = angular frequency,

k = wave number.

- Relation Between Phase and Group Velocity

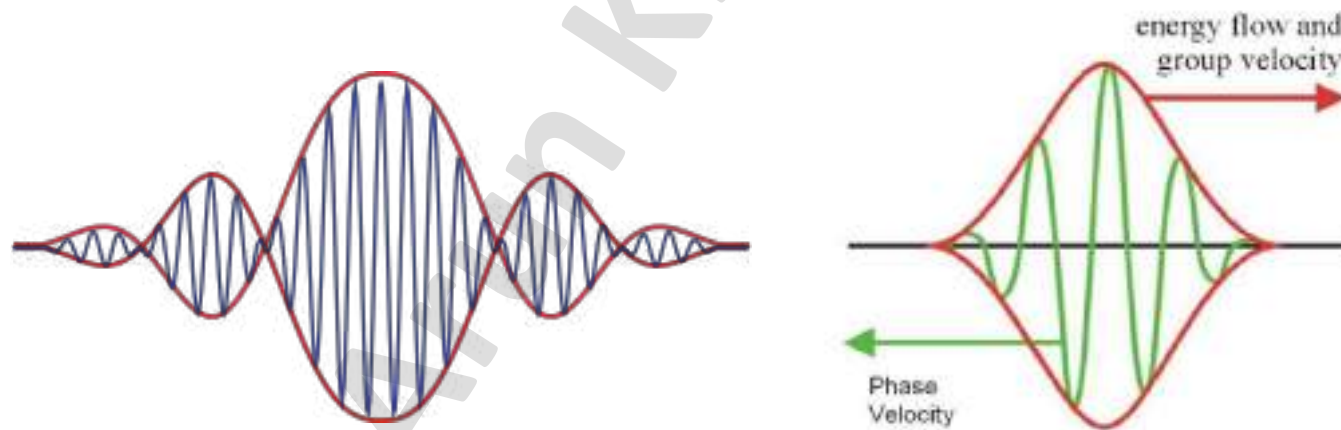


Fig. 4: Phase velocity and Group velocity

- The phase velocity refers to the speed of the individual components of the wave.
- The group velocity refers to the speed at which the overall wave packet (representing the particle) propagates.
- In many cases, the group velocity is associated with the velocity of the particle, while the phase velocity is not directly related to the particle's velocity.

- Group Velocity Interpretation

- Group velocity represents the velocity of the packet's energy or information, and it is generally more physically relevant in describing the motion of a particle.
- In a dispersive medium, the phase velocity and group velocity may not be the same. The group velocity is often the velocity at which the energy of the wave packet propagates.

- Example of the Relationship Between Phase and Group Velocity

- Let's say a wave packet is made of waves with different frequencies and wavelengths. Each component wave will have a different phase velocity. However, the overall wave packet will travel with a velocity determined by the group velocity.
- If the dispersion relation $\omega(k)$ is known (i.e., how the angular frequency depends on the wave number), the group velocity can be derived by differentiating the dispersion relation with respect to k .
- For instance, if the relation between $\omega = Ak^2$, where A is a constant, the phase velocity and group velocity would be:

Phase velocity:

$$v_p = \frac{\omega}{k} = Ak$$

Group velocity:

$$v_g = \frac{d\omega}{dk} = 2Ak$$

- Thus, the group velocity and phase velocity would depend on the wave number k in different ways.
- Phase Velocity (v_p): The velocity of the phase of the wave, given by $v_p = \frac{\omega}{k}$. It can exceed the speed of light but does not carry energy or information.
- Group Velocity (v_g): The velocity of the wave packet (envelope) or the velocity of information/energy transfer, given by $v_g = \frac{d\omega}{dk}$. It is typically the velocity associated with the particle represented by the wave packet.
- The concepts of phase velocity and group velocity are essential in understanding the propagation of wave packets in quantum mechanics. While the phase velocity describes the motion of individual components of the wave, the group velocity represents the motion of the entire wave packet and is often related to the particle's motion. These concepts are crucial in understanding phenomena such as dispersion and the behavior of quantum particles.

8. Heisenberg's Uncertainty Principle

- The Heisenberg Uncertainty Principle is one of the cornerstone concepts of quantum mechanics. It asserts that it is fundamentally impossible to precisely measure certain pairs of physical properties of a particle, such as its position and momentum, simultaneously. This principle was introduced by the German physicist Werner Heisenberg in 1927 and has profound implications on our understanding of the quantum world.

- Statement of the Uncertainty Principle

The uncertainty principle states that there is a fundamental limit to how accurately we can measure certain pairs of quantum variables. The most common pair is position (x) and momentum (p) of a particle. The uncertainty principle can be expressed mathematically as:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} \quad \dots(17)$$

where:

Δx is the uncertainty in the position,

Δp is the uncertainty in the momentum,

\hbar is the reduced Planck's constant ($\hbar = \frac{h}{2\pi}$, where h is Planck's constant).

- This equation indicates that the more precisely the position of a particle is measured (Δx is small), the less precisely its momentum can be known (Δp is large), and vice versa.

- Implications of Heisenberg's Uncertainty Principle

- **Measurement Limits:** The uncertainty principle asserts that certain pairs of physical quantities, like position and momentum, cannot be simultaneously measured with infinite precision. This is not due to experimental limitations but rather is a fundamental property of nature at microscopic scales.
- **Quantum Nature:** This principle is crucial for understanding the behavior of particles at the quantum level. While it can be ignored in the macroscopic world (e.g., everyday objects), it holds significant importance in the quantum world of atoms and subatomic particles.
- **Wave-Particle Duality:** The principle is intimately connected with the wave-particle duality of matter. Since particles such as electrons also exhibit wave-like properties, their precise position and momentum cannot both be defined exactly at the same time. This is because waves have a spread-out nature, and attempting to pinpoint the exact position of a wave-like particle disturbs its momentum.
- **Energy-Time Uncertainty:** The uncertainty principle also extends to the energy-time uncertainty relation, which states that it is impossible to measure the energy of a system exactly over a finite time period. This is expressed as:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2} \quad \dots(18)$$

where,

ΔE is the uncertainty in energy and

Δt is the uncertainty in time.

This relation implies that for processes occurring in a very short time, the uncertainty in energy is large.

- Simultaneous Measurements:

In quantum mechanics, the simultaneous measurement of certain properties (like position and momentum) leads to uncertainties in the values, such that their product cannot be smaller than a certain constant. This means that there is a limit to how accurately we can know both properties at the same time. For example, if the uncertainty in the position measurement is extremely small, the uncertainty in momentum measurement must be large, and vice versa.

- Physical Interpretation

- The uncertainty principle emphasizes the intrinsic uncertainty or "fuzziness" in the quantum world. It suggests that quantum objects, such as electrons, cannot be precisely pinpointed in terms of both position and momentum simultaneously. This is in stark contrast to classical mechanics, where such measurements could be made with arbitrary precision.
- The principle also suggests that the very act of measurement can disturb the system being measured. For instance, trying to measure the position of an electron with great accuracy inevitably disturbs its momentum, introducing uncertainty.

- Practical Examples

- **Electron in an Atom:** For an electron bound in an atom, the Heisenberg uncertainty principle explains why electrons do not collapse into the nucleus. If we were able to determine the electron's position precisely (close



to the nucleus), the uncertainty in its momentum would become so large that the electron would have extremely high velocity, making it impossible for the electron to remain in a stable orbit.

- Microscopic Particles: At the quantum scale, microscopic particles like electrons, protons, and neutrons exhibit wave-like properties. When we try to measure their position or momentum, we are constrained by the uncertainty principle, meaning we cannot have both values with high precision at the same time.
- Particle Accelerators: In particle accelerators, scientists can measure particles' position and momentum with high precision. However, even in these advanced experiments, the uncertainty principle imposes a limit on how well both quantities can be known simultaneously, especially for particles at high velocities.
- The Heisenberg Uncertainty Principle is a fundamental concept that reflects the limitations of our knowledge about quantum systems. It challenges our classical understanding of determinism and introduces a probabilistic framework where uncertainties are inherent in the measurements of certain pairs of properties like position and momentum. This principle has far-reaching consequences in various fields of physics, particularly in quantum mechanics, and has altered the way we view the behavior of particles at microscopic scales.

9. Introduction to Quantum Mechanics

- Quantum mechanics addresses the complex nature of light and matter at the atomic and subatomic levels. Light, which exhibits both particle and wave properties, posed a mystery that classical physics could not resolve.
- Quantum mechanics provides the theoretical framework to solve this dilemma, establishing the concept of wave-particle duality. To understand quantum phenomena, knowledge of Bohr's atomic theory, wave motion, and de Broglie's hypothesis is essential.
- De Broglie proposed that particles such as electrons exhibit wave-like characteristics, which led Erwin Schrödinger to develop the **Schrödinger wave equation**. This equation forms the cornerstone of quantum mechanics, offering a way to describe how matter behaves and interacts with energy on a microscopic scale.
- One of the fundamental principles of quantum mechanics is that electrons are not just particles, but also waves. At its core, quantum mechanics suggests that it is impossible to precisely determine the exact location of an electron. Instead, we can only calculate the probability of finding the electron in a certain region of space at any given time.

10. A wave function

- A wave function in quantum physics is a fundamental mathematical concept that describes the quantum state of an isolated system.
- It encapsulates all the information about a system's state, such as the position, momentum, and energy of particles. The wave function is a complex-valued probability amplitude, meaning it represents the likelihood of different outcomes for various measurements made on the system. The square of the absolute value of the wave function gives the probability density of finding a particle in a particular state or location.
- In most cases, the wave function is denoted by the Greek letters ψ (psi) for the lowercase version and Ψ (Psi) for the uppercase version. These symbols are used to represent the wave function in both the position and momentum representations. The wave function depends on the degrees of freedom of the system, corresponding to a set of commuting observables, which are quantities that can be simultaneously measured without interfering with each other (like position and momentum in specific cases).
- Once the appropriate representation for the system is chosen, the wave function can be derived from the quantum state. This allows physicists to calculate the probabilities of possible measurement outcomes, providing a statistical description of the system's behavior.

- Thus, the wave function plays a central role in predicting the behavior of quantum systems and understanding phenomena such as interference, superposition, and quantization.

11. Interpretation of wave function Ψ

- The interpretation of the wave function (Ψ) in quantum mechanics plays a crucial role in understanding the behavior of matter at the microscopic level. Matter waves, associated with particles like electrons, do not behave like electromagnetic or sound waves. Rather, they represent a fundamental concept of wave-like behavior in particles, although the exact physical quantity responsible for generating matter waves remains unclear.
- To mathematically describe these waves, Erwin Schrödinger introduced the wave function Ψ , which mathematically represents the oscillations of these matter waves. The wave function is a function of both position and time, providing a comprehensive description of a quantum system's state.
- The magnitude of the wave function is associated with the probability of finding a particle in a specific location at a given time.
- The square of the amplitude of the wave function ($|\Psi|^2$) gives the probability density, which means that regions where the amplitude is larger correspond to a higher likelihood of finding the particle.
- Therefore, the greater the amplitude of Ψ , the higher the probability of locating the particle at that particular point in space and time.
- However, since the wave function can take on both positive and negative values, care must be taken when interpreting its amplitude. A negative amplitude could imply a negative probability, which is physically meaningless.
- To resolve this, the probability is derived from the square of the wave function's magnitude, ensuring that the probability remains a positive real number.
- Thus, the wave function is central to quantum mechanics because it encapsulates the probabilistic nature of quantum systems, providing valuable insight into the likelihood of various outcomes in a given system.

i) Ψ represents the wave as a function of position and time.

- Greater is the amplitude of wave function Ψ , higher is the probability of finding the particle at that position and time.
- Amplitude can be positive or negative.
- The negative amplitude gives rise to negative probability which is meaningless.
- Ψ is complex but $|\Psi|^2 = \Psi\Psi^*$ is always real and positive.
- $|\Psi|^2$ can have any value between 0 and 1.
- $|\Psi|^2 = 0$ particle is absent, $|\Psi|^2 = 1$ particle is present.
- $|\Psi|^2$ represent probability density.

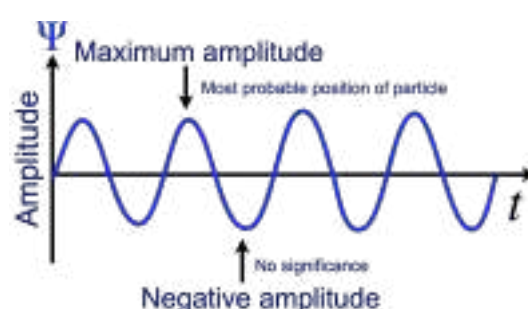


Fig. 5: Wave as a function of position and time

ii) Probability interpretation of wave function Ψ

- A probability interpretation of the wave function was given by Max Born. Born's probability interpretation claims that the probability density that a particle will be found is equal to the square of the absolute value of the wave function. Namely, the probability that the particle will be found in the small volume dV shown in Fig.6.
- Here, the word, "probability" was used this however does not mean that the particle, e.g. an electron, exists in a form of a "particle" or "corpuscle" and this particle moves in accordance with the degree of probability. An electron is neither mere "particle" nor mere "wave". An electron exists with particle-wave duality. The word "probability" used above denotes the chance that the particle will be found in the volume dV when it is detected.

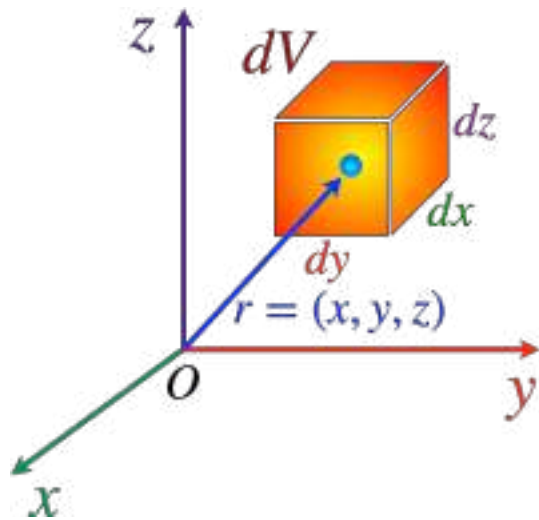


Fig. 6: A particle in a volume

- Suppose a small volume (box) $dV = dx dy dz$ with three edges of dx , dy and dz at a coordinate point $r = (x, y, z)$ in a three-dimensional space. Let the probability that a particle will be found in this volume at a time t be $P(x, y, z, t) dx dy dz$.
- The function $P(x, y, z, t)$ is considered as the probability in the unit volume in the neighborhood of the point (x, y, z) , and is sometimes called the *probability density*.

iii) $|\Psi|^2$ is known as probability density and Ψ is the probability amplitude.

- The probability interpretation of the wave function is a fundamental concept in quantum mechanics, largely introduced by Max Born. It provides a statistical framework for understanding the behavior of particles at the microscopic level. In quantum mechanics, the wave function Ψ (psi) represents the state of a particle or system, but it does not directly give the position or momentum of a particle. Instead, the square of the magnitude of the wave function ($|\Psi|^2$) provides the probability density for finding a particle at a particular location and time. This interpretation fundamentally departs from classical physics, where particles are considered to have well-defined positions and velocities.

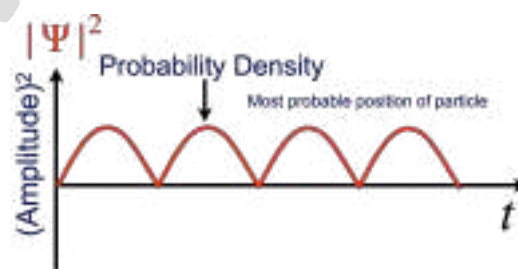


Fig. 7: Probability density

- The wave function $\Psi(x, t)$ is a complex-valued function that depends on both position (x) and time (t). The square of the magnitude of the wave function $|\Psi(x, t)|^2$ gives the probability density of finding a particle at position x at a particular time t . This means that $|\Psi(x, t)|^2$ is not the probability itself, but the probability density, meaning it must be integrated over a region of space to obtain the actual probability of finding the particle in that region. The square of the magnitude of a wave function $|\Psi|^2$ gives the probability of finding the particle in that region. The probability P of finding the particle in an infinitesimal volume $dV = dx, dy, dz$ is given by ;

$$P \propto |\Psi(x, y, z)|^2 dV \quad \dots(19)$$

Since the particle is certainly somewhere in the space, the probability $P = 1$.

- Normalization:

- The total probability of finding the particle somewhere in space must equal 1. This requirement means that the wave function must be normalized so that:

- The probability,

$$\int_{-\infty}^{+\infty} |\Psi|^2 dV = 1 \quad \dots(20)$$

- This ensures that the particle must be somewhere in space, as the probability of finding it anywhere in the entire universe is 100%.
- The wave function Ψ is in general a complex function. But the probability must be real.
- Therefore, Ψ is multiplied by its complex conjugate Ψ^* . Thus,

$$\int_{-\infty}^{+\infty} \Psi \cdot \Psi^* dV = 1 \quad \dots(21)$$

- Thus although Ψ has no physical significance but $|\Psi|^2$ gives the probability density of the particle i.e. probability of finding the atomic particle in a particular region.
- Probability density is represented by;

$$|\Psi(x, y, z)|^2 dV = \text{Probability density,}$$

The **normalisation condition** implies that the sum of the probabilities over all values of x, y, z must be unity;

$$\iiint_{-\infty}^{+\infty} |\Psi|^2 dx dy dz = 1 \quad \dots(22)$$

Whenever the wave functions are normalised, $|\Psi|^2 dV$ equals the probability that a particle will be found in an elemental volume dV .

12. Conditions to be satisfied by wave function

- The wave function (Ψ) in quantum mechanics must satisfy certain conditions to be physically meaningful and mathematically consistent. These conditions ensure that the wave function accurately describes the quantum system and allows valid predictions of measurable quantities. The key conditions are as follows:

- Single-Valued:

The wave function Ψ must be single-valued at any given point in space and time.

This means that for any position x , the wave function must have only one value.

This ensures that the probability density $|\Psi(x, t)|^2$ is well-defined.

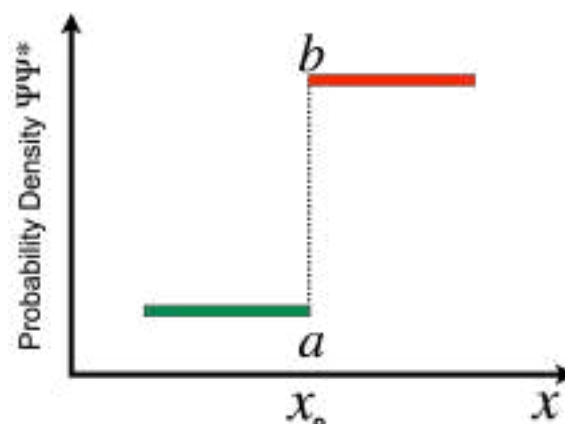


Fig. 8: Wave function as a single-valued

- Continuous:

The wave function Ψ and its space derivatives $\frac{\partial \Psi}{\partial x}$, $\frac{\partial \Psi}{\partial y}$ and $\frac{\partial \Psi}{\partial z}$ should be continuous across any boundary.

Discontinuities in the wave function or its derivative would result in undefined probabilities or unphysical behaviour.

This condition ensures smooth variations of the wave function and is necessary for the validity of Schrödinger's equation.

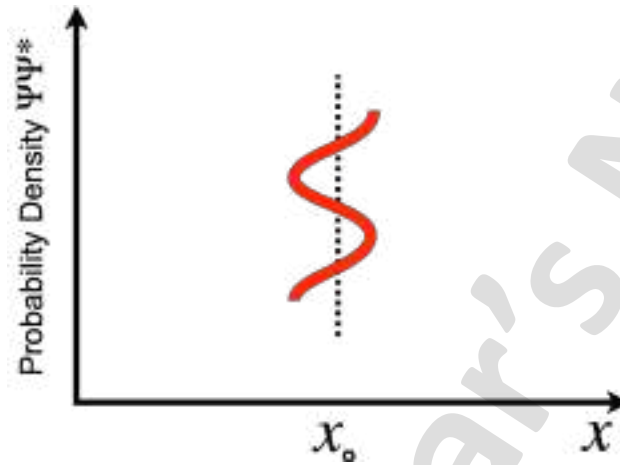


Fig. 9: Variation of a wave function

- Finite:

The wave function Ψ must be finite everywhere in space.

Even if $x \rightarrow \infty$ or $-\infty$, $y \rightarrow \infty$ or $-\infty$, $z \rightarrow \infty$ or $-\infty$, the wave function should not tend to infinity.

It must remain finite for all values of x, y, z .

Infinite values of the wave function are physically meaningless, as they would imply an infinite probability density.

- Normalizable:

The wave function Ψ must be normalizable, meaning the total probability of finding the particle anywhere in space must equal 1. Mathematically, this is expressed as:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$$

If the wave function is not normalizable, it cannot represent a physical state.

- Square Integrable:

The wave function $|\Psi(x, t)|^2$ must be integrable over all space, meaning the integral of its square over the entire domain must converge to a finite value:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx < \infty$$

This ensures that the probability density is finite and well-defined.

- Boundary Conditions:

The wave function must satisfy the boundary conditions imposed by the physical system.

For example: In a particle-in-a-box problem, the wave function must be zero at the boundaries of the box because the particle cannot exist outside it. In infinite potential wells, the wave function vanishes at the boundaries where the potential is infinite.

- Physical Constraints:

The wave function must correspond to the specific constraints of the quantum system it describes.

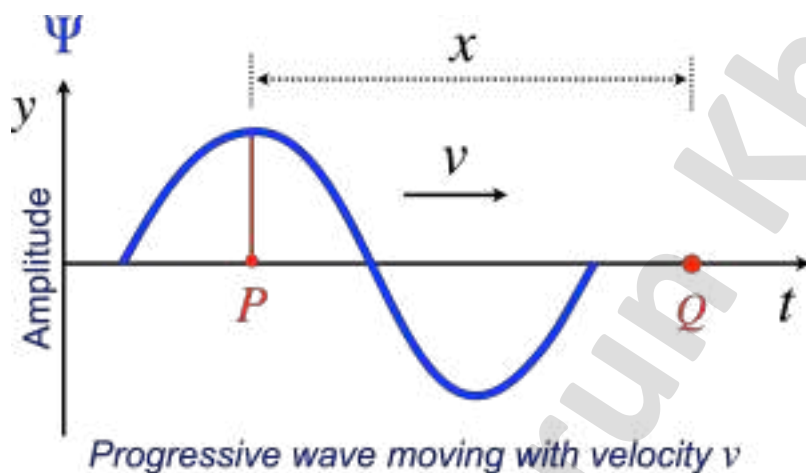
For instance: It must respect the symmetry of the problem (e.g., symmetric or antisymmetric wave functions for bosons and fermions, respectively).

In bound states, the wave function must decay to zero as $x \rightarrow \pm \infty$ ensuring the particle is localized.

- These conditions ensure that the wave function is physically meaningful, mathematically consistent, and capable of describing a quantum system accurately. If any of these conditions are violated, the wave function cannot represent a valid quantum state.

13. Schrödinger's Time-Independent Equation

- The Schrödinger time-independent equation is a key mathematical formulation in quantum mechanics that describes the quantum state of a system in a stationary energy state. It is used to determine the allowed energy levels and the corresponding wave functions for a particle in a given potential field.
- Schrödinger developed wave equations for the matter waves that are associated with a moving particle. They are basically a linear partial differential equation developed to understand the nature of matter waves in a quantum-mechanical system.
- Schrödinger's equation defines the wave properties of sub atomic particles and also predicts particle-like behaviour. They predict the future behaviour of a dynamic system.



Consider the wave is propagating forward with velocity v . If P is the origin of the wave, then the particle at Q at a distance x from P will receive the wave x/v seconds later that P did as shown in figure. When mechanical wave passes through a medium, the medium particle performs simple harmonic motion (S.H.M.) given by equation;

$$y = A \cdot \cos \cdot \omega t \quad \dots(23)$$

Fig. 10: A progressive wave

Where; A is amplitude of the oscillation and $\omega = 2\pi\nu$ where ν is frequency.

The displacement of wave at time t and distance x from the origin will be;

$$y = A \cos \left(\omega \left(t - \frac{x}{v} \right) \right) \quad \dots (24)$$

The general complex wave function is:

$$\psi = A e^{-i\omega(t - \frac{x}{v})}$$

Note:

For answer in examination, skip steps 1 to 5 and directly use equation 25.

Steps 1 to 5 are for your understanding only.



Let's solve this step by step and derive the wave equation from the given function.

Step 1: Given Wave Function

The displacement of wave at time t and distance x from the origin will be;

$$y = A \cos \left(\omega \left(t - \frac{x}{v} \right) \right)$$

where:

A is the amplitude,

ω is the angular frequency,

v is the velocity of the wave,

x is the spatial coordinate,

t is time.

Step 2: Compute the Second Time Derivative $\frac{d^2y}{dt^2}$

First, differentiate y with respect to t :

$$\frac{dy}{dt} = -A\omega \sin \omega \left(t - \frac{x}{v} \right)$$

Differentiate again to get the second derivative:

$$\frac{d^2y}{dt^2} = -A\omega^2 \cos \omega \left(t - \frac{x}{v} \right) \text{ Since } y = A \cos \omega \left(t - \frac{x}{v} \right), \text{ we get:}$$

$$\frac{d^2y}{dt^2} = -\omega^2 y$$

Step 3: Compute the Second Spatial Derivative $\frac{d^2y}{dx^2}$

Differentiate y with respect to x :

$$\frac{dy}{dx} = -A\omega \frac{1}{v} \sin \omega \left(t - \frac{x}{v} \right)$$

Differentiate again:

$$\frac{d^2y}{dx^2} = -A\omega^2 \frac{1}{v^2} \cos \omega \left(t - \frac{x}{v} \right)$$

Since $y = A \cos \omega \left(t - \frac{x}{v} \right)$, we get:

$$\frac{d^2y}{dx^2} = -\frac{\omega^2}{v^2} y$$

Step 4: Establish the Wave Equation

From the two second derivatives:

$$\frac{d^2y}{dt^2} = -\omega^2 y, \quad \frac{d^2y}{dx^2} = -\frac{\omega^2}{v^2} y \implies v^2 \frac{d^2y}{dx^2} = -\omega^2 y$$

$$\text{Equating both equations; } \frac{d^2y}{dt^2} = v^2 \frac{d^2y}{dx^2}$$

which is the fundamental wave equation.

Step 5: Expressing the Solution in Complex Form

The general complex wave function is:

$$\psi = A e^{-i\omega \left(t - \frac{x}{v} \right)}$$



To derive above the general complex wave function:

A typical harmonic wave propagating in the positive x -direction is given by:

$$y = A \cos \left(\omega \left(t - \frac{x}{v} \right) \right)$$

Instead of using trigonometric functions, we use,

Euler's formula: $e^{i\theta} = \cos \theta + i \sin \theta$ and its conjugate: $e^{-i\theta} = \cos \theta - i \sin \theta$

From Euler's formula:

$$\cos \theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

Thus, our real wave equation:

$$y = A \cos \left(\omega \left(t - \frac{x}{v} \right) \right) \text{ can be rewritten using complex exponentials as:}$$

$$y = \text{Re} \left(A e^{i\omega(t - \frac{x}{v})} \right)$$

where Re denotes taking the real part.

However, in many applications (especially in quantum mechanics and signal processing), it is convenient to work with the full complex form rather than just the real part. Thus, we consider:

$\psi = A e^{-i\omega(t - \frac{x}{v})}$ which is the general complex wave function.

This represents a traveling wave propagating in the positive x -direction.

Justification for the Negative Exponent

The choice of negative exponent in:

$\psi = A e^{-i\omega(t - \frac{x}{v})}$ is conventionally used for a forward-traveling wave.

- For a wave moving in the positive x -direction, the phase decreases with increasing x , which corresponds to $e^{-i\omega(t - x/v)}$.
- For a wave moving in the negative x -direction, the phase increases with x , which corresponds to $e^{-i\omega(t + x/v)}$

Thus $e^{-i\omega(t - \frac{x}{v})}$ correctly describes a wave propagating forward in the positive x -direction.

We differentiate $\psi = A e^{-i\omega(t - \frac{x}{v})}$ twice with respect to t

$$\frac{d\psi}{dt} = -i\omega A e^{-i\omega(t - \frac{x}{v})}$$

$$\frac{d^2\psi}{dt^2} = -\omega^2 A e^{-i\omega(t - \frac{x}{v})} = -\omega^2 \psi$$

Now, differentiating twice with respect to x :

$$\frac{d\psi}{dx} = -i\omega \frac{1}{v} A e^{-i\omega(t - \frac{x}{v})}$$

$$\frac{d^2\psi}{dx^2} = -\frac{\omega^2}{v^2} A e^{-i\omega(t - \frac{x}{v})} = -\frac{\omega^2}{v^2} \psi$$

Thus,

$$\frac{d^2\psi}{dt^2} = v^2 \frac{d^2\psi}{dx^2}$$

which confirms that ψ is a valid solution of the wave equation.

Thus, the solution to the wave equation is:

$$\psi = A e^{-i\omega(t - \frac{x}{v})} \quad \dots(24)$$



The wave equation of such wave is ; $\frac{d^2y}{dt^2} = v^2 \frac{d^2y}{dx^2}$ or $\frac{d^2\psi}{dt^2} = v^2 \frac{d^2\psi}{dx^2}$... (25)

The solution of equation (25) can be written as;

$$\psi = Ae^{-i\omega(t - \frac{x}{v})} \quad \dots (26)$$

a) Partial differential equation for wave function from equation

Let a wave function ψ is associated with matter waves. The wave function ψ depend on position coordinates x, y, z and time t . The differential equation for matter wave motion with wave function ψ and velocity v can be written as,

$$\frac{\partial^2\psi}{\partial t^2} = v^2 \left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} \right) \quad \dots (27)$$

This is a partial differential equation (PDE) because it involves partial derivatives of the function $\psi(x, y, z, t)$ with respect to multiple independent variables: time t and space coordinates x, y, z .

$$\frac{\partial^2\psi}{\partial t^2} = v^2 \nabla^2 \psi \quad \dots (28)$$

Where $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ is known as Laplace operator.

b) Differentiation of wave function ψ .

The wave function ψ can be expressed as a function of space (x, y, z) and time t as.

$$\psi(x, y, z, t) = \psi_0(x, y, z)e^{-i\omega t} \quad \text{or} \quad \text{simply } \psi = \psi_0 e^{-i\omega t} \quad \dots (29)$$

$$\text{Differentiating } \frac{\partial\psi}{\partial t} = \psi_0 e^{-i\omega t} (-i\omega)$$

Differentiating again

$$\frac{\partial^2\psi}{\partial t^2} = \psi_0 e^{-i\omega t} (-i\omega)^2$$

$$\text{or } \frac{\partial^2\psi}{\partial t^2} = -\omega^2 \psi_0 e^{-i\omega t}$$

From equation (29);

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2 \psi \quad \dots (30)$$

c) Differential equation for wave function ψ .

From equation (28) and (30)

$$v^2 \nabla^2 \psi = -\omega^2 \psi \quad \text{Dividing by } v^2;$$

$$\nabla^2 \psi = -\frac{\omega^2}{v^2} \psi$$

$$\nabla^2 \psi + \frac{\omega^2}{v^2} \psi = 0 \quad \text{Dividing by } v = \nu\lambda \text{ and } \omega = 2\pi\nu;$$

$$\nabla^2 \psi + \frac{(2\pi\nu)^2}{(\nu\lambda)^2} \psi = 0$$



$$\nabla^2 \psi + \frac{4\pi^2 \nu^2}{\lambda^2} \psi = 0$$

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0 \quad \text{Substituting } \lambda = \frac{h}{mv};$$

$$\nabla^2 \psi + \frac{4\pi^2}{\left(\frac{h}{mv}\right)^2} \psi = 0$$

$$\therefore \nabla^2 \psi + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad \dots(31)$$

d) Total energy (E) of particle.

Now, the total energy of particle E, is the sum of kinetic energy K.E. and potential energy (P.E.), hence;

$$E = KE + PE$$

$$E = \frac{1}{2}mv^2 + V$$

$$2E = mv^2 + 2V$$

$$mv^2 = 2E - 2V$$

$$mv^2 = 2(E - V)$$

Multiplying by m;

$$m^2 v^2 = 2m(E - V) \quad \dots(32)$$

e) Schrödinger's time-independent equation

Substituting the value of the total energy of the particle E from equation (32) into equation (31);

$$\therefore \nabla^2 \psi + \frac{4\pi^2 2m(E - V)}{h^2} \psi = 0$$

$$\therefore \nabla^2 \psi + 2m \left(\frac{4\pi^2}{h^2} \right) (E - V) \psi = 0$$

$$\therefore \nabla^2 \psi + \frac{2m(E - V)}{\left(\frac{h}{2\pi}\right)^2} \psi = 0$$

Now, $\hbar = \frac{h}{2\pi}$ is known as reduced **Plank's constant**, hence,

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad \dots(33)$$

This is known as **Schrödinger's time independent equation**.

The wave function ψ and Laplace operator $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ depends on space coordinates x, y, z

and does not depend on time.

14. Particle in infinite potential well (rigid box)

- The infinite potential well, also known as the rigid box is a classic example in quantum mechanics used to illustrate the quantization of energy levels. It describes a particle confined in a one-dimensional box where the potential is infinite outside the box and zero inside the box.

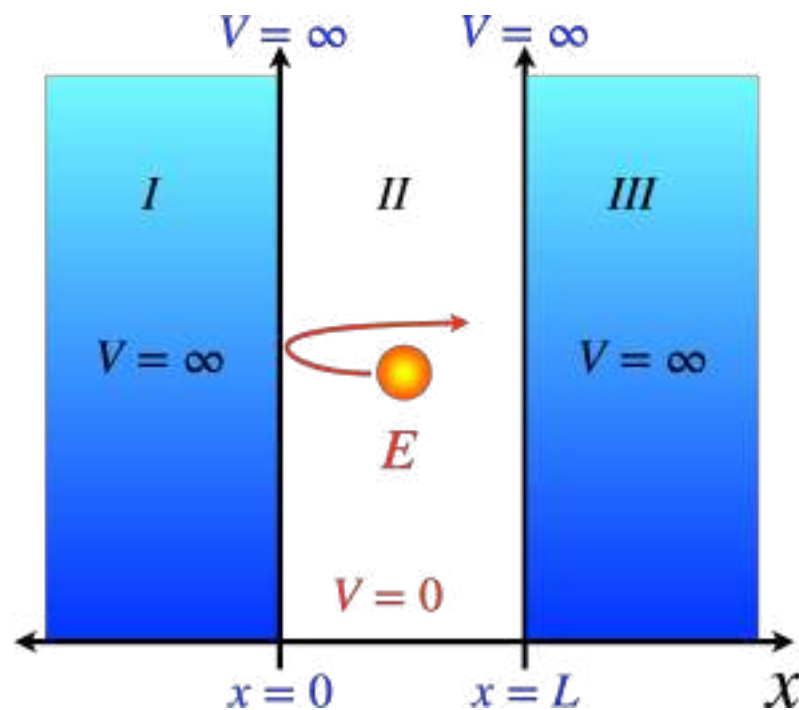


Fig. 11: Particle in infinite potential well

- Consider a particle is enclosed in a potential well of rigid box having infinite potential,
 $\therefore V = \infty$.
- Inside the box motion of particle is restricted between $x = 0$ and $x = L$.
- Assuming the collision of the particle with walls as elastic, total energy of the particle E remains constant.
- The potential energy of the particle is infinite outside the box and it can be considered as zero inside the box
 $\therefore V = 0$.
- Thus, the boundary conditions for potential energy are
- $V(x) = 0$ for $0 < x < L$
- $V(x) = \infty$ for $x \leq 0$ and $x \geq L$ (otherwise)

- Hence potential energy function $V(x)$ is defined as:

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty, & \text{otherwise} \end{cases}$$

Where: L is the width of the well,

$V(x) = \infty$ outside the well confines the particle to $0 \leq x \leq L$.

- The wave function is associated with the particle. As particle cannot leave the box, hence its probability outside the box is zero. Thus, boundary conditions for wave function are:

$$\psi(x) = 0 \text{ for } x \leq 0 \text{ and } \psi(x) = 0 \text{ for } x \geq L.$$

- To find out the wave function of the particle inside the box, we have to apply Schrödinger's time independent equation.

- Step I: Schrödinger's Time-Independent Equation

Schrödinger's time independent equation is;

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad \dots(34)$$

Let, Laplacian operator is; $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$

As particle is moving in one-dimension along x -axis, y and z coordinates are zero; T

hus, $y = 0$, $z = 0$, and

Laplace's operator is; $\nabla^2 = \frac{\partial^2}{\partial x^2}$



Equation (34) thus reduces to ; $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$.

Inside the box, potential energy of particle $V = 0$; hence $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$... (35)

Let assume; $\frac{2mE}{\hbar^2} = k^2$... (36)

Thus equation (35) reduces to; $\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$... (37)

Using the D-Operator Method:

Consider, $D = \frac{\partial}{\partial x}$, Squaring, $\therefore D^2 = \frac{\partial^2}{\partial x^2}$; Equation (37) becomes;

$$\therefore D^2 \psi + k^2 \psi = 0$$

$$\therefore (D + k)^2 \psi = 0 \text{ This is homogeneous differential equation.}$$

Consider, $D^2 + k^2 = 0$

$$\therefore D^2 = -k^2$$

$$\therefore D = \pm ik$$

Thus, the general solution is:

Equation (37) is a second order differential equation. Its general solution can be written as;

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \dots (38)$$

where; A and B are constants.

Step II : Apply Boundary Conditions:

The wavefunction must vanish at the boundaries $x = 0$ and $x = L$, i.e.,

$$\psi(0) = 0 \quad \text{and} \quad \psi(L) = 0$$

Condition at $x=0$:

$$\psi(0) = Ae^{i(0)} + Be^{-i(0)} = A + B = 0$$

which gives:

$$B = -A$$

Thus, the wavefunction simplifies to $B = -Ae^{-ikx}$ hence equation (38) can be written as,

$$\psi(x) = Ae^{ikx} - Ae^{-ikx}$$

$$\therefore \psi(x) = A(e^{ikx} - e^{-ikx})$$

Using Euler's formula,

$$e^{ikx} - e^{-ikx} = 2i \sin(kx)$$

so the wavefunction takes the form:

$$\psi(x) = C \sin(kx) \quad \dots (39)$$

where, $C = 2iA$ is a constant.

**Condition at $x=L$:**

$$\psi(L) = C \sin(kL) = 0$$

For a nontrivial solution ($C \neq 0$), we must have:

$$\sin(kL) = 0$$

which implies:

$$kL = n\pi, \quad n = 1, 2, 3, \dots$$

Thus,

$$k = \frac{n\pi}{L} \quad \dots(40)$$

Step III: Obtain the Energy Expression

From equation (36):

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{Substituting equation (40)}$$

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE}{\hbar^2}$$

Solving for

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

Using $\hbar = \frac{h}{2\pi}$, so that $\hbar^2 = \frac{h^2}{4\pi^2}$, we get:

$$E_n = \frac{n^2 h^2}{8mL^2}$$

Conclusion

Thus, using the D-operator method, we have derived the energy levels of a particle in an infinite potential well:

$$E_n = \frac{n^2 h^2}{8mL^2}, \quad n = 1, 2, 3, \dots \quad \dots(41)$$

These discrete energy levels indicate the quantization of energy in a rigid box.

- Important points:

- Energy Quantization: The energy levels depend on n^2 , meaning higher quantum numbers correspond to higher energies.
- Zero-Point Energy: The lowest energy state ($n = 1$) has a finite energy:

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad \text{This is due to quantum confinement.}$$

- Wave-Particle Duality: The particle's behavior is described by wave functions, meaning it doesn't have a fixed position but a probability distribution.
- This model is fundamental in quantum mechanics, explaining quantum confinement in nanotechnology, semiconductors, and quantum dots.

- Energy levels of particle in infinite potential well (rigid box)

- As n is integer, from above it is clear that the particle inside an infinite potential well can have only certain discrete values of energies. However, the minimum value of energy can never be zero as $n \neq 0$. These values of energies are known as energy eigen values.

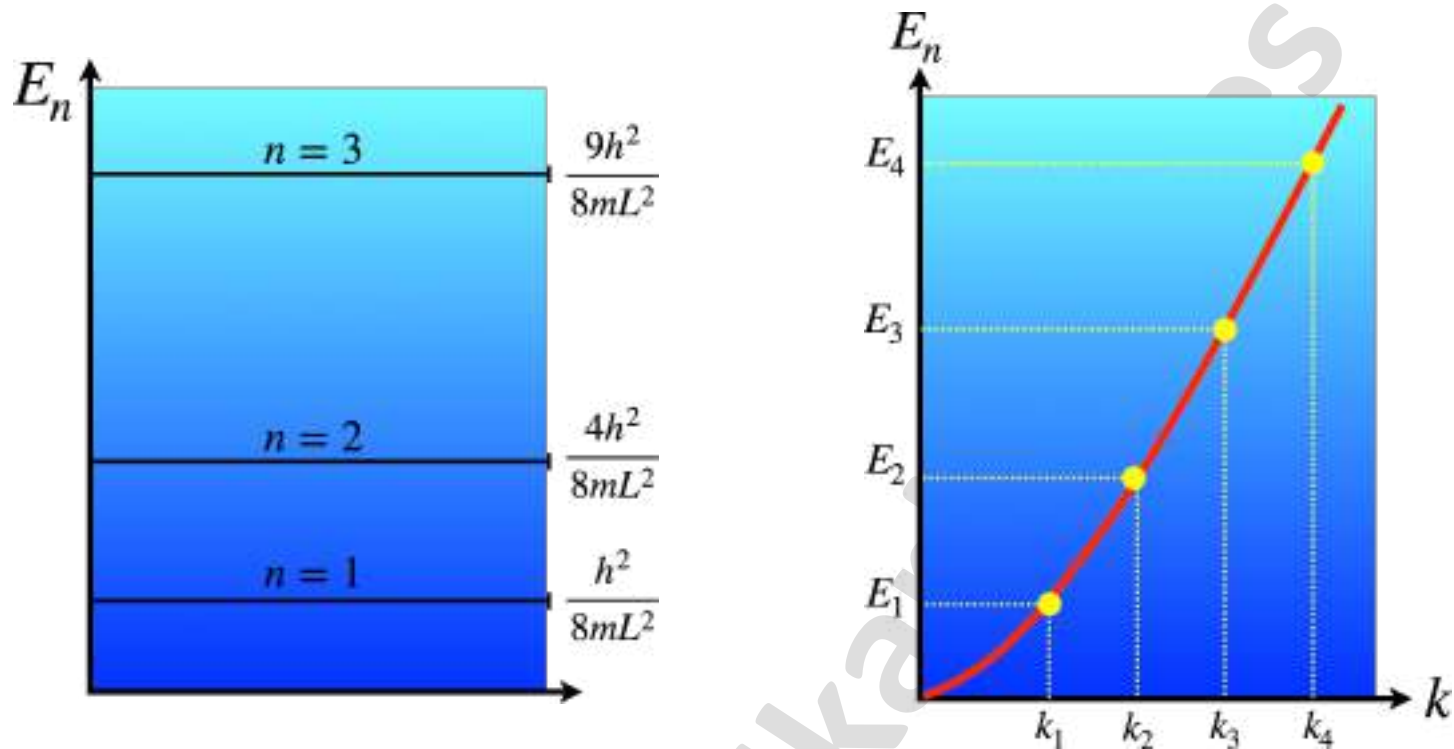


Fig. 12 : Energy levels of particle in infinite potential well (rigid box)

- E_1, E_2, E_3 and E_4 are energy states. K_1, K_2, K_3 and K_4 are wave numbers. The energy of a particle in a box (yellow circles) and a free particle (red line) both depend upon wavenumber in the same way. However, the particle in a box may only have certain, discrete energy levels.

- Step-IV: Wave function of particle inside the box

From equation (39), the wave function ψ of the particle inside the rigid box is given by;

$$\psi(x) = A \sin kx.$$

In the equation, $kL = n\pi$, where, $n = 1, 2, 3, \dots$ and $n \neq 0$ as it may lead to either,

$$\text{Thus; } k = \frac{n\pi}{L};$$

$$\psi(x) = A \sin \frac{n\pi}{L}x \quad \dots(42)$$

- Thus for each energy value E_n , there is a wave function ψ_n which is known as eigen function. The particle can be found at any location inside the box. It means its probability of finding inside the box is one.

$$\text{As, } \psi(x) = A \sin kx$$

$$\int_{x=0}^{x=L} |\psi_n|^2 dx = 1$$

$$\int_{x=0}^{x=L} A^2 \sin^2 \left(\frac{n\pi x}{L} \right) dx = 1$$

$$A^2 \int_{x=0}^{x=L} \sin^2 \left(\frac{n\pi x}{L} \right) dx = 1$$



Using, $\sin^2\theta = \frac{1}{2}(1 - \cos^2\theta)$

$$\frac{A^2}{2} \int_{x=0}^{x=L} \left(1 - \cos \frac{2n\pi x}{L}\right) dx = 1$$

$$\frac{A^2}{2} \int_{x=0}^{x=L} \left(dx - \cos \frac{2n\pi x}{L} dx\right) = 1$$

$$\frac{A^2}{2} \left[\int_{x=0}^{x=L} dx - \int_{x=0}^{x=L} \cos \frac{2n\pi x}{L} dx \right] = 1$$

$$\frac{A^2}{2} \left[x - \frac{L}{2\pi n} \sin \frac{2\pi n x}{L} \right]_0^L = 1$$

$$\frac{A^2}{2} \left[L - \frac{L}{2\pi n} \sin \frac{2\pi n L}{L} - \left(0 - \frac{L}{2\pi n} \sin \frac{2\pi n 0}{L} \right) \right] = 1$$

As; $\sin 2\pi n = 1$; $\sin 0 = 0$

$$\frac{A^2}{2} L = 1$$

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

Substituting value of A in equation (42)

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Hence the normalized wave function is given by:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi x}{L} \right) \quad \dots(43)$$

Where, $n = 1, 2, 3, \dots$, and the wave functions are orthonormal.

- The equation (43) represents the wave function ψ of the particle enclosed in rigid box of length L . As ψ gives negative probability, probability density i.e. $|\psi|^2$ determines the position of the particle inside the box.

- The wave function and probability function for particle in infinite potential well (rigid box)

- The wave function ψ and probability density $|\psi|^2$ of the particle ψ can be plotted as shown in figure. The locations where probability densities show peaks are the most probable position of the particle.
- According to classical mechanics, a particle with any energy can be present at any location inside the box. Quantum mechanically, probability of the particle being present in the box is different according to its quantum number n . For example, at $n = 1$, $|\psi|^2$ i.e. the probability of finding the particle is maximum at $L/2$. Similarly, at $n = 2$, $|\psi|^2$ i.e. probability of finding the particle is maximum at $L/4$ and $L = 3L/4$.

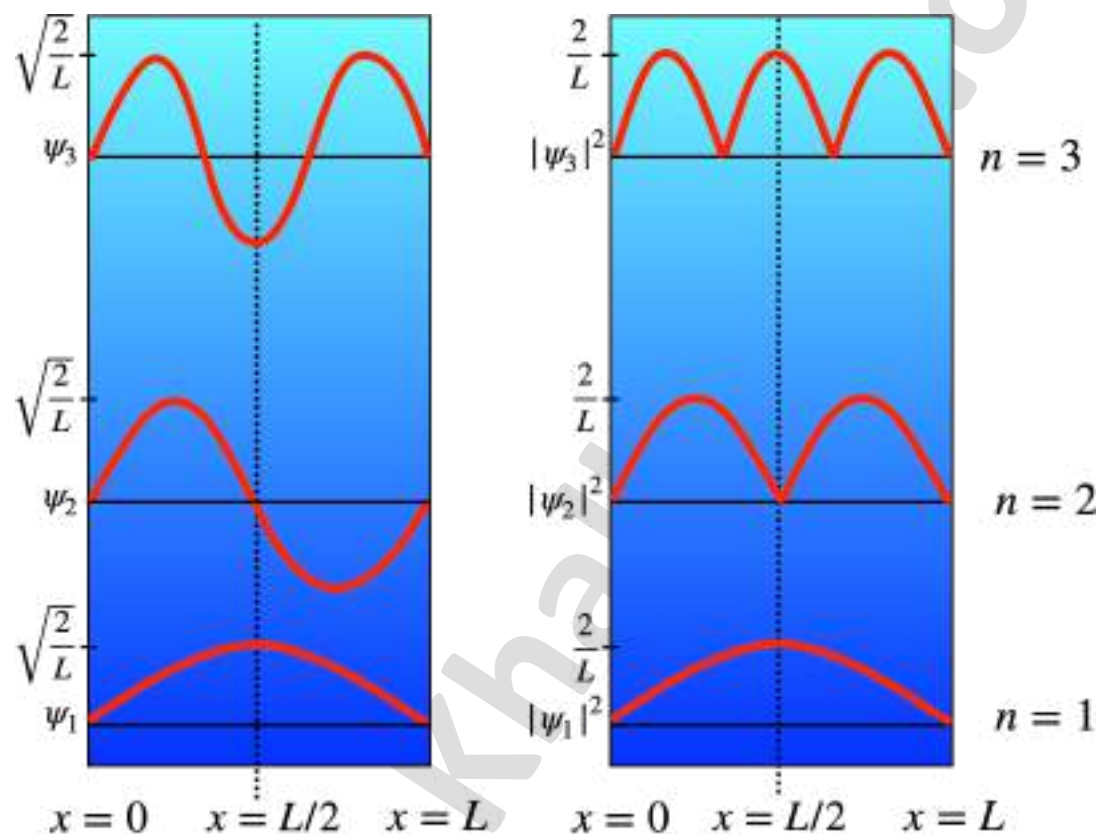


Fig. 13: Wave Function and Probability Function for particle in infinite potential well (rigid box)

- In an infinite potential well, the quantum states of a particle are characterized by the wave function $\Psi_n(x)$ and the probability density $|\Psi_n(x)|^2$. The first three quantum states exhibit distinct wave and probability distributions:

For $n = 1$ (Ground State):

- The wave function has a single peak with no internal nodes, and the probability density is maximum at the center ($x = L/2$) and zero at the walls. This means the particle is most likely found near the middle of the well.

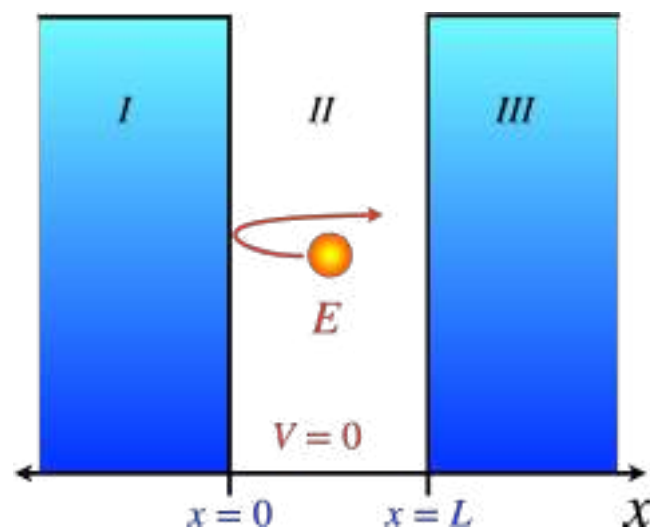
For $n = 2$ (First Excited State):

- The wave function has one node at $x = L/2$, meaning the probability of finding the particle at the center is zero. The probability density shows two peaks, with the highest probability of finding the particle in two symmetric regions on either side of the center i.e. at $L/4$ and $L = 3L/4$.

For $n = 3$ (Second Excited State):

- The wave function has two nodes at $x = L/3$ and $x = 2L/3$, dividing the well into three regions of oscillation. The probability density has three peaks, meaning the particle is likely to be found in three distinct areas, with zero probability at the nodes.
- As the quantum number n increases, the number of nodes and the complexity of the probability distribution increase, reflecting the wave-like nature of quantum particles confined in a potential well.

15. Particle in finite potential well (rigid box)



- The finite potential well is a fundamental quantum mechanical model used to describe a particle trapped in a region with finite potential barriers. Unlike the infinite potential well, where the particle is strictly confined, in a finite well, there is a nonzero probability of the particle existing outside the well due to quantum tunneling.
- Consider a particle is enclosed in a potential well (rigid box) having **finite** potential $\therefore V = 0$. Inside the well (box) motion of particle is restricted between $x = 0$ and $x = L$. The potential energy of the particle is $V = V_0$ outside the box and it can be considered $V = 0$ inside the well (box). Assuming the collision of the particle with walls as elastic, total energy of the particle E can exceed V_0 .

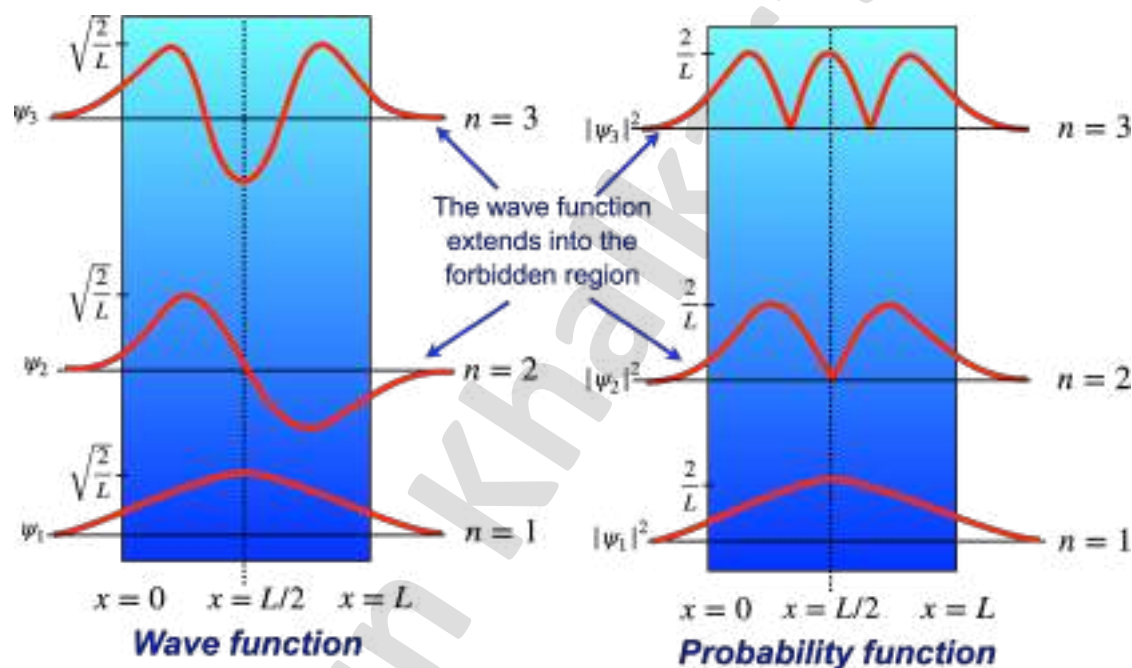


Fig. 14: Wave function and probability function

- The wave functions ψ_I , ψ_{II} , ψ_{III} and corresponding probability density curves are as follows :
- It can be seen that the wave functions ψ_I are not equal to zero outside the box. Thus, even though the particle energy E is smaller than the value of potential outside the well (box), there is still a definite probability that the particle be found outside the well (box).
- In other words, even though the particle does not have sufficient energy to cross potential barrier the well (box), it may nevertheless somehow penetrate them and leak out. The wave functions of a particle in a box, with walls are zero at the walls. But when the confining box has non-rigid walls, the wave functions of the particle are not equal to zero at the walls. This means that the particle wave functions are somewhat longer in the case of non-rigid box than the wave the corresponding energy levels of particle when it is confined to a rigid box.
- When the particle comes out of the well (box), its kinetic energy is reduced (as potential outside is V_0) ($K.E. = E - V_0$). Lower K.E. implies lower energy and hence lower frequency in turn longer wave function. Thus, the wave function associated with matter waves are longer when particle comes outside the box than when it is inside the well (box). Thus, the behaviour of the particle is similar to radiation. When radiation encounters a boundary separating two media, a part of it is reflected and a part is transmitted.
- Similarly, a matter wave encounters a boundary separating two regions where its potential changes, the possibility of reflection as well as transmission is there.

16. Quantum Tunneling

- Quantum tunneling is a fundamental quantum mechanical phenomenon where a particle penetrates and passes through a potential barrier even when its total energy is less than the barrier height. This is a direct consequence of wave-particle duality, as described by Schrödinger's equation.
- In classical physics, if a particle does not have enough energy to overcome a barrier, it would be completely reflected. However, quantum mechanics predicts that there is a finite probability for the particle to appear on the other side of the barrier, meaning it has "tunneled" through it.
- **Wave Function Behavior:** According to quantum mechanics, particles behave as waves. When a wave encounters a barrier, part of it is reflected, and part of it penetrates into the barrier. Inside the barrier, the wave function decays exponentially but does not become zero. If the barrier is thin enough, the wave function can continue on the other side, meaning the particle has "tunneled" through.
- **Applications of Quantum Tunneling:**
 - Alpha Decay: In radioactive elements, alpha particles tunnel out of the nucleus, leading to nuclear decay.
 - Nuclear Fusion: In stars, hydrogen nuclei overcome electrostatic repulsion and fuse due to tunneling.
 - Tunnel Diodes: Used in high-speed electronic circuits due to their ability to conduct via tunneling.
 - Quantum Computing: Exploits tunneling effects to perform computations at unprecedented speeds.
 - Scanning Tunneling Microscope (STM): Uses tunneling to visualize atomic surfaces with incredible precision.
- Quantum tunneling defies classical intuition but is essential for both fundamental physics and technological advancements.
- **Analogy:**
 - To understand the phenomenon, particles attempting to travel between potential barriers can be compared to a ball trying to roll over a hill; quantum mechanics and classical mechanics differ in their treatment of this scenario.
 - Classical mechanics predicts that particles that do not have enough energy to classically surmount a barrier will not be able to reach the other side. Thus, a ball without sufficient energy to surmount the hill would roll back down. Or, lacking the energy to penetrate a wall, it would bounce back (reflection) or in the extreme case, bury itself inside the wall (absorption).
 - In quantum mechanics, these particles can, with a very small probability, tunnel to the other side, thus crossing the barrier. Here, the "ball" could, in a sense, borrow energy from its surroundings to tunnel through the wall or "roll over the hill", paying it back by making the reflected electrons more energetic than they otherwise would have been.

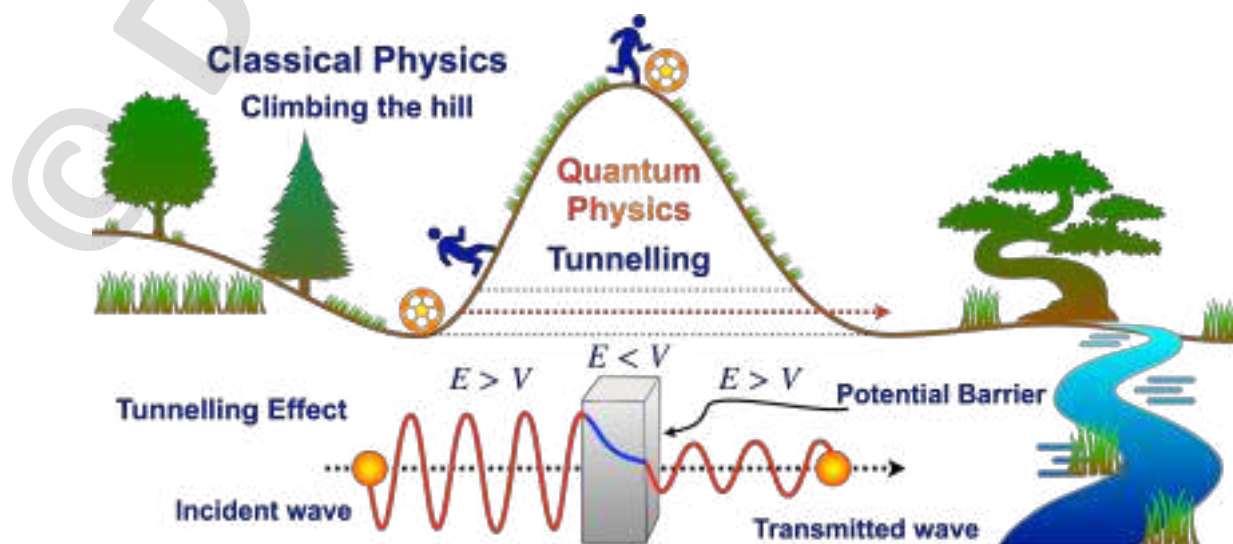


Fig. 15: Tunnelling effect

- Tunnel effect:

- Let us consider a potential barrier as shown in Fig. 16 (a) and Fig. (b).
- Suppose that an incident particle with energy E coming from the left collides with the potential barrier. The energy E is assumed to be lower than the top of the barrier. In the classical mechanics, the particle is completely reflected by the potential barrier.
- In quantum mechanics, some probability will be reflected, but the other penetrates the barrier and pass through into the right-hand side region to proceed to the far right. This is the **tunnel effect**.

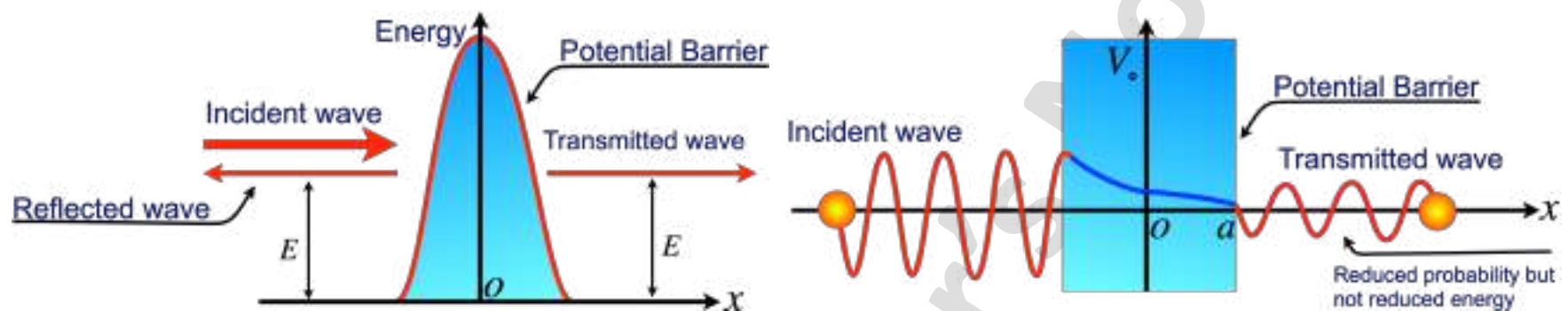


Fig. 16: (a): Incident particle with energy collides with the potential barrier, (b): Tunnel effect

- Application of tunnelling effect:

Scanning Tunneling Microscope (STM):

- The quantum tunnelling phenomenon at metallic surfaces, which we have just described, is the physical principle behind the operation of the scanning tunnelling microscope (STM), invented in 1981 by Gerd Binnig and Heinrich Rohrer.
- A metal tip usually made out of tungsten is placed at a very small distance above a conducting or semiconducting surface. This distance acts as a potential barrier for tunnelling. The space between the tip and the surface normally is vacuum. When electrons tunnel from the metal tip to the surface, a current is created and monitored by a computer as shown in Fig.17.
- The current depends on the distance between the tip and the surface, which is controlled by a piezoelectric cylinder. If there is a strong current, the tip will move away from the surface. The increase of the potential barrier will decrease the probability of tunnelling and decrease the current. If the current becomes too weak, the tip moves closer to the surface. The potential barrier will be reduced and the current will increase. The variations in the current as the tip moves over the sample are reconstructed by the computer to produce a topological image of the scanned surface.
- In Fig. a scanning tip (a needle, usually made of tungsten, platinum-iridium, or gold); a piezoelectric device that controls the tip's elevation in a typical range of 0.4 to 0.7 nm above the surface to be scanned; some device that controls the motion of the tip along the surface; and a computer to display images. While the sample is kept at a suitable voltage bias, the scanning tip moves along the surface and the tunneling-electron current between the tip and the surface is registered at each position.
- In STM, a surface at a constant potential is being scanned by a narrow tip moving along the surface. When the STM tip moves close to surface atoms, electrons can tunnel from the surface to the tip. This tunneling-electron current is continually monitored while the tip is in motion. The amount of current at location (x,y) gives information about the elevation of the tip above the surface at this location. In this way, a detailed topographical map of the surface is created and displayed on a computer monitor.

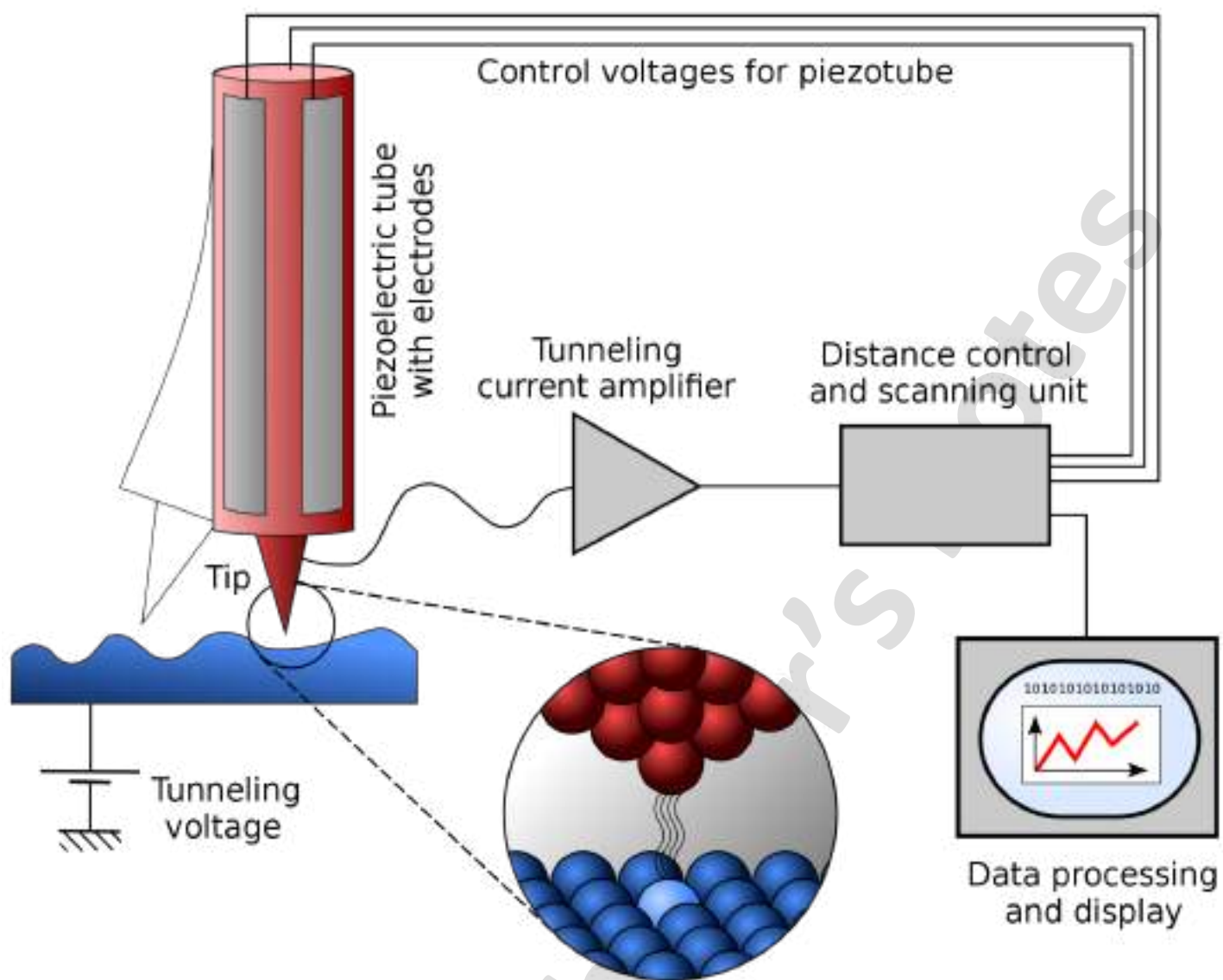
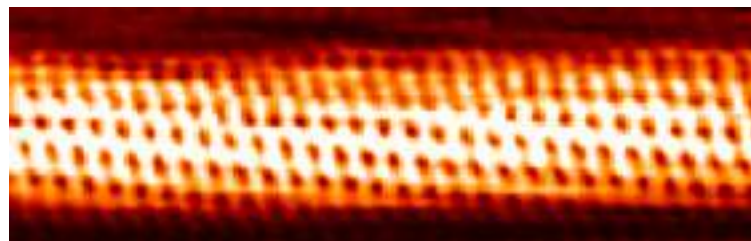
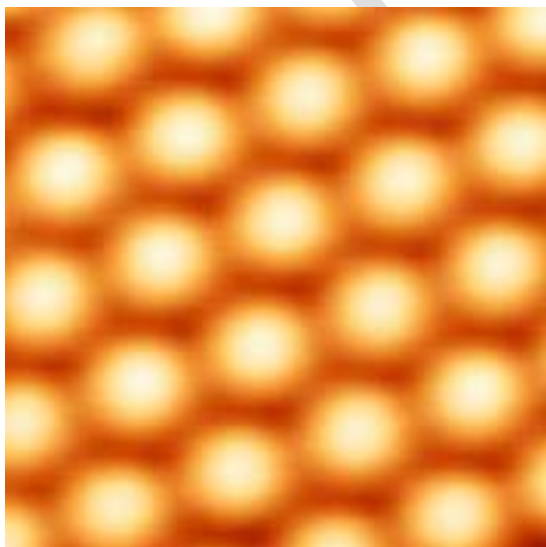


Fig. 17: Schematic diagram of a scanning tunnelling microscope

- The amount of the current depends on the probability of electron tunneling from the surface to the tip, which, in turn, depends on the elevation of the tip above the surface. Hence, at each tip position, the distance from the tip to the surface is measured by measuring how many electrons tunnel out from the surface to the tip. This method can give an unprecedented resolution of about 0.001 nm, which is about 1% of the average diameter of an atom. In this way, we can see individual atoms on the surface, as in the image of silicon and Carbon nanotube are shown in Fig. 18.



**Fig. 18: a) The silicon atoms on the surface of a crystal of silicon carbide (SiC). Image obtained using STM.
b) An STM image of a single-walled carbon nanotube**

**- Working Principle of STM:**

- Sharp Metal Tip: A fine, conducting tip (usually tungsten or platinum-iridium) is brought extremely close to the surface of a sample (within nanometers).
- Bias Voltage: A small voltage is applied between the tip and the sample, creating an electric field.
- Quantum Tunnelling: Due to the proximity, electrons tunnel from the tip to the sample (or vice versa), generating a tunnelling current.
- Current Measurement: The tunnelling current depends on the distance between the tip and the surface atoms. If the tip moves over an atom, the current increases; if it moves into a lower region, the current decreases.
- Atomic Resolution Imaging: By scanning the tip across the surface and maintaining a constant current, an atomic-scale map of the surface is generated.

- Modes of Operation:

- Constant Current Mode: The tip height is adjusted to keep the tunneling current constant, providing topographic details of the surface.
- Constant Height Mode: The tip remains at a fixed height, and variations in tunneling current are used to generate the image.

- Applications of STM:

- Surface Analysis: STM can provide atomic-level resolution of surfaces, allowing researchers to study the structure of materials at the atomic scale. This is particularly useful in materials science for investigating metals, semiconductors, and thin films.
- Nanotechnology: STM is often used in the fabrication and manipulation of nanostructures. It can manipulate individual atoms and molecules, making it an essential tool in the development of nanodevices and nanoscale circuits.
- Surface Chemistry and Reactions: STM can monitor and study surface reactions, including the interaction of atoms or molecules with surfaces. This has applications in catalysis, corrosion studies, and understanding chemical processes at the atomic level.
- Quantum Dots and Nanostructures: STM is widely used to study and characterize quantum dots and other nanostructures. It helps researchers to understand electronic properties, such as conductance and electron transport, which are critical in quantum computing and optoelectronics.
- Biomolecular Imaging: STM is used in biophysics and chemistry to study the structures of biological molecules, like proteins and DNA, at the atomic scale. It has potential applications in drug design, bioengineering, and molecular biology.
- Semiconductor Research: In the semiconductor industry, STM is used to study surfaces of materials used in electronics, such as silicon wafers. It aids in understanding defects, interfaces, and electronic properties, which are critical for the development of advanced semiconductor devices.
- Atomic-Scale Imaging of Magnetic Properties: STM allows the imaging of magnetic properties at the atomic scale. This is important for the development of spintronic devices, which rely on the electron's spin rather than charge for information storage and processing.
- Materials Science: STM plays a significant role in studying materials' surface properties, including crystallography, roughness, defects, and electronic properties, which is crucial for designing new materials with specific properties.

**- Advantages of STM:**

- **Unmatched Resolution:** One of the most remarkable advantages of STM is its atomic-scale resolution. It can image individual atoms, which is beyond the capability of most other microscopy techniques. STM allows researchers to visualize structures at the atomic level, providing insight into atomic arrangements, defects, and surface structures that were previously inaccessible.
- **Real-time Surface Analysis:** STM not only provides high-resolution images but also allows for real-time observation of surface morphology and dynamic processes. This is particularly useful for studying the growth of materials, chemical reactions, and even the movement of molecules or atoms on surfaces. Researchers can watch how atoms and molecules interact with each other and how structures evolve in real-time, which is invaluable for understanding surface phenomena.
- **Atomic Manipulation:** STM's atomic manipulation capability is a groundbreaking feature. In addition to imaging, STM can manipulate individual atoms on a surface. For example, IBM's famous quantum corral experiment demonstrated the ability to move individual atoms to create stable structures, like a "corral" for electrons. This atomic-level control is essential for nanotechnology, where precision is key to building molecular machines, nano-devices, and even for developing quantum computers.
- **High Sensitivity to Surface Properties:** STM can provide detailed information about the electronic properties of surfaces. It is sensitive to surface conductivity, charge density, and local electronic states, making it an ideal tool for studying semiconductors, superconductors, and materials with complex electronic behaviors. STM can also be used to investigate magnetism at the atomic scale, helping in the development of spintronic devices.
- **Non-destructive Imaging:** Unlike some other techniques that may damage or alter the sample (e.g., electron microscopy), STM provides non-destructive imaging, preserving the surface as it is. This makes STM ideal for studying delicate or valuable materials without compromising their integrity.
- **Versatility:** STM can be applied to a wide variety of materials, including metals, semiconductors, insulators, and even biological samples (when properly prepared). Its versatility allows it to be used across many different disciplines, from materials science to biophysics to quantum computing.

- Limitations of STM:

- **Sample Preparation:** STM requires the sample to be conductive or at least semi-conductive. This can limit its applicability to certain materials. For non-conductive samples, special preparations (such as coating the sample with a conductive layer) may be needed, which can affect the accuracy of the measurements.
- **Limited to Flat Surfaces:** STM is primarily designed for imaging flat surfaces with smooth topographies. Although it can scan rough surfaces, it may not be as effective on highly irregular or rough samples, as the tip might lose its sharpness or fail to maintain a stable tunneling current.
- **Environmental Conditions:** STM requires a highly controlled environment for accurate imaging. It often needs to be operated in ultra-high vacuum (UHV), at low temperatures, or under controlled atmospheric conditions to avoid interference from contaminants like air molecules or water vapor. These stringent conditions make the system costly and sometimes difficult to use for certain applications.
- **Tip Condition and Wear:** The STM tip is crucial for high-resolution imaging, and maintaining its sharpness can be challenging. Over time, the tip can become worn, which can degrade the resolution and accuracy of the measurements. Additionally, the tip may interact with the sample in ways that alter the image if it is not in perfect condition.
- **Limited Imaging Depth:** STM images the surface of a sample, but it does not provide information about the internal structure. This means that while STM offers incredible detail of surface features, it cannot probe deeper



layers or give insight into the bulk material's properties. For internal structure analysis, other techniques like Transmission Electron Microscopy (TEM) may be needed.

- **Slow Imaging Process:** STM imaging can be relatively slow, especially when imaging large areas. The scanning process involves moving the tip across the surface, which can take time to generate high-resolution images. For large-scale imaging or fast processes, STM might not be the most efficient technique.
- **Size of the Scan Area:** STM typically operates over small scan areas (on the order of micrometers to nanometers). While this allows for high resolution, it also means that for larger surfaces, multiple scans are required, which can be time-consuming and computationally intensive.
- **Difficulty with Biological Samples:** STM can be challenging for imaging delicate biological samples because they are often soft, complex, or poorly conductive. Special sample preparations and conditions are needed to study biological molecules, and the tip's interaction with these samples might distort the biological structures.
- **Surface Sensitivity:** STM is very sensitive to surface features, but it might not provide information about subsurface structures. In addition, small surface contaminants or oxidation layers can obscure the true atomic arrangement, making it harder to interpret the data accurately.



17. Solved Problems

de Broglie wave

Problem 1: An electron beam is accelerated from rest through a potential difference of 200V. This beam is passed through a diffraction grating of spacing 3\AA .

(i) Calculate the associated wavelength.

(ii) At what angle of deviation from the incident direction will be the first maximum observed?

Solution:

(i) The wavelength of the waves associated with the electron beam is given by;

$$\lambda = \frac{h}{\sqrt{2m_e eV}} = \frac{6.626 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 1.602 \times 10^{-19} \text{ C} \times 200 \text{ V}}} = 0.86 \text{\AA}$$

(ii) The diffraction is governed by equation $2d \sin \theta = m\lambda$; for first order $m = 1$.

$$2d \sin \theta = \lambda \therefore \theta = \sin^{-1} \left(\frac{\lambda}{2d} \right) \therefore \theta = \sin^{-1} \left(\frac{0.86 \times 10^{-10} \text{ m}}{2 \times 3 \times 10^{-10} \text{ m}} \right) = 8.31^\circ$$

Problem 2: An enclosure filled with helium is heated to 400K. A beam of He-atoms emerges out of the enclosure. Calculate the de Broglie wavelength corresponding to He atoms. Mass of He atom is $6.7 \times 10^{-27} \text{ kg}$.

Solution:

$$\text{De Broglie wavelength is; } \lambda = \frac{h}{\sqrt{2mkT}}$$

$$\lambda = \frac{6.626 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 6.7 \times 10^{-27} \text{ kg} \times 1.376 \times 10^{-21} \text{ J/deg} \times 400}} = 0.769 \text{\AA}$$

Problem 3: Calculate the de Broglie wavelength of (i) an electron accelerated through a potential difference of 182V and (ii) a 1kg object moving with a speed 1m/s. Comparing the results explain why the wave nature of matter is not more apparent in daily observations?

Solution:

$$(i) \lambda_e = \frac{h}{\sqrt{2emV}}$$

$$\lambda_e = \frac{6.626 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 1.602 \times 10^{-19} \text{ C} \times 9.11 \times 10^{-31} \text{ kg} \times 182 \text{ V}}} = \frac{6.626 \times 10^{-34} \text{ J.s}}{7.29 \times 10^{-24} \text{ kg.m/s}} = 0.91 \times 10^{-10} \frac{\text{kg.m}^2/\text{s}}{\text{kg.m/s}}$$

$$= 9.11 \times 10^{-11} \text{ m} \therefore \lambda_e = 0.91 \text{\AA}$$

$$(ii) \lambda_m = \frac{h}{mv}$$

$$\lambda_m = \frac{6.626 \times 10^{-34} \text{ J.s}}{1 \text{ kg} \times 1 \text{ m/s}} = 6.626 \times 10^{-34} \frac{\text{kg.m}^2/\text{s}}{\text{kg.m/s}} = 6.626 \times 10^{-34} \text{ m} \therefore \lambda_m = 6.626 \times 10^{-34} \text{ m}$$



Problem 4: What is de Broglie wavelength of an electron when accelerated through a potential difference of 10,000 volts?

Solution:

Potential Difference = 10,000V. Hence $\lambda = \frac{12.27}{\sqrt{V}} = \frac{12.27}{\sqrt{10,000}} = 0.1227 \text{ \AA}$

Problem 5: Compute the de Broglie wavelength of an electron whose kinetic energy is 10 eV.

Solution: The kinetic energy $E_k = \frac{p^2}{2m}$

$$p = \sqrt{2mE_k} = \sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 10 \text{ eV} \times 1.6 \times 10^{-19} \text{ J/eV}} = 1.707 \times 10^{-24} \text{ kg m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34} \text{ J.s}}{1.707 \times 10^{-24} \text{ kg m/s}} = 3.88 \times 10^{-10} \text{ m} = 0.39 \text{ nm}$$

Problem 6: An electron and a proton have the same non-relativistic kinetic energy. Show that the proton has a shorter de Broglie wavelength.

Solution: The kinetic energy $E_k = \frac{p^2}{2m}$ or $p = \sqrt{2mE_k}$

The de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE_k}}$; Since both have the same kinetic energy, $\frac{\lambda_e}{\lambda_p} = \sqrt{\frac{m_p}{m_e}}$

Since $m_p > m_e$, we have $\lambda_p < \lambda_e$

Heisenberg's Uncertainty Principle

Problem 7: Uncertainty in time of an excited atom is about 10^{-8} s . What are the uncertainties in energy and in frequency of the radiation?

Solution:

$$\Delta E \Delta t \approx \frac{h}{4\pi} \therefore \Delta E = \frac{6.626 \times 10^{-34} \text{ J.s}}{10^{-8}} \text{ eV} = 6.58 \times 10^{-8} \text{ eV} = 1.054 \times 10^{-26} \text{ J}$$

$$\therefore \Delta \nu = \frac{\Delta E}{h} = \frac{1.054 \times 10^{-26} \text{ J}}{6.626 \times 10^{-34} \text{ J.s}} = 15.9 \text{ MHz}$$

Problem 8: An electron is confined to a potential well of width 10nm. Calculate minimum uncertainty in its velocity.

Solution:

$$\Delta x \Delta p \approx \frac{h}{4\pi} \therefore \Delta x \cdot m \Delta v \approx \frac{h}{4\pi} \therefore \Delta v = \frac{h}{4\pi m \cdot \Delta x}$$

$$\Delta v = \frac{6.626 \times 10^{-34} \text{ J.s}}{4 \times 3.14 \times 9.11 \times 10^{-31} \text{ kg} \times 10 \times 10^{-9} \text{ m}} \therefore \Delta v = 5.79 \text{ km/s}$$



Problem 9: If the kinetic energy of an electron is 1eV , must be measured within 0.0001eV , what accuracy can its position be measured simultaneously?

Solution:

$$E = \frac{p^2}{2m} \therefore \Delta E = \frac{2p\Delta p}{2m} \therefore \Delta p = \frac{m\Delta E}{p} \therefore \Delta x \Delta p = \frac{h}{2\pi}$$

$$\therefore \Delta x = \frac{h}{2\pi \cdot \Delta p} = \frac{h}{2\pi} \cdot \frac{p}{m\Delta E} = \frac{h\sqrt{2mE}}{2\pi m\Delta E} = \frac{h}{\pi\Delta E} \cdot \sqrt{\frac{E}{2m}}$$

$$\therefore \Delta x = \frac{6.626 \times 10^{-34} \text{ J.s}}{3.14 \times 0.0001 \times 1.602 \times 10^{-19} \text{ J}} \cdot \sqrt{\frac{1.602 \times 10^{-19} \text{ J}}{2 \times 9.11 \times 10^{-31} \text{ kg}}} \therefore \Delta x = 1.95 \mu\text{m}$$

Problem 10: An electron and a 150gm base ball are travelling at a velocity of 220m/s , measured to an accuracy of 0.065% . Calculate and compare uncertainty in position of each.

Solution:

The uncertainty in velocity

$$\Delta v = v \times 0.065 \% = 220\text{m/s} \times \frac{0.065}{100} = 0.143\text{m/s}$$

(i) The uncertainty in position of electron is;

$$\Delta x_e = \frac{\hbar}{2m\Delta v} = \frac{1.05 \times 10^{-34} \text{ J.s}}{2 \times 9.11 \times 10^{-31} \text{ kg} \times 0.143\text{m/s}} \therefore \Delta x_e = 0.4\text{mm}.$$

(ii) The uncertainty in position of baseball is;

$$\Delta x_B = \frac{\hbar}{2M\Delta v} = \frac{1.05 \times 10^{-34} \text{ J.s}}{2 \times 0.15\text{kg} \times 0.143\text{m/s}} \therefore \Delta x_B = 2.5 \times 10^{-33}\text{m}.$$

Problem 11: An electron moves with a constant speed $v = 1.1 \times 10^6 \text{ m/s}$ in a straight line. If the speed is measured to a precision of 0.1 per cent, what is the maximum precision with which its position could be simultaneously measured?

Solution:

The momentum of the electron

$$p = mv$$

$$p = 9.11 \times 10^{-31} \text{ kg} \times 1.1 \times 10^6 \text{ m/s} = 10^{-24} \text{ kg m/s}$$

$$\Delta p = \frac{0.1}{100} \times 10^{-24} \text{ kg m/s} = 10^{-27} \text{ kg m/s}$$

$$\Delta x = \frac{\hbar}{2\Delta p} = \frac{1.054 \times 10^{-34} \text{ J.s}}{2 \times 10^{-27} \text{ kg m/s}} = 0.53 \times 10^{-7} \text{ m}$$



Problem 12: An electron remains in an excited state of an atom for 10^{-8} s. What is the minimum uncertainty in the energy of the state in eV?

Solution:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2} \quad \text{as } \Delta t \approx 10^{-8} \text{ s}$$

$$\Delta E \geq \frac{\hbar}{2 \cdot \Delta t} \quad \text{hence } \Delta E \geq \frac{1.05 \times 10^{-34} \text{ J}}{2 \times 10^{-8} \text{ s}} = 3.28 \times 10^{-7} \text{ eV}$$

Problem 13: A particle constrained to move along x-axis in the region $0 < x < a$ has a wave function,

$$\Psi(x) = N \sin\left(\frac{n\pi x}{a}\right) \quad \text{where } n \text{ is an integer. Normalize the wave function.}$$

Solution:

The normalization condition gives

$$N^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$N^2 \int_0^a \frac{1}{2} \left(1 - \cos\frac{2n\pi x}{a}\right) dx = 1$$

$$N^2 \frac{a}{2} = 1 \quad \text{or} \quad N = \sqrt{\frac{2}{a}}$$

The normalized wave function

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Particle in infinite potential well

Problem 14: Find the probability that a particle trapped in a box L wide can be found between $0.45L$ and $0.55L$ for the ground state and first excited state.

Solution:

$$\text{Formula: } \psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$P = \frac{2}{L} \int_{x_1}^{x_2} \sin^2\left(\frac{n\pi x}{L}\right) dx \therefore P = \frac{1}{L} \int_{x_1}^{x_2} \left(1 - \cos\frac{n\pi x}{L}\right) dx \therefore P = \frac{1}{L} [x]_{x_1}^{x_2} - \frac{1}{2n\pi} \left[\sin\frac{2n\pi x}{L}\right]_{x_1}^{x_2}$$

$$P = \frac{1}{L} [x_2 - x_1] - \frac{1}{2n\pi} \left[\sin\frac{2n\pi x_2}{L} - \sin\frac{2n\pi x_1}{L}\right]$$

For ground state $n = 1$, hence above equation can be written as;

$$P = \frac{1}{L} [0.55L - 0.45L] - \frac{1}{2\pi} \left[\sin\frac{2 \times 180^\circ \times 0.55L}{L} - \sin\frac{2 \times 180^\circ \times 0.45L}{L}\right]$$



$$P = 0.1 - \frac{1}{2 \times 3.143} (-0.309 - 0.309) = \mathbf{0.198}$$

For 1st excited state $n = 2$, hence above equation can be written as;

$$P = \frac{1}{L} [0.55L - 0.45L] - \frac{1}{4\pi} \left[\sin \frac{4 \times 180^\circ \times 0.55L}{L} - \sin \frac{4 \times 180^\circ \times 0.45L}{L} \right]$$

$$P = 0.1 - \frac{1}{4 \times 3.143} (0.5878 - 0.5878) = \mathbf{0.0065}$$

Problem 15: Find the lowest energy of an electron confined to move in a one dimensional box of length 1\AA . Express the result in eV.

Solution:

The energy values of electron in one dimensional box are given by $E_n = \frac{n^2 h^2}{8mL^2}$;

For the lowest energy level $n = 1$.

$$E_1 = \frac{1^2 (6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (10^{-10} \text{ m})^2} = 6 \times 10^{-18} = \frac{6 \times 10^{-18} \text{ J}}{1.6 \times 10^{-19}} \text{ eV} \therefore E_1 = \mathbf{37.5 \text{ eV}}$$

Problem 16: An electron is confined to move in a one dimensional potential well of length 5\AA . Find the quantised energy values for the three lowest energy states. Express the result in eV.

Solution:

The quantised energy values of electron in 1-D potential well are given by $E_n = \frac{n^2 h^2}{8mL^2}$;

$$\text{For Ground state; } n = 1; E_1 = \frac{1^2 h^2}{8mL^2} = \frac{h^2}{8mL^2} = \frac{(6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (5 \times 10^{-10} \text{ m})^2}$$

$$\text{For Ground state; } n = 1; E_1 = 2.41 \times 10^{-19} \text{ J} = \mathbf{1.5 \text{ eV}}$$

$$\text{For Energy for 1st excited state; } n = 2; E_2 = \frac{2^2 h^2}{8mL^2} = \frac{4h^2}{8mL^2} = 4 \times E_1 = 4 \times 1.5 \text{ eV} = \mathbf{6 \text{ eV}}$$

$$\text{For Energy for 2nd excited state; } n = 3; E_3 = \frac{3^2 h^2}{8mL^2} = \frac{9h^2}{8mL^2} = 9 \times E_1 = 9 \times 1.5 \text{ eV} = \mathbf{13.5 \text{ eV}}$$

$$E_1 = \mathbf{1.5 \text{ eV}} \quad E_2 = \mathbf{6 \text{ eV}} \quad E_3 = \mathbf{13.5 \text{ eV}}$$

Problem 17: An electron is trapped in a one-dimensional box of length 0.1 nm . Calculate the energy required to excite the electron from its ground state to the third excited state.

Solution:

The quantised energy values of electron in 1-D potential well are given by $E_n = \frac{n^2 h^2}{8mL^2}$;



$$\text{For Ground state; } n = 1; E_1 = \frac{1^2 h^2}{8mL^2} = \frac{h^2}{8mL^2} = \frac{(6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (0.1 \times 10^{-9} \text{ m})^2}$$

$$\text{For Ground state; } n = 1; E_1 = 60.3 \times 10^{-19} \text{ J} = \mathbf{37.65 \text{ eV}}$$

$$\text{For 3rd excited state; } n = 4; E_4 = \frac{4^2 h^2}{8mL^2} = \frac{16 \times (6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (0.1 \times 10^{-9} \text{ m})^2}$$

$$\text{For 3rd excited state; } n = 4; E_4 = \mathbf{601.6 \text{ eV}}$$

The energy required to excite the electron from its ground state to the third excited state;

$$\mathbf{E_4 - E_1 = 601.6 \text{ eV} - 37.6 \text{ eV} = 564 \text{ eV}}$$

Problem 18: An electron is confined to move between two rigid walls separated by 1 nm. Find the de Broglie wavelength representing the first two allowed energy states of the electron and the corresponding energies.

Solution:

The eigen values of electron energy confined in a potential well are given by

$$E_n = \frac{n^2 h^2}{8mL^2};$$

Energy of the 1st allowed state; $n = 1$;

$$E_1 = \frac{1^2 h^2}{8mL^2} = \frac{h^2}{8mL^2} = \frac{(6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (1 \times 10^{-9} \text{ m})^2} = \mathbf{6.03 \times 10^{-20} \text{ J}}$$

Energy of the 2nd allowed state; $n = 2$;

$$E_2 = \frac{2^2 h^2}{8mL^2} = \frac{4 \times (6.626 \times 10^{-34} \text{ J.s})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} (1 \times 10^{-9} \text{ m})^2} = \mathbf{2.4 \times 10^{-19} \text{ J}}$$

De Broglie wavelength of the electron at the 1st energy level,

$$\lambda_1 = \frac{h}{\sqrt{2mE_1}} = \frac{6.626 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 6.03 \times 10^{-20} \text{ J}}} = \mathbf{2 \text{ nm}}$$

De Broglie wavelength of the electron at the 2nd energy level,

$$\lambda_2 = \frac{h}{\sqrt{2mE_2}} = \frac{6.626 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 2.4 \times 10^{-19} \text{ J}}} = \mathbf{1 \text{ nm}}$$

Problem 19: An electron is moving in a one-dimensional box of width $2 \times 10^{-10} \text{ m}$. If the wave function of the first

excited state $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$, what is the probability of finding the electron between $x = 0$ and $x = 10^{-10} \text{ m}$ in that state.



Solution: The required probability $= \frac{2}{a} \int_{x_1}^{x_2} \sin^2 \frac{2\pi x}{a} dx$

where $x_1 = 0$, $x_2 = 1 \times 10^{-10} \text{ m}$, $a = 2 \times 10^{-10} \text{ m}$

$$\text{Probability} = \frac{2}{a} \int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos \frac{4\pi x}{a} \right) dx$$

$$= \frac{2}{a} \cdot \frac{1}{2} \cdot x_2 - \frac{2}{a} \cdot \frac{1}{2} \frac{a}{4\pi} \sin \frac{4\pi x_2}{a}$$

$$= \frac{1}{2}$$

Problem 20: A proton and an alpha particle are accelerated through the same potential difference. Show that the ratio of wavelengths associated with proton and alpha particles respectively is $2\sqrt{2}$. Assume the mass of the alpha particle is 4 times the mass of a proton.

Solution:

The mass of the alpha particle is 4 times the mass of a proton, $m_\alpha = 4m_p$

$$\lambda_p = \frac{1}{\sqrt{2m_p \cdot e}} \text{ and}$$

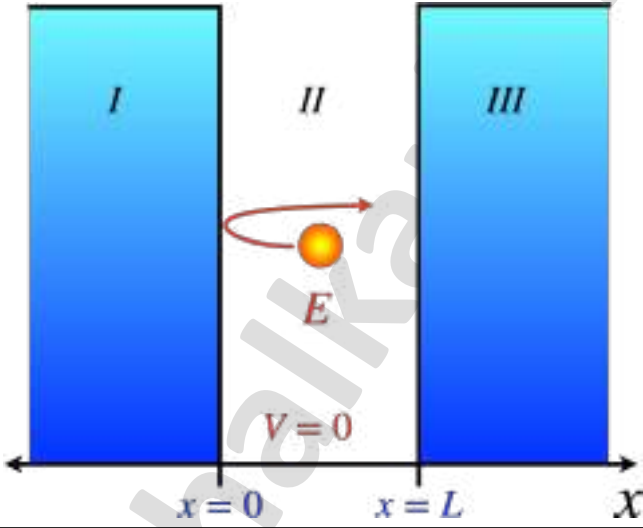
$$\lambda_\alpha = \frac{1}{\sqrt{2m_\alpha \cdot e}} = \frac{1}{\sqrt{2 \cdot (4m_p) \cdot e}}$$

$$\text{Hence } \frac{\lambda_p}{\lambda_\alpha} = \frac{1}{\sqrt{2m_p \cdot e}} \times \frac{\sqrt{2(4m_p) \cdot e}}{1} = \sqrt{8} = 2\sqrt{2}$$

$$\frac{\lambda_p}{\lambda_\alpha} = \sqrt{8} = 2\sqrt{2}$$



Sr. No	Question statement
1	State De Broglie hypothesis. Obtain an expression for wavelength of matter waves for a charged particle accelerated through a potential difference V volt
2	Explain properties of matter waves.
3	What is a wave group. Define phase velocity and group velocity.
4	State and explain Heisenberg's uncertainty principle
5	What is wave function Ψ ? What is its physical significance? What conditions should it satisfy to represent matter waves associated with a moving particle?
6	What is a normalised wavefunction? What conditions a well behaved wavefunction should satisfy to represent a matter wave function?
7	A particle is described by the following wavefunction: $\psi(x) = A \sin(kx)$ for $0 \leq x \leq L$ $\psi(x) = B e^{-\alpha x}$ for $x \geq L$ where A, B, k , and α are constants, L is the position where the wavefunction changes form. i) Check if the wavefunction is continuous at $x = L$ ii) Find the relationship between A and B for the wavefunction to be continuous at $x = L$
8	Derive Schrodinger's time independent wave equation.
9	Apply Schrodinger's time independent wave equation to a particle confined to a rigid box of length L to obtain energy values associated with it.
10	How Schrodinger equation applied to a particle in a rigid box of length L leads to discrete energy levels?
11	Apply Schrodinger's time independent wave equation to a particle confined to a non-rigid box of length L . Write wave equation for all three regions. Also write solutions to these.
12	Why must a matter wave function be single valued?
13	Draw a wave function and probability curves associated with a particle confined to an infinite potential well. Interpret the curves.
14	Draw a wave function associated with a particle confined to an infinite potential well and a finite potential well, for lowest three energy levels. Hence, compare the two.
15	Analyse the wavefunctions of a particle in an infinite potential well by drawing and comparing the first three energy states.
16	Draw a wave function and probability density curves associated with a particle confined to a finite potential well. Interpret the curves.
17	With the help of quantum tunnelling, explain the principle of working in STM.
18	Draw a diagram for a particle with energy E , confined to a finite potential well of height V_0 and width L . The potential function inside the well is zero. Hence, write Schrodinger's time independent wave equation for matter wave function associated with this particle.
19	Write an expression for energy values of a particle confined to a rigid box. How the energy associated with a particle confined to a rigid box differs from a classical particle
20	Draw a neat labeled diagram of a wavefunction associated with a particle confined to a rigid and non-rigid box, for lowest three energy levels. Use these curves to compare the energy of the particle in rigid and non-rigid box.
21	A particle is confined within a region of space of length 5 nm . Calculate the minimum uncertainty in the particle's momentum using Heisenberg's Uncertainty Principle.
22	An electron is confined to a region of space with a width of 1 nm . What is the minimum uncertainty in the electron's velocity?
23	An electron is moving with a velocity of $2 \times 10^6 \text{ m/s}$. Calculate its de Broglie wavelength. $m = 9.1 \times 10^{-31} \text{ kg}$, $h = 6.63 \times 10^{-34} \text{ J.s}$

24	The lowest energy of an electron confined to a rigid box is 38 eV . Determine the width of rigid box.
25	An electron is confined to an infinite potential well of 2 \AA . Calculate its minimum energy and momentum.
26	An electron is confined in a 1-dimensional infinite potential well with a width of 2 nm . Calculate the first three energy eigenvalues for the particle. Then, analyse how the energy eigenvalues would change if the width of the well were increased to 4 nm . $m = 9.1 \times 10^{-31}\text{ kg}$
27	Compute the uncertainty in the location of a 2 gm mass moving with a speed of 1.5 m/s and also for an electron with a speed of $0.5 \times 10^8\text{ m/s}$ Given: $P = 10^{-3}$. Comment on result.
28	<p>Consider a particle with energy E, confined to a finite potential well of height V_0 and width L, as shown in figure. The potential function inside the well is zero. Hence, write Schrodinger's time independent wave equation for matter wave function associated with this particle and its solution.</p> 

UNIT 3: MAGNETISM AND SUPERCONDUCTIVITY

1. Introduction to Magnetism

- Magnetism is a fundamental physical phenomenon arising from the motion of electric charges, which results in attractive or repulsive forces between objects. It is one of the key aspects of electromagnetism, a major branch of physics that studies the interactions between electric fields and magnetic fields. Magnets, the most familiar sources of magnetic force, possess a magnetic field that can influence other materials, particularly those containing iron, nickel, or cobalt.
- At the atomic level, magnetism is primarily caused by the movement of electrons, especially their spin and orbital motion around the nucleus. This behavior leads to the formation of magnetic dipoles within atoms, which collectively contribute to the magnetic properties of materials. Depending on how these dipoles align, materials can exhibit different types of magnetism, such as ferromagnetism, paramagnetism, and diamagnetism.
- Magnetism plays a crucial role in numerous applications in modern technology. It is the foundation for the operation of electric motors, generators, transformers, magnetic storage devices, and even in medical imaging techniques like MRI. Understanding magnetism not only helps in exploring the natural forces of the universe but also in advancing technologies that drive our daily lives.

2. Basic Terms and Definitions in Magnetism

- Magnet:

An object that produces a magnetic field and can attract materials like iron, nickel, and cobalt. Magnets can be natural (like lodestone) or artificial.

- Magnetic Poles:

The regions at the ends of a magnet where the magnetic force is strongest, known as the North Pole (N) and South Pole (S). Like poles repel, unlike poles attract.

- Magnetic Field (B):

The region around a magnet where magnetic forces can be detected. It is represented by magnetic field lines and measured in Tesla (T).

- Magnetic Field Lines:

Imaginary lines that show the direction of the magnetic field, flowing from the north pole to the south pole of a magnet. The closer the lines, the stronger the field.

- Magnetic Dipole:

A system with two opposite magnetic poles, like a bar magnet. Earth itself behaves like a giant magnetic dipole.

- Magnetic Dipole Moment (μ):

A vector quantity that represents the strength and orientation of a magnetic dipole. It is calculated as:

$$\mu = m \times 2l \quad \dots(1)$$

- where m is the magnetic pole strength and $2l$ is the distance between the poles.

- It is defined as the maximum amount of torque caused by magnetic force on a dipole that arises per unit value of surrounding magnetic field in vacuum.

$$\vec{\tau}_{mag} = \mu \times \vec{B} \quad \dots(2)$$

- The unit for dipole moment is ampere-square metre.

- As shown in Fig. 1, the magnetic dipole moment is $\mu = I \times A$.

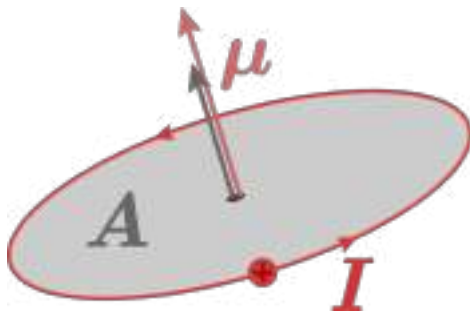


Fig. 1: Magnetic Dipole Moment

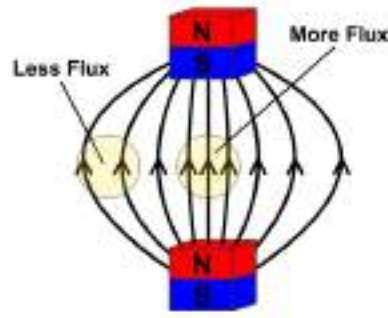


Fig. 2: Magnetic Flux

$$B = \frac{\Phi}{A}$$

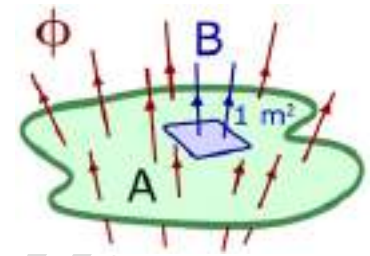


Fig. 3: Magnetic Flux Density (B)

- Magnetic Flux (Φ):

Magnetic flux is a measurement of the total magnetic field which passes through a given area. It is given by:

$$\Phi = B \cdot A \cdot \cos(\theta) \quad \dots(3)$$

where B is the magnetic field, A is the area, and θ is the angle between the field and the normal to the surface.

The SI unit of magnetic flux is the Weber (Wb).

- Magnetic Flux Density (B):

Magnetic induction is the number of lines of force through a unit area of a perpendicular cross-section. Thus;

The SI unit of B is Weber per square meter (Wb/m^2) and CGS unit is Tesla (T); 1 Gauss = 10^{-4} Tesla. Measured in Tesla (T).

- Magnetic Field Strength (H):

The strength (or intensity) of magnetic field at any point in magnetic field is force experienced by a unit north pole placed at that point. It is given by:

$$H = \frac{I}{2\pi r} \quad \dots(4)$$

where I is the current and r is the distance from the conductor. The unit of H is ampere-turns per meter (A/m) in SI system. Measured in A/m (Ampere per meter).

- Magnetization (M):

The magnetic moment per unit volume of a material, representing how strongly a material is magnetized:

$$M = \frac{\mu}{V} \quad \dots(5)$$

where μ is the magnetic moment and V is the volume.

The unit of magnetisation in SI system is amperes per meter (A/m).

As magnetisation is induced by magnetic field, M is proportional to H .

$$\text{Thus, } M \propto H \text{ or } M = \chi H, \quad \dots(6)$$

Where, χ is called as **magnetic susceptibility**.

- Magnetic Susceptibility (χ):

A dimensionless quantity that indicates how much a material will become magnetized in an external magnetic field:

$$\chi = \frac{M}{H} \quad \dots(7)$$

where M is the magnetization and H is the magnetic field strength.

It is also defined as **magnetisation (M) produced in the material per unit applied magnetic field (H)**.



- Magnetic Induction (B):

Also known as magnetic flux density, it represents the magnetic effect produced by a magnetic field on a material. It is related to the magnetic field strength as:

$$B = \mu H \quad \dots(8)$$

- Relation Between B and H :

The magnetic flux density B and magnetic field strength H are related through permeability μ :

$$B = \mu H$$

where μ is the permeability of the medium.

The magnetic induction B produced inside the material is given by;

$$B = \mu_0(H + M)$$

Where, μ_0 is known as permeability of the free space.

$$B = \mu_0 \left(1 + \frac{M}{H} \right) H$$

$$B = \mu_0 (1 + \chi) H \quad \dots(9)$$

It is equal to $4\pi \times 10^{-7}$ Henry per meter (H/m).

- Permeability (μ):

A measure of how easily magnetic field lines can pass through a material. High-permeability materials allow stronger magnetic fields.

- Absolute Permeability (μ):

The measure of how easily a material can support the formation of a magnetic field within itself. For a vacuum, it's denoted as; $\mu_0 = 4\pi \times 10^{-7} H/m$

The absolute permeability of the material is a measure of the degree of which the field lines penetrate (or permeate) the material.

It is defined as **the ratio of magnetic induction B in the medium to the magnetising field H .**

$$\text{Thus, } \mu_a = \frac{B}{H} \quad \dots(10)$$

The unit of absolute permeability is Henry per meter (H/m).

- Relative Permeability (μ_r):

The relative permeability of a material is defined as the ratio of absolute permeability of the material to the permeability of free space.

$$\mu_r = \frac{\mu_a}{\mu_0} \quad \dots(11)$$

μ_r is only a number and has no units. Its value for air or vacuum is one.

- Relation Between μ_a and μ_r :

The absolute permeability and relative permeability are related as:

$$\mu_a = \mu_0 \mu_r \quad \dots(12)$$

- Relation between μ_r and χ

Magnetic Induction; $B = \mu_0 (1 + \chi) H$ or $B = \mu_a H$

Thus; $\mu_a = \mu_o(1 + \chi)$

$$\text{as; } \mu_r = \frac{\mu_a}{\mu_o};$$

$$\mu_r = 1 + \chi \quad \dots(13)$$

- **Retentivity:**

The ability of a material to retain its magnetization after the external magnetic field is removed.

- **Coercivity:**

The measure of the resistance of a magnetic material to becoming demagnetized.

- **Ferromagnetism:**

Strong magnetic behavior where materials can become permanently magnetized (e.g., iron, cobalt, nickel).

- **Paramagnetism:**

Weak magnetic attraction observed in materials that lose their magnetism when the external field is removed.

- **Diamagnetism:**

A property where materials create a weak magnetic field opposite to an applied external field, causing slight repulsion.

- **Electromagnet:**

A magnet created when an electric current flows through a coil of wire, producing a magnetic field. The field disappears when the current is turned off.

3. Origin of Magnetization

- The magnetic properties of solids arise due to the behavior of electrons undergoing different types of motion within atoms. These motions generate magnetic moments, which collectively contribute to the magnetization of the material. The magnetic properties of materials come from the motion of electrons inside atoms. These motions create tiny magnetic fields, which add up to give a material its overall magnetism. There are three main types of electron motions that contribute to this phenomenon:

- **Orbital Motion of Electrons:**

- Electrons move around the nucleus of an atom in specific paths called orbits. Think of it like planets revolving around the sun. This circular motion of charged particles (electrons) creates a tiny current loop, just like current flowing through a wire coil generates a magnetic field. Each electron's orbit acts like a miniature magnet, producing a magnetic field called the orbital magnetic dipole moment. When we sum up the contributions from all electrons in the atom, we get the total orbital magnetic moment. The stronger the electron's motion around the nucleus, the stronger the magnetic effect from the orbital motion.

- **Spin Motion of Electrons:**

- Besides revolving around the nucleus, each electron also spins around its own axis, much like how Earth spins while revolving around the Sun. This property is known as electron spin. The spinning electron generates its own tiny magnetic field, called the spin magnetic moment. Interestingly, this spin contribution is often stronger than the orbital contribution because the electron's spin is a fundamental property, not dependent on its motion through space. In many magnetic materials (like iron), the spin magnetic moment is the dominant factor that causes strong magnetism.

- Nuclear Spin

- Just like electrons, the nucleus of an atom can also spin. This motion creates a small magnetic field, known as the nuclear magnetic moment. Although the nucleus is much larger than an electron, it carries a very tiny charge compared to the electron's motion. As a result, its magnetic contribution is about 1/2000th of that of the electrons. Because the nuclear magnetic moment is so small, we usually ignore it when discussing the magnetism of materials. However, it becomes important in certain advanced technologies like Nuclear Magnetic Resonance (NMR) and MRI in medical imaging.
- The magnetism of any material mainly comes from i) The orbital motion of electrons (like tiny current loops). ii) The spin motion of electrons (acting like tiny spinning magnets). iii) The nuclear spin does add a little, but it's so small that it's not significant in most cases.

4. Classification of Magnetism

- Magnetism in materials can be classified based on how they respond to an external magnetic field. This response depends on the arrangement and behavior of the electrons' magnetic moments within the material. The three main types of magnetism are:

- Diamagnetism
- Paramagnetism
- Ferromagnetism

i) Diamagnetism

- Diamagnetism is a weak form of magnetism that occurs in all materials but is usually very small and easily overshadowed by other types of magnetism. Diamagnetic materials are repelled by a magnetic field. It arises due to the change in the orbital motion of electrons when an external magnetic field is applied. This change creates tiny currents that generate a magnetic field in the opposite direction to the applied field.

- Characteristics:

- Weakly repelled by magnetic fields.
- Magnetic susceptibility (χ) is negative i.e. $\chi < 0$. It is due to the repulsion experienced by diamagnetic materials when placed in a magnetic field.
- No permanent magnetic moment in the absence of an external field.
- Effect disappears when the external magnetic field is removed.
- The relative permeability is slightly less than one i.e. $\mu_r < 1$.
- The magnetic susceptibility is temperature independent and which has negative value.

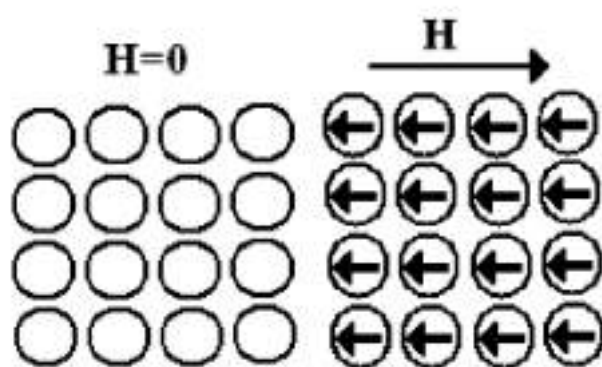


Fig. 4: Domain structure

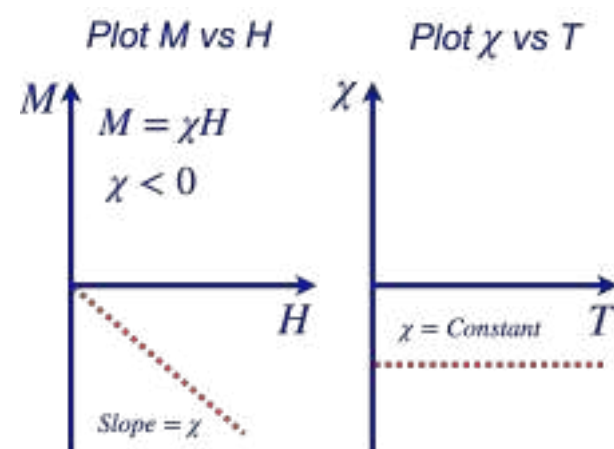


Fig. 5: Effect of temperature on M and χ

- Examples:

Bismuth, copper, silver, gold, lead, water, quartz, and graphite.

ii) Paramagnetism

- Paramagnetism occurs in materials that have unpaired electrons, which create tiny magnetic moments. These materials are weakly attracted to an external magnetic field. It is caused by the alignment of magnetic dipoles (due to unpaired electrons) in the direction of the applied magnetic field. However, this alignment is disordered because of thermal motion, making the effect weak.
- **Characteristics:**
 - Weakly attracted to magnetic fields.
 - Magnetic susceptibility (χ) is positive but small i.e. $\chi < 0$.
 - It is due to the slight attraction of magnetic field when placed in a magnetic field.
 - No permanent magnetism after removing the external field.
 - Magnetic behavior decreases with increasing temperature (due to thermal agitation disrupting alignment).
 - The **relative permeability** of these materials is slightly above than one i.e. $\mu_r > 1$.
 - A temperature dependent susceptibility which known as the **Curie Law**.

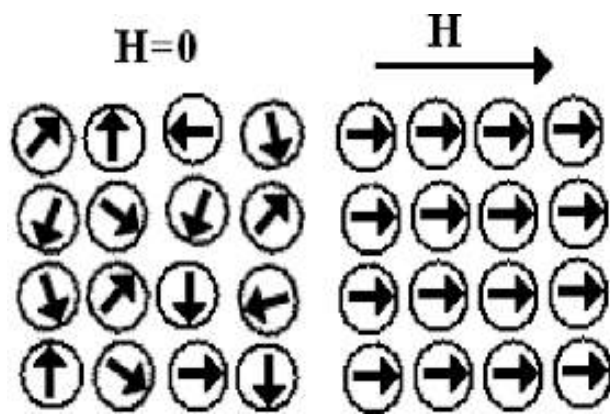


Fig. 6: Domain structure

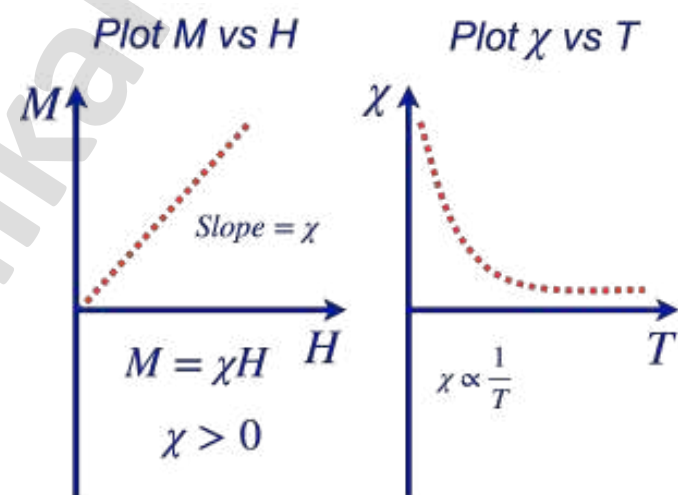


Fig. 7: Effect of temperature on M and χ

- **Examples:**
Aluminum, platinum, magnesium, manganese, and oxygen.

iii) Ferromagnetism

- Ferromagnetism is the strongest form of magnetism. Ferromagnetic materials are strongly attracted to magnetic fields and can become permanently magnetized, even after the external field is removed. It results from the parallel alignment of magnetic dipoles in large regions called domains. In ferromagnetic materials, these domains naturally align in the same direction, leading to strong magnetization.
- **Characteristics:**
 - Strongly attracted to magnetic fields.
 - Magnetic susceptibility (χ) is very large and positive.
 - Can retain permanent magnetism (hysteresis effect).
 - The relative permeabilities of these materials are much greater than one and dependent on the field strengths i.e. $\mu_r > 1$.
 - The ferromagnetic susceptibility is greater than one and positive i.e. $\chi \gg 1$. It is due to the large attraction of magnetic field when placed in a magnetic field.
 - Has a Curie temperature: Above this temperature, the material loses its ferromagnetic properties and becomes paramagnetic.

- Above the **Curie temperature** (T_c), ferromagnetic materials behave as *paramagnetic materials* and their *susceptibility* is given by the **Curie-Weiss law**, defined as,

$$\chi = \frac{C}{T - T_c}$$

...(14)

- where C is material constant, T and T_c are Temperature and Curie temperatures.
- **Examples:**
Iron, cobalt, nickel, gadolinium, and their alloys.

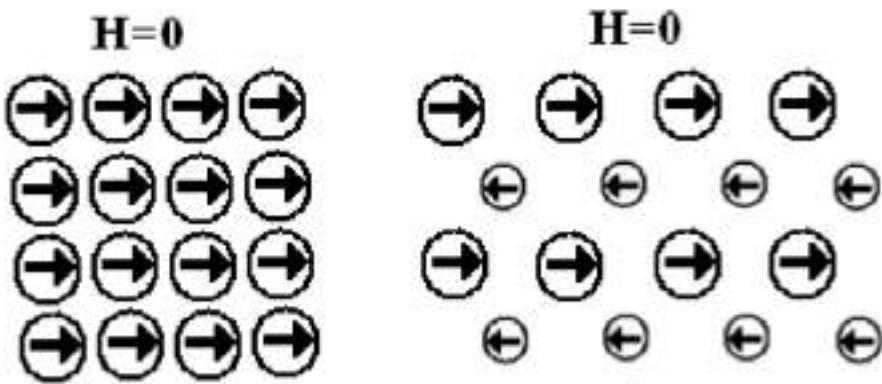
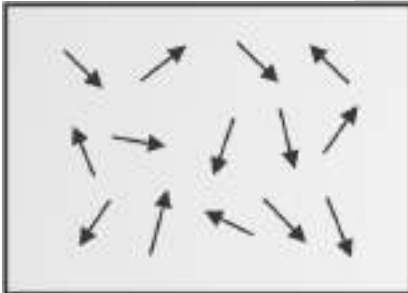
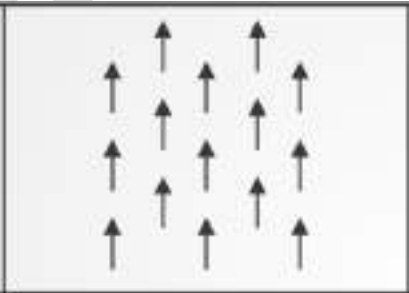
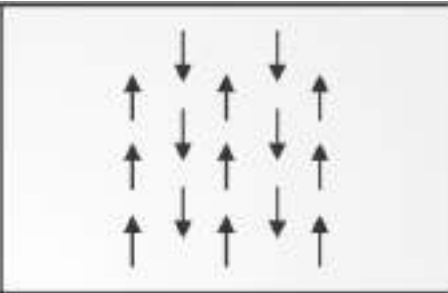
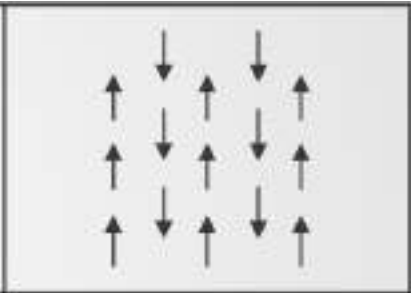


Fig. 8: Domain structure

- Comparison Table

Property	Diamagnetism	Paramagnetism	Ferromagnetism
Response to Field	Weakly repelled	Weakly attracted	Strongly attracted
Magnetic Moment	None (no unpaired electrons)	Due to unpaired electrons	Due to unpaired electrons and domain alignment
Susceptibility (χ)	Negative	Positive (small)	Positive (large)
Effect of Temperature	No effect	Decreases with temperature	Disappears above Curie temperature
Permanent Magnetism	No	No	Yes
Examples	Copper, gold, bismuth	Aluminum, platinum, oxygen	Iron, cobalt, nickel

- The orientation of spins in magnetic materials

			
Paramagnetic Materials : In this case, magnetic dipole moments are oriented randomly and interaction is negligible	Ferromagnetic Materials : In this case, all magnetic dipole moments are oriented in the same direction	Antiferromagnetic Materials : In this case, magnetic dipole moments are of equal magnitude but oriented in opposite direction to each other	Ferrimagnetic Materials : In this case, magnetic dipole moments are of different magnitude and oriented in opposite direction

5. Temperature Dependent Magnetic Transitions

- The magnetic properties of materials are strongly influenced by temperature. As temperature changes, the thermal energy affects the alignment of magnetic moments (spins), leading to transitions between different magnetic states. These transitions are known as temperature-dependent magnetic transitions and are characterized by specific critical temperatures.

- The key magnetic transitions include:

- Curie Temperature (T_C)

- Neel Temperature (T_N)

i) Curie Temperature (T_C)

- The Curie temperature is the temperature above which a ferromagnetic or ferrimagnetic material loses its permanent magnetism and becomes paramagnetic.
- Below T_C : The magnetic moments are aligned in the same direction due to strong exchange interactions, resulting in spontaneous magnetization.
- At and Above T_C : Thermal agitation becomes strong enough to disrupt the alignment of spins, causing the material to behave like a paramagnet (random spin orientation).
- Irreversible transition: The loss of magnetization is not recovered unless the material is cooled below T_C .
- The drastic drop in magnetization at T_C .
- Magnetic susceptibility (χ) follows the Curie-Weiss law above T_C :

$$\chi = \frac{C}{T - T_C} \quad \dots(15)$$

- where C is the Curie constant.

- Examples:

- Iron ($T_C \approx 770^\circ\text{C}$)

- Nickel ($T_C \approx 358^\circ\text{C}$)

- Cobalt ($T_C \approx 1,115^\circ\text{C}$)

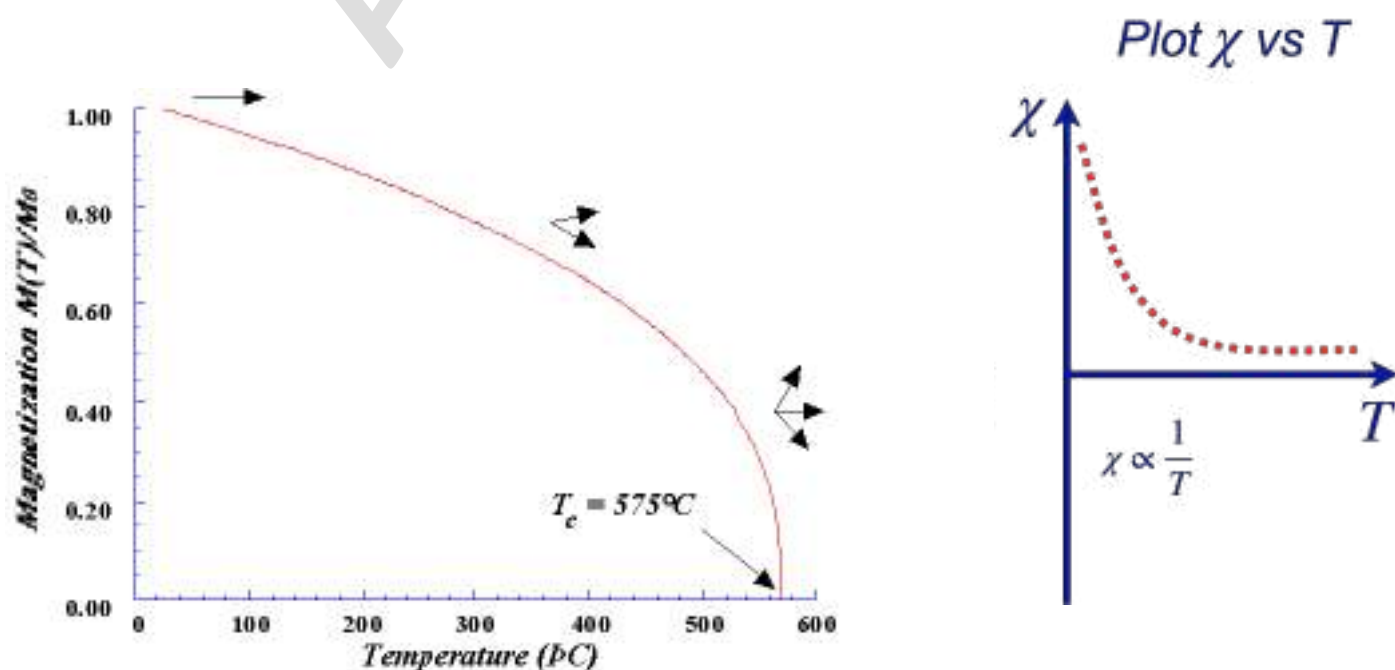


Fig.9: a) Magnetisation vs Temperature

b) Magnetic susceptibility (χ) vs Temperature

ii) Neel Temperature (T_N)

- Definition: The Neel temperature is the critical temperature above which an antiferromagnetic material becomes paramagnetic. The clue to antiferromagnetism is the behaviour of susceptibility above a critical temperature, called the Néel temperature (T_N).
- Below T_N : Magnetic moments of adjacent atoms or ions are aligned in an antiparallel fashion (opposite directions), cancelling each other out.
- At and Above T_N : Thermal energy disrupts this ordered antiparallel alignment, leading to random spin orientation similar to paramagnetic behaviour.
- At Néel temperature, the thermal energy becomes sufficient enough to destroy the microscopic magnetic ordering within the material.
- A sharp change in magnetic susceptibility at T_N . Unlike ferromagnets, no net magnetization exists even below T_N because spins are opposite.
- Examples:
 - Manganese oxide (MnO) ($T_N \approx 122K$)
 - Nickel oxide (NiO) ($T_N \approx 523K$)
 - Hematite ($T_N \approx 956K$)

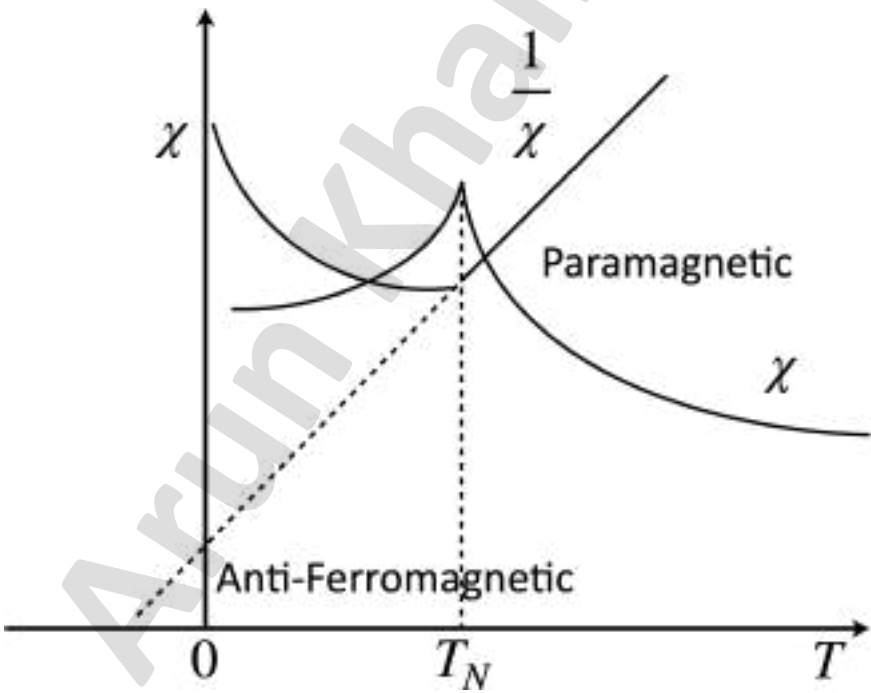


Fig. 10: Magnetic susceptibility (χ) vs Temperature

Parameter	Curie Temperature (T_C)	Neel Temperature (T_N)
Applies to	Ferromagnetic/Ferrimagnetic materials	Antiferromagnetic materials
Transition	Ferromagnetic \rightarrow Paramagnetic	Antiferromagnetic \rightarrow Paramagnetic
Spin Behavior	Parallel alignment \rightarrow Random	Antiparallel alignment \rightarrow Random
Permanent Magnetism	Lost above T_C	No permanent magnetism below or above T_N
Example	Iron ($T_C = 770^\circ C$)	MnO ($T_N = 122K$)

6. Magnetic Hysteresis

- The term "hysteresis" comes from the Greek word meaning "to lag behind." In the context of magnetism, magnetic hysteresis refers to the phenomenon where the magnetization (M) of a ferromagnetic material lags behind the applied magnetic field (H) during the process of magnetization and demagnetization.
- This lagging behaviour is a characteristic feature of ferromagnetic materials and can be visualized using a hysteresis loop, also known as the M vs. H curve or $B - H$ curve (where B is the magnetic flux density).
- When a ferromagnetic material is subjected to an external magnetic field (H), the material's magnetic domains (regions where magnetic moments are aligned) start to align with the field, causing an increase in magnetization (M).
- However, when the magnetic field is reduced to zero, the material does not return to its original unmagnetized state. This is because some domains remain partially aligned, resulting in residual magnetization.
- To completely demagnetize the material, a reverse magnetic field must be applied. The process of increasing, decreasing, and reversing the magnetic field forms a loop on the M vs. H graph, known as the **hysteresis loop**.
- The microscopic ordering of electron spins characteristic of ferromagnetic materials leads to the formation of regions of magnetic alignment called domains.

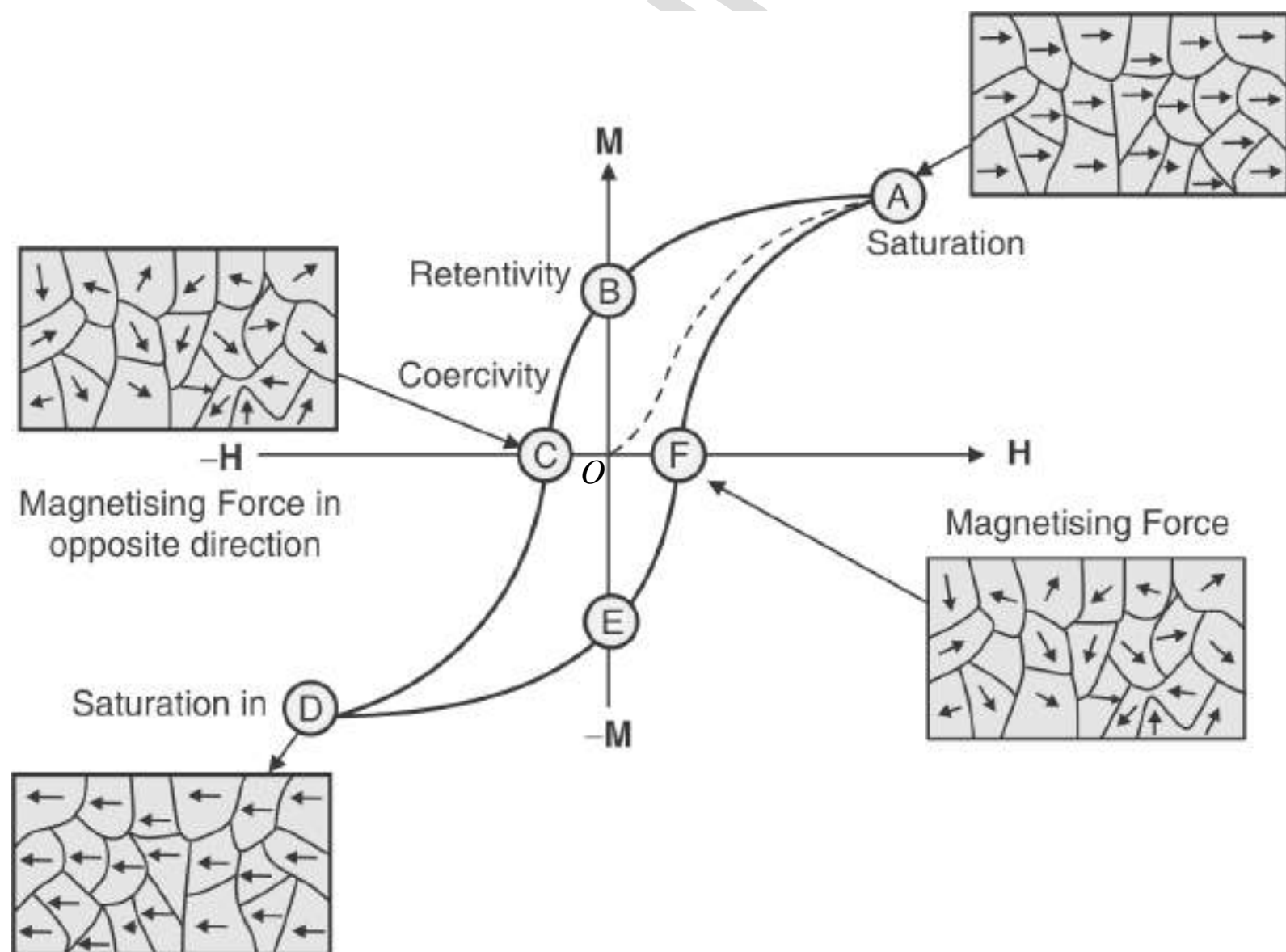


Fig. 11: Hysteresis M vs H curve



- **Path Analysis of the Hysteresis Loop**
- **Initial Magnetization Curve (Path OA):**
 - When the magnetic field H is increased from zero, the material's magnetization M increases as well. This is because magnetic dipole moments (tiny magnets within the material) begin to align with the direction of the applied field. The path followed is from O to A, showing a rapid increase in magnetization initially, which gradually slows down as the dipoles become more aligned.
- **Saturation Magnetization (Point A):**
 - At a particular value of H , all the magnetic dipoles in the material are fully aligned in the direction of the field. Beyond this point, further alignment is not possible, even if H is increased. This state is called **saturation magnetization**, and point A is known as the saturation point.
- **Reducing Magnetic Field (Path AB):**
 - When the magnetic field is reduced from point A towards zero, the material's magnetization does not decrease to zero immediately. Instead, it follows path AB, showing that the material retains some magnetization even after the external field is removed. This residual magnetization is called **retentivity or residual magnetism** (M_r).
- **Applying Reverse Magnetic Field (Path BC):**
 - To completely demagnetize the material, a reverse magnetic field must be applied. As the reverse field increases, the magnetization decreases, following path BC. At point C, the magnetization becomes zero. The magnitude of the reverse field required to bring the magnetization to zero is called the coercive force (H_c), and the property is known as **coercivity**.
- **Saturation in Opposite Direction (Path CD):**
 - If the reverse magnetic field is further increased, the magnetic dipoles align in the opposite direction, and the material reaches saturation magnetization in the negative direction at point D.
- **Reducing Reverse Magnetic Field (Path DE):**
 - Reducing the reverse field towards zero causes the magnetization to follow path DE, where the material again retains some residual magnetization in the opposite direction.
- **Reapplying Positive Magnetic Field (Path EF → FA):**
 - Applying the magnetic field in the positive direction again causes magnetization to increase, following path EF. Eventually, the material reaches positive saturation at point A, completing the hysteresis loop.
- **Soft Magnetic Materials:**
 - Narrow hysteresis loop.
 - Low coercivity and low retentivity.
 - Easily magnetized and demagnetized.
 - Applications: Transformer cores, electromagnets, inductors.
- **Hard Magnetic Materials:**
 - Wide hysteresis loop.
 - High coercivity and high retentivity.
 - Difficult to demagnetize (ideal for permanent magnets).
 - Applications: Permanent magnets, magnetic storage devices, electric motors.

7. Magnetoresistance and Giant Magnetoresistance (GMR)

- Magnetoresistance (MR)

- Magnetoresistance is a physical phenomenon where the electrical resistance of a material changes when subjected to an external magnetic field. This effect occurs due to the influence of the magnetic field on the motion of charge carriers (electrons) within the material.

- Giant Magnetoresistance (GMR)

- In 1988, scientists Albert Fert and Peter Grünberg discovered a revolutionary effect known as Giant Magnetoresistance (GMR), which significantly advanced the field of magnetic storage and spintronics.
- GMR is an enhanced form of magnetoresistance observed in magnetic multilayer structures made of alternating ferromagnetic and non-magnetic layers, typically on the nanometer scale.

- Structure of GMR Materials:

- Multilayer Films: Alternating layers of:

- Ferromagnetic materials (e.g., Iron (Fe), Cobalt (Co)).
- Non-magnetic spacer layers (e.g., Chromium (Cr), Copper (Cu)).

- Example Systems:

- Fe/Cr multilayers.
- Co/Cu multilayers.

- Working Principle:

- In zero magnetic field, the magnetic moments of adjacent ferromagnetic layers are often aligned antiparallel, causing high electrical resistance due to electron scattering.
- When an external magnetic field is applied, these moments become aligned parallel, which reduces electron scattering and lowers the resistance.
- The change in resistance is much larger than in conventional magnetoresistance, hence the name "Giant" Magnetoresistance.
- Reduction in the thickness of the Cr layer (non-magnetic spacer) in Fe/Cr multilayers leads to a larger change in resistance under a magnetic field.
- This behavior is depicted in Fig. 12 (typically showing resistance vs. magnetic field curves).

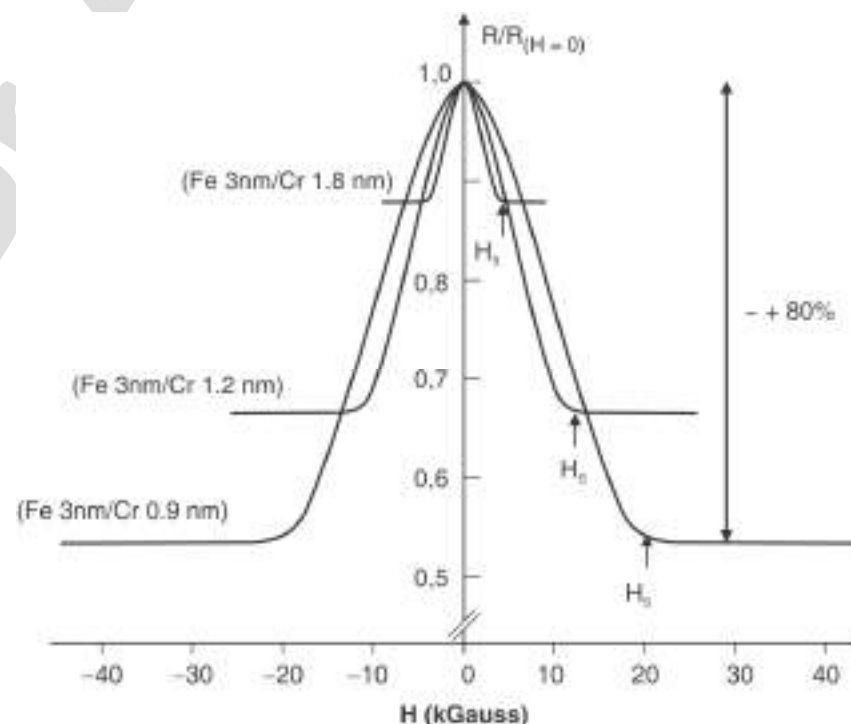


Fig. 12 Resistance vs. magnetic field curves.

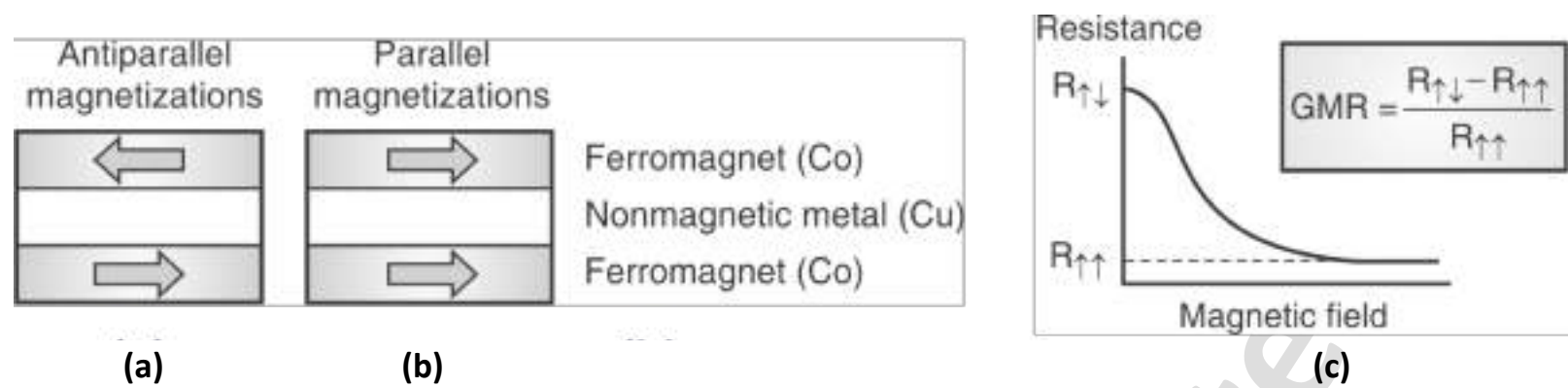


Fig. 13: A schematic three-layer structure Co|Cu|Co.

- A schematic three-layer structure is shown in Fig.12. Nonmagnetic and conducting Cu layer is deposited between two ferromagnetic Co layers.
- In absence of the magnetic field spins from unpaired electrons in ferromagnetic materials align anti parallel to each other as shown in Fig (a). While when field is applied, the spins align in the direction parallel to the field direction to give the material the total magnetic moment.
- It is well known that Copper is good electrical conductor, however at a few atom thicknesses, electron scattering causes significant reduction in the resistance. It was also found that resistance to the flow of current in the direction perpendicular to these layers is very high.
- When magnetic field is applied parallel to the layers, magnetic moments in successive ferromagnetic layers align in the direction of magnetic field as shown in Fig. (b). Thus causes the decrease in resistance of the multilayer's as shown in Fig. (c).
- The value of GMR is calculated using the resistance measured by applying magnetic field in parallel and anti parallel direction using formula,

$$GMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}} \quad \dots(16)$$

- The GMR effect occurs because conduction electron passes easily through the magnetic layer if it encounters the electrons with parallel orientation of the spin in the direction of magnetic field as shown in Fig. 12(b) and this process reduces the resistance. While if it encounters with electrons having antiparallel spin, it experiences the high resistance as shown in Fig. 12. This also can be easily seen from Fig. 13.

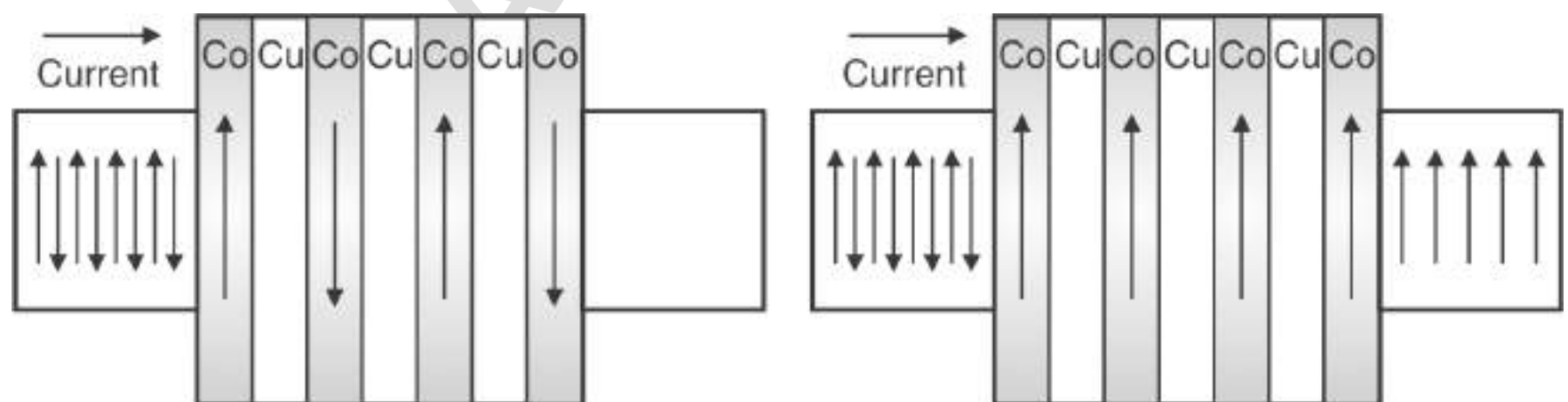


Fig. 13: Conduction electron passes through Co|Cu layers structure

- **Importance of GMR**
- Unlike traditional magnetoresistance, GMR works effectively at room temperature and with moderate magnetic fields, making it highly suitable for real-world applications.
- The discovery of GMR revolutionized data storage technology.

- Applications of Giant Magnetoresistance (GMR)

- Giant Magnetoresistance (GMR) has revolutionized various industries due to its ability to detect small changes in magnetic fields with high sensitivity. Here are the key applications:
- **Hard Disk Drives (HDDs):**
 - GMR read heads enabled massive increases in data storage density.
 - Allowed for the development of compact, high-capacity drives.
- **Magnetic Sensors:**
 - Used in automotive systems (e.g., wheel speed sensors), biomedical devices, and position sensors.
- **MRAM (Magnetoresistive Random-Access Memory):**
 - A type of non-volatile memory that retains data without power.
- **Spintronics:**
 - A revolutionary field of electronics that manipulates the spin of electrons in addition to their charge.
 - GMR forms the foundation of many spintronic devices.

8. Magneto-Caloric Effect (MCE)

- The Magneto-Caloric Effect (MCE) is a phenomenon where a change in the magnetic field applied to certain materials causes a change in their temperature. This effect is a result of the interaction between the material's magnetic moments and the external magnetic field, leading to either heating or cooling.
- **Concept:**
 - Applying a magnetic field → Material heats up (due to magnetic moment alignment).
 - Removing the magnetic field → Material cools down (due to magnetic moment disorder).
- **Working mechanism of Magneto-Caloric Effect:**
 - The MCE is based on the principles of thermodynamics and magnetism.
- **In the Absence of a Magnetic Field:** The magnetic moments (tiny magnetic dipoles) in the material are randomly oriented, representing high entropy (disorder).
- **When a Magnetic Field is Applied (Isothermal Magnetization):** The magnetic moments align with the external field, leading to reduced entropy (more order). This alignment releases energy as heat, causing the material's temperature to increase.
- **When the Magnetic Field is Removed (Adiabatic Demagnetization):** The magnetic moments return to a random orientation, increasing the system's entropy. This process absorbs heat from the surroundings, causing the material's temperature to drop.
- **Thermodynamic Explanation**
 - The MCE is related to the change in entropy (ΔS) and temperature (ΔT) of a material due to a change in the applied magnetic field (ΔH).
- **Equation:**

$$\Delta T = -\frac{T}{C} \left(\frac{\partial S}{\partial H} \right)_T \Delta H \quad \dots(17)$$

Where: ΔT = Change in temperature, T = Absolute temperature, C = Heat capacity of the material,
 S = Entropy, H = Magnetic field.

- The sign of ΔT depends on whether the field is being applied (heating) or removed (cooling).

- We can illustrate the cooling produced by adiabatic demagnetization using temperature- entropy diagram of the paramagnetic substance for $H = 0$ and $H = H$ as shown in Fig. 14.

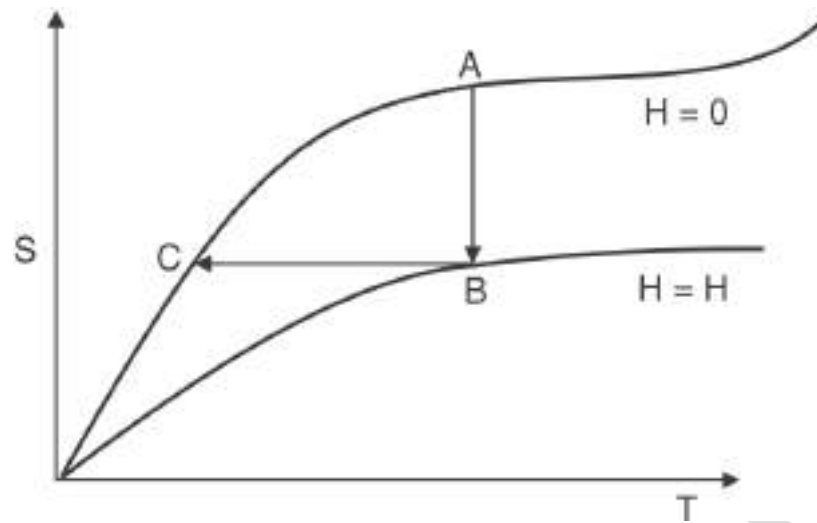


Fig. 14: temperature- entropy diagram of the paramagnetic substance for $H = 0$ and $H = H$.

- The change in entropy during isothermal magnetization is represented by the arrow AB, which shows that during isothermal magnetization entropy of the substance decreases. Now if the field is switched off, the substance demagnetizes adiabatically, temperature of the system falls while entropy remains constant as represented by the arrow BC.
- According to Curie law, the susceptibility of the paramagnetic substance is given by,

$$\chi = \frac{C}{T}. \quad \dots(18)$$

- From above equation, susceptibility of paramagnetic substance increases with decrease in temperature. Hence magneto-caloric effect increases if the initial temperature of the substance is lowered. Thus if the Curie law is true up to liquid helium temperature, and if the subject is adiabatically demagnetized, a large cooling should result and the temperature lower than that of liquid helium can be produced. In general, fall in temperature of paramagnetic substance during adiabatic demagnetization is given by,

$$T_f - T_i = \frac{-C_V}{T_i C_H} H_i^2 \quad \dots(19)$$

Where:

T_f = final temperature after demagnetization

T_i = initial temperature before demagnetization

C_V = heat capacity at constant volume

C_H = heat capacity at constant magnetic field

H_i = initial magnetic field strength

- $T_f - T_i$ is negative or $T_f < T_i$ means the fall in temperature is greater for low value of initial temperature and high value of initial magnetization.
- $H = 0$ Curve: Represents the entropy when no magnetic field is applied (high entropy state).
- $H = H$ Curve: Represents the entropy when the magnetic field is applied (low entropy state).
- Cooling Effect: The vertical drop from point A to B represents the decrease in temperature during adiabatic demagnetization.

- Materials Exhibiting MCE

- Paramagnetic Materials: Show MCE at very low temperatures (used in scientific cooling applications). Example: Gadolinium salts.
- Ferromagnetic Materials: Exhibit strong MCE near their Curie temperature (temperature at which they lose ferromagnetism). Example: Gadolinium (Gd), LaFeSi-based alloys, MnFeP-based compounds.
- Magnetocaloric Alloys: Engineered materials with enhanced MCE for commercial applications.

- Applications of the Magneto-Caloric Effect

- Magnetic Refrigeration: Eco-friendly cooling technology that eliminates harmful refrigerant gases. More energy-efficient than traditional vapor-compression refrigeration systems.
- Used in: Refrigerators, Air conditioners, Cryogenic cooling systems
- Cryogenics: Used for ultra-low temperature cooling in scientific research, space technology, and quantum computing.
- Magnetic Heat Pumps: Emerging technology for heating and cooling in industrial applications.
- Space Technology: Efficient cooling systems for satellites and space probes.

9. Adiabatic Demagnetization

- Adiabatic demagnetization is a technique used to achieve extremely low temperatures, often in the microkelvin range ($10^{-5} K$). This method relies on the thermodynamic behavior of paramagnetic salts under varying magnetic fields.

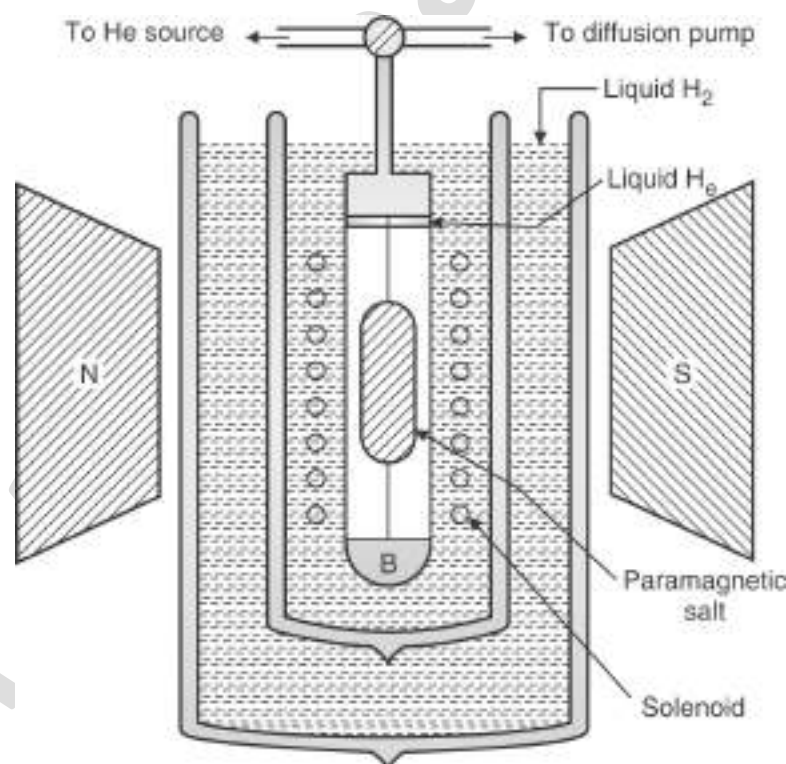


Fig. 15: Production of Low Temperature by Adiabatic Demagnetization.

- Experimental Setup:

- Paramagnetic Material:

- A paramagnetic salt, such as gadolinium sulfate $Gd_2(SO_4)_3 \cdot 8H_2O$, is used. It is pressed into a spheroidal shape to simplify magnetic property calculations.

- Suspension System:

- The spheroid is suspended inside a glass bulb (B), which can be connected either to: A helium gas supply (for thermal conduction), or A diffusion pump (for creating thermal isolation).

**- Thermal Shielding:**

- Bulb B is surrounded by a Dewar flask containing liquid helium (for initial cooling). This is further enclosed by another Dewar flask containing liquid hydrogen, providing an extra layer of thermal insulation.

- Magnetic Field Source:

- The entire setup is placed between the pole pieces (N and S) of a strong electromagnet, which can apply and remove the magnetic field as needed.

- Temperature Measurement:

- A co-axial solenoid coil around bulb B is used to measure the temperature indirectly through the magnetic susceptibility of the paramagnetic material.

- Working Principle:**- Initial Magnetization (Isothermal Process):**

- Helium gas is introduced into bulb B to facilitate heat exchange. The magnetic field is switched ON, causing the paramagnetic salt to become highly magnetized. This process releases the heat of magnetization, which is carried away by the helium gas to the surrounding liquid helium bath. As a result, the paramagnetic material cools back down to the temperature of liquid helium (~ 4.2 K).

- Thermal Isolation:

- After achieving thermal equilibrium, the helium gas is pumped out, creating a vacuum around the specimen. This step thermally isolates the paramagnetic material from the environment, ensuring no heat exchange occurs during the next stage.

- Adiabatic Demagnetization (Isentropic Process):

- The magnetic field is gradually switched OFF. Since the system is thermally isolated, the process is adiabatic (no heat exchange with surroundings) and isentropic (constant entropy). As the magnetic field decreases, the alignment of magnetic dipoles reduces, leading to an increase in their disorder. This increased disorder absorbs internal thermal energy, causing the temperature of the paramagnetic material to drop significantly.

- Temperature Measurement:

- The final temperature is measured based on the magnetic susceptibility, which varies with temperature. Using the solenoid coil, precise changes in susceptibility help determine the temperature, which can reach values as low as 10^{-5} K.
- The process relies on the fact that reducing the magnetic field in an isolated system causes internal energy redistribution, lowering the temperature. The system remains at constant entropy during demagnetization, leading to cooling as the magnetic disorder increases.

- Applications:

- Cryogenics: Achieving ultra-low temperatures for scientific experiments.
- Quantum Physics: Studying quantum phenomena at near-absolute zero.
- Magnetic Refrigeration: Prototype technologies based on similar principles.

1. Introduction to Superconductivity

- In 1909, Heike Kamerlingh Onnes successfully liquefied helium for the first time, introducing a novel refrigeration technique capable of achieving temperatures in the range of a few Kelvin. This breakthrough opened new avenues for low-temperature physics and enabled the discovery of remarkable phenomena.
- One of the most significant discoveries resulting from this advancement was superconductivity. In 1911, while studying the electrical resistance of metals at low temperatures, Onnes observed that the electrical resistance of highly purified mercury suddenly vanished at 4.15 K, as illustrated in Fig 1. This phenomenon, characterized by the abrupt drop to zero electrical resistance, is known as superconductivity. Materials exhibiting this property are referred to as superconductors.

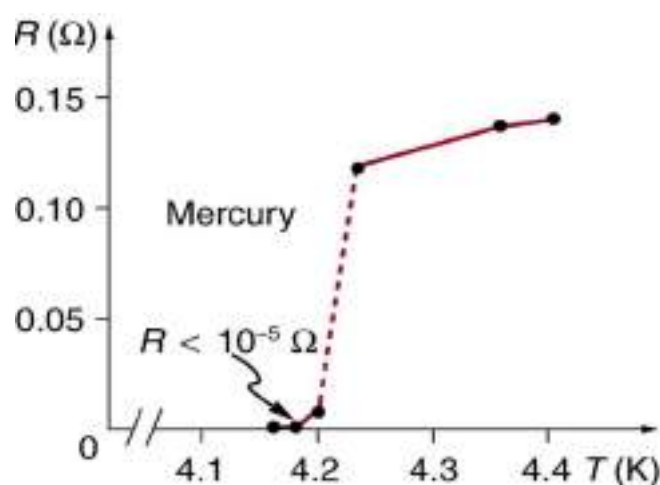


Fig. 1: A graph of resistivity Vs temperature for Hg.

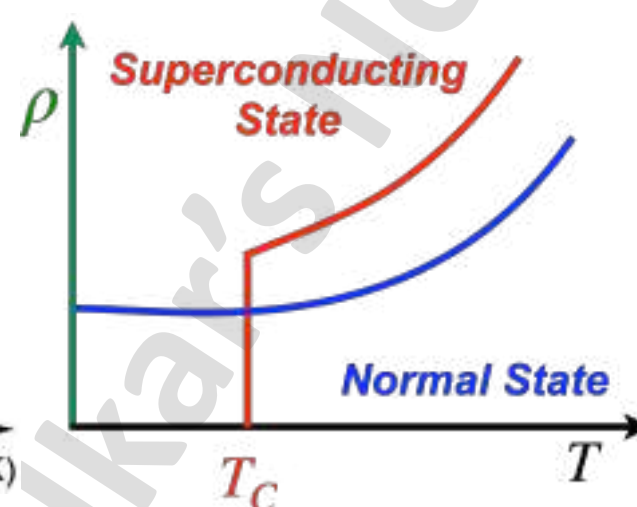


Fig. 2: Behaviour of resistivity (ρ) for superconductors

- Since its discovery, superconductivity has been the subject of extensive experimental investigations and theoretical interpretations. It remains one of the most celebrated fields in physics, having been recognized with five Nobel Prizes. Notably, Heike Kamerlingh Onnes received the Nobel Prize in Physics in 1913 "for his investigations on the properties of matter at low temperatures which led to the production of liquid helium."
- Conventional superconductors exhibit critical temperatures ranging from less than 1 K to around 20 K. For instance, solid mercury has a critical temperature of 4.15 K. The study of superconductivity continues to evolve, with ongoing research focused on discovering new materials and understanding the underlying mechanisms that govern this fascinating phenomenon.
- **Superconductivity** is defined as the complete disappearance of electrical resistance in certain materials when they are cooled below a characteristic temperature, known as the transition temperature or critical temperature (T_c). A superconductor, therefore, is a material that demonstrates this unique property.
- In addition to the absence of electrical resistance, superconductivity is accompanied by the expulsion of magnetic flux fields, a phenomenon known as the **Meissner effect**. This combination of properties results in remarkable electrical and magnetic behaviours, distinguishing superconductors from conventional conductive materials.
- **Behaviour of Resistivity (ρ) for Superconductors**
- Fig. 2 shows the resistivity (ρ) of superconductors exhibits a distinct behaviour compared to conventional conductive materials. As a superconductor is cooled down, its resistivity decreases gradually, similar to that of normal conductors, until it reaches the critical temperature (T_c). At T_c , the resistivity drops abruptly to zero, indicating the onset of the superconducting state.
- This transition from a finite resistivity to zero resistivity occurs over an extremely narrow temperature range, often less than a fraction of a Kelvin. Once in the superconducting state, the material maintains zero electrical

resistivity as long as the temperature remains below T_c and external magnetic fields and currents are within critical limits.

- In contrast, normal conductors exhibit a continuous decrease in resistivity as temperature decreases, but they never reach zero due to scattering mechanisms like electron-phonon interactions and impurities. Superconductors, however, overcome these scattering mechanisms entirely below T_c , allowing for perfect electrical conductivity.
- The behavior of resistivity in superconductors can be graphically represented, showing a sharp transition at T_c , distinguishing them clearly from normal conductive materials. This property is fundamental to the unique applications of superconductors in technologies such as MRI machines, particle accelerators, and quantum computing.

2. BCS theory of Superconductivity

- A theory of superconductivity was developed in the 1950s by John Bardeen, Leon Cooper, and J. Robert Schrieffer, this theory is known as the BCS theory.
- Cooper showed that if there is any attractive interaction between two electrons at the Fermi level, then the electrons can form a bound state in which their total energy is less than $2E_F$. Two such electrons are known as a **Cooper pair**.
- **Formation of Cooper pairs:**
- The transition of a metal from the normal to the superconducting state has the nature of a condensation of the electrons. Multiple electrons can't collect into a single state because of the Pauli exclusion principle. Froehlich was first to suggest that the electrons act as pairs coupled by lattice vibrations in the material. This coupling is viewed as an exchange of **phonons** (quantized units of vibrational energy). The boson-like behaviour of such electron pairs was further investigated by Cooper and they are called "**Cooper pairs**".

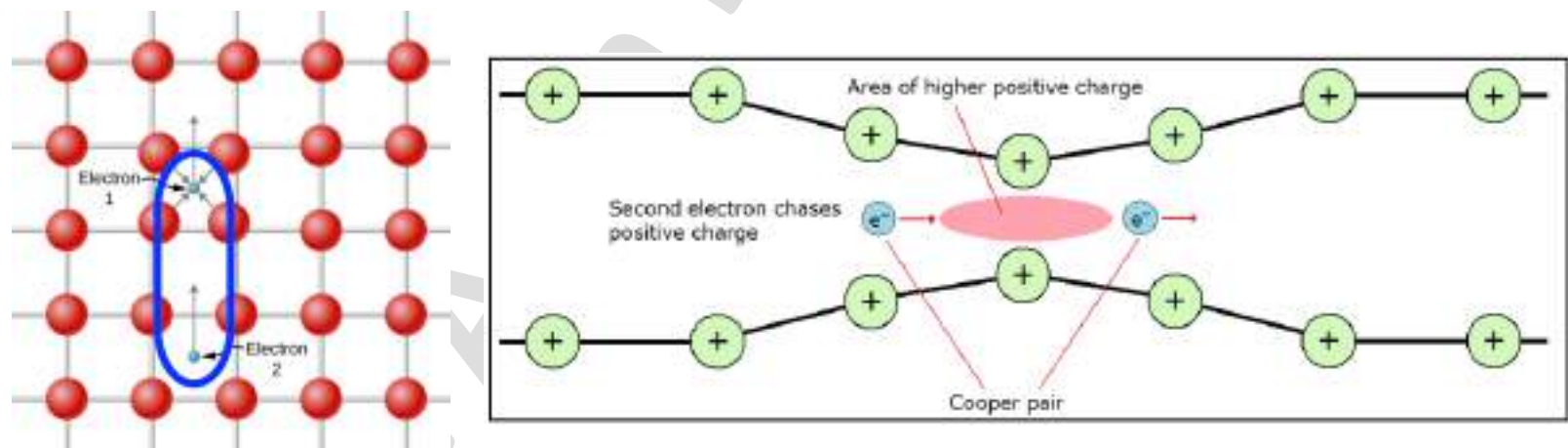


Fig. 3: a) Formation of Cooper pairs b) Electrons coupled through a phonon is called a Cooper pair.

- As shown in Fig. 3, electron 1 slightly displaces the positively charged atomic nuclei toward itself as it travels past because of the Coulomb attraction.
- Electron 2 "sees" a region with a higher density of positive charge relative to the surroundings and is therefore attracted into this region to electron 1.
- A Cooper pair can form as a result of the displacement of positive atomic nuclei.
- **Electron-Lattice-Electron interaction in superconductivity**
- The electron-lattice-electron interaction is the fundamental mechanism behind the formation of Cooper pairs in superconductors, as described in the BCS theory. Electrons moving through a metal lattice interact with the positively charged ions that form the crystal structure. This interaction leads to the creation of lattice vibrations, known as **phonons**.

- **Step 1: Electron 1 Distorts the Lattice:** As Electron 1 moves through the lattice, its negative charge attracts nearby positive ions, causing a slight local distortion of the lattice. This distortion creates a region of increased positive charge density in the vicinity of Electron 1.
- **Step 2: Lattice Responds (Phonon Emission):** The displaced ions oscillate, creating a phonon, which is essentially a quantum of the lattice vibration.
- **Step 3: Electron 2 Feels the Attraction:** After Electron 1 moves on, Electron 2 enters the region of increased positive charge. Electron 2 is attracted to this region due to the higher positive potential left behind by the lattice distortion.
- **Effective Electron-Electron Attraction:** Although Electrons 1 and 2 never directly attract each other, the lattice distortion acts as a mediator, creating an indirect attractive force. This effective attraction is strong enough at low temperatures to overcome the natural Coulomb repulsion between the electrons. The exchange of phonons between the electrons is the key to this attractive interaction.
- **Feynman Diagram Representation**

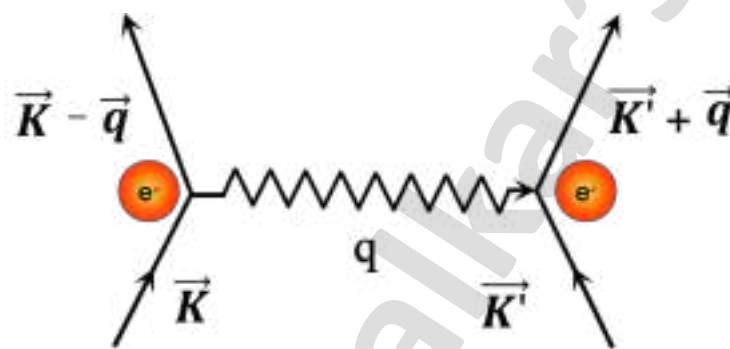


Fig. 4: Feynman diagram

- Fig. 4 shows a Feynman diagram which visually represents the indirect attractive interaction between two electrons mediated by a phonon. This interaction is key to the formation of Cooper pairs in superconductors.
- Consider an electron 1 with momentum \vec{k} passing through the lattice of positively charged ions. It attracts the lattice and loses its momentum \vec{q} to the lattice. In this interaction positive charge density in the vicinity of electron 1 will increase. Thus after this interaction the momentum of electron 1 will become $(\vec{k} - \vec{q})$.
- Now, as lattice receives momentum \vec{q} from electron 1 and starts vibrating. Also due to large positive charge accumulation in a region electron 2 already having momentum \vec{k}' , will be attracted and it will receive $+\vec{q}$ momentum from the lattice. Thus after this interaction the momentum of electron 2 will become $(\vec{k}' + \vec{q})$.
- At long distances, this attraction between electrons due to the displaced ions can overcome the electrons' repulsion due to their negative charge, and cause them to pair up. The effective net attraction between the normally repulsive electrons produces a pair binding energy on the order of milli-electron volts, enough to keep them paired at extremely low temperature.
- The energy of the pairing interaction is quite weak, of the order of 10^{-3} eV , and thermal energy can easily break the pairs. So only at low temperatures, in metal and other substrates, are a significant number of the electrons in *Cooper pairs*. The electrons in a pair are not necessarily close together; because the interaction is long range, paired electrons may still be many hundreds of nanometers apart.
- This distance is usually greater than the average inter-electron distance; so many Cooper pairs can occupy the same space. Electrons have spin $-1/2$, so they are **fermions**, but the total spin of a Cooper pair is integer (0 or 1) so it is a composite **boson**. This means the wave functions are symmetric under particle interchange. Therefore unlike electrons, multiple Cooper pairs are allowed to be in the same quantum state.
- This pair condensation is the basis for the BCS theory of superconductivity.

3. The BCS theory is able to explain properties of superconductors such as;

- Zero electrical resistance
- Persistent Current
- Critical Temperature (T_C)
- Critical Magnetic Field (H_C)
- Critical current (I_C)
- Meissner Effect
- Magnetic Penetration Depth or (London Penetration Depth)
- Flux Quantisation
- Entropy
- Isotope Effect.

i) Zero electrical resistance

- The electrical resistivity of the materials can be measured by using the Four probe resistivity measurements. The setup for electrical resistivity measurements is shown in Fig 5. At room temperature (300 K) material exhibits some finite resistance; when current is passed through the material due to this resistance voltage is developed in the material. Now if the temperature of the material is lowered from room temperature, the resistance of the material decreases and hence the voltage. Further if we continue lowering the temperature, at certain temperature the resistance of the material drops to zero which can be confirmed from zero voltage reading in the voltmeter.

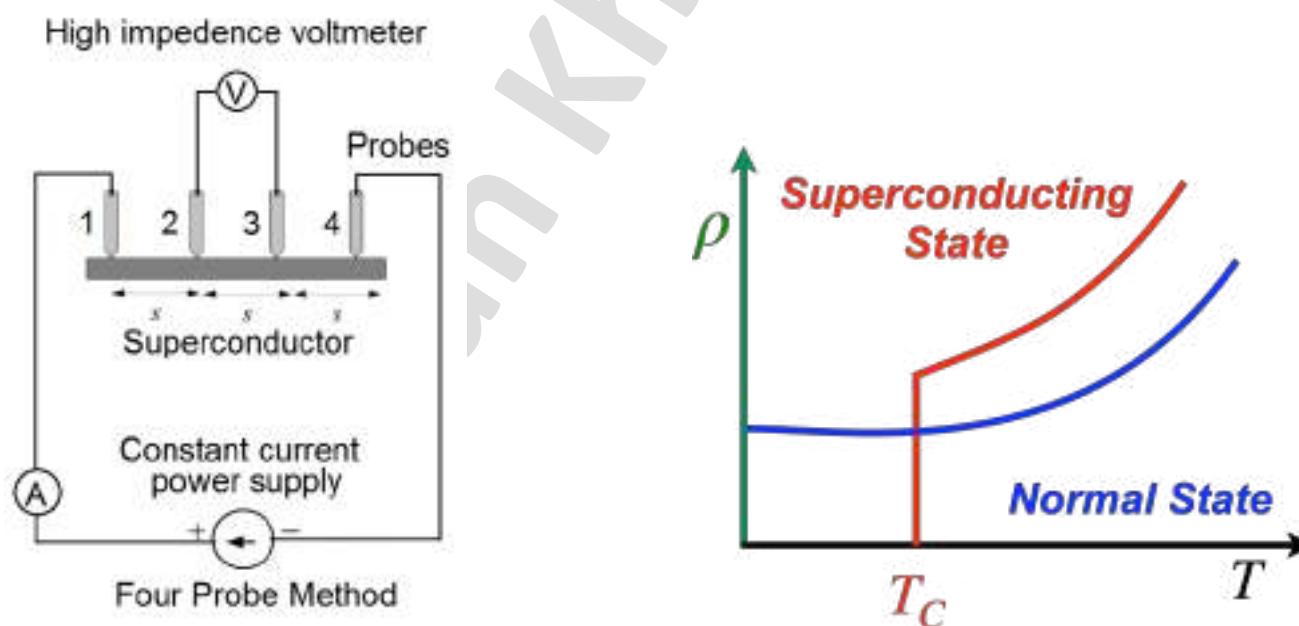


Fig. 5: a) Zero Electrical Resistance measurement by Four-Probe Method, b) Resistivity (ρ) vs Temperature (T)

- The temperature at which the resistance of the materials drops suddenly to zero is called as the Critical Temperature (T_C) of the superconductor. The material remains in superconducting state below this temperature while becomes normal conductor above this temperature.
- Thus in general, a zero electrical resistivity is a fundamental property of the superconductivity.
- It should be noted that, even at low temperatures ($0K$), the normal conductors like copper show residual resistance due to defects and impurities present in it. Hence, further attempts were made to detect whether any small residual resistance exists in the superconducting state of the material. This was done by observing whether the current decays after few years.

- The variation of resistance of superconductor with temperature measured by four probe method. The current is passed in superconductor through current probes (1 and 4).
- Voltage developed is measured with voltage probes (2 and 3). The resistance of superconductor can be calculated by **Ohm's law**;

$$R = \frac{V}{I} \quad \dots(1)$$

- **For a superconducting ring**, If it is kept in a magnetic field and is cooled below the critical temperatures so that it goes into a superconducting state. When external magnetic field is switched off, current is induced in the ring. In general if R is the resistance of the ring then the current in the ring was expected to decay exponential with time given by an equation,

$$I_t = I_0 e^{\frac{-Rt}{L}} \quad \dots(2)$$

where, I_t is current at time t ,

I_0 is initial current and

L is the inductance.

- **Normal state**: A voltage is developed across voltage probes and Ohm's law is obeyed. Above T_c The material behaves like a normal conductor with finite resistance.
- **At T_c** : A sharp drop in resistance is observed.
- **Superconducting state**: The resistance of superconductor vanishes ($R = 0$) and hence the voltage across voltage probes disappear i.e. ($V = 0$) while current continues to flow. Below T_c the resistance drops to zero, confirming superconductivity.
- However one should keep in mind that the current flowing in the superconducting loop clearly cannot be measured by inserting an ammeter into the loop, since this would introduce a resistance and the current would rapidly decay.
- So other option is to detect the magnitude of the magnetic field as it is directly proportional to the current circulating in the loop, and the field can be measured without drawing energy from the circuit.

ii) Persistent Current

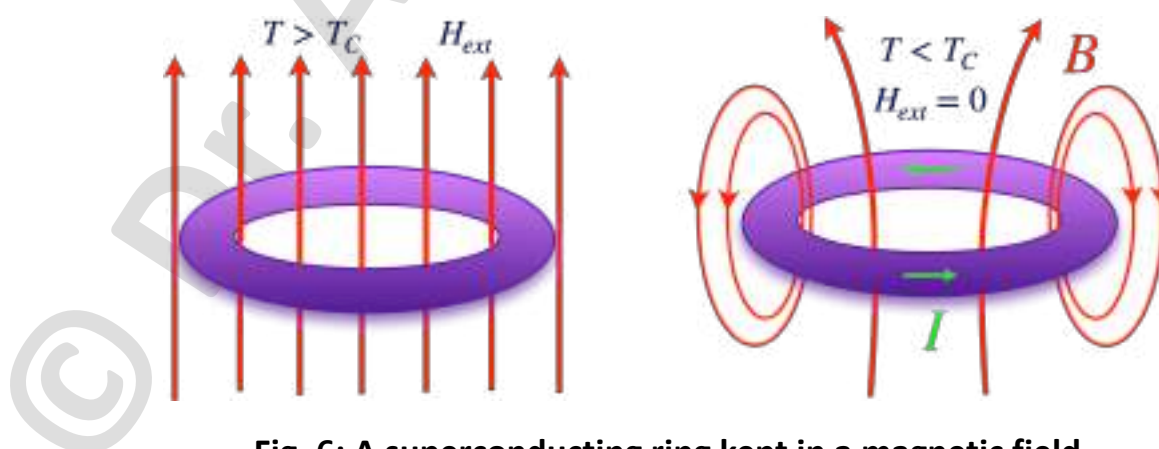


Fig. 6: A superconducting ring kept in a magnetic field

a) Normal State, b) Superconducting state with I persistent current

- A persistent current is an electrical current that flows indefinitely without any loss of energy. This remarkable phenomenon occurs in the superconducting state, where the material's resistance drops to zero.
- A persistent current is a current that continues to flow without diminishing in strength over time. It can persist for years or even indefinitely in a closed superconducting loop.

- In the superconducting state, the resistance (R) is zero: $R = 0$. As a result, there are no resistive losses in the form of heat (I^2R losses).
- No Energy Dissipation: Since $R = 0$, the power loss due to resistance is also zero: $P = I^2R = 0$. This allows the current to maintain its magnitude without any external power source.
- Experiments of this type have been carried out over periods of years, as $R = 0$, no I^2R losses and the magnetic field and hence the superconducting current has always remained constant within the precision of the measuring equipment. Such current is called as a **Persistent Current**, and is characteristic of the superconducting state. Calculations showed that this current will persist for 10^5 years. The current which flows without diminishing in strength is called persistent current.

iii) Critical Temperature (T_c)

- The critical temperature is a fundamental property of superconductors. It is the temperature below which a material enters the superconducting state, exhibiting zero electrical resistivity and expelling magnetic fields (Meissner effect).
- The critical temperature is the temperature at which a material's electrical resistivity drops abruptly to zero.
- **Mathematically:**

$$\rho(T) = 0 \quad \text{for} \quad T < T_c$$
 where $\rho(T)$ is the temperature-dependent resistivity.
- **Phase Transition:**
- The transition at T_c is sudden and complete, resembling a phase transition (like water freezing into ice).
- It is classified as a second-order phase transition because it involves no latent heat but shows discontinuities in properties like specific heat.
- **Superconducting Phase:**
- Above T_c : The material behaves like a normal conductor with finite resistivity due to electron scattering.
- Below T_c : The material becomes superconducting with zero resistance and perfect diamagnetism.
- Several materials exhibit superconducting phase transitions at low temperatures as shown in the following table.

Material	Gallium	Aluminum	Indium	Tin	Mercury	Lead	Niobium
T_c (K)	1.1	1.2	3.4	3.7	4.2	7.2	9.3

iv) Critical Magnetic Field (H_c)

- The critical magnetic field (H_c) is a key property of superconductors. It represents the maximum magnetic field strength that a superconductor can withstand while remaining in its superconducting state. Beyond this field, the material loses superconductivity and reverts to its normal, resistive state.
- The critical magnetic field is the threshold magnetic field above which superconductivity is destroyed.
- **Superconducting State (Zero Resistance)**
- $H < H_c \Rightarrow$ Superconducting State (Zero Resistance) $H < H_c \Rightarrow$ Superconducting State (Zero Resistance).
- **Normal State (Finite Resistance)**
- $H \geq H_c \Rightarrow$ Normal State (Finite Resistance) $H \geq H_c \Rightarrow$ Normal State (Finite Resistance).
- This is because the external magnetic field disrupts the Cooper pairs responsible for superconductivity.

- Temperature Dependence of Critical Magnetic Field

- The critical magnetic field decreases as the temperature approaches the critical temperature. The relationship is given by:

$$H_c(T) = H_c(0) \left[1 - \left(\frac{T}{T_c} \right)^2 \right] \quad \dots(3)$$

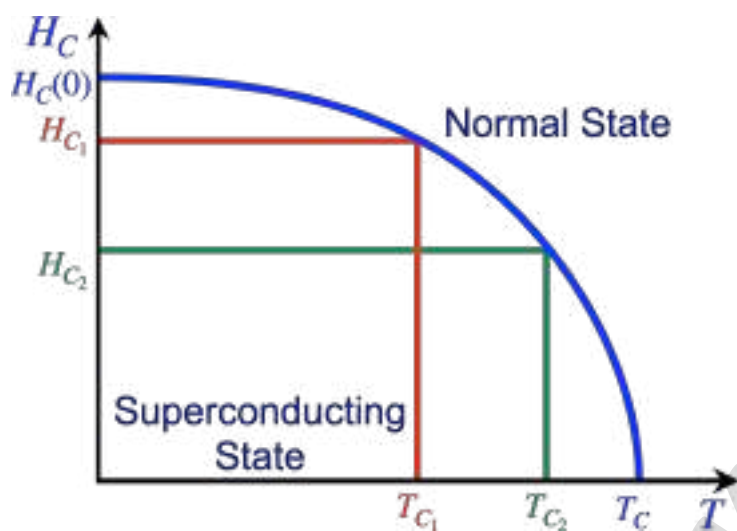
- where:

$H_c(T)$ = Critical magnetic field at temperature T

$H_c(0)$ = Critical magnetic field at absolute zero (0K)

T_c = Critical temperature of the superconductor

- Fig. 7: Graphical Representation:



- At $T = 0K$, the field is at its maximum $H_c(0)$.
- At $T = T_c$, the critical magnetic field drops to zero, and material becomes normal even without any external field.
- Type I Superconductor: Sharp transition at H_c .
- Type II Superconductor: Mixed state between H_{c1} and H_{c2}

v) Critical Current (I_c)

- The critical current (I_c) is the maximum electric current that can flow through a superconductor without destroying its superconducting state. When the current exceeds this limit, the superconductor transitions back to its normal resistive state due to the generation of a magnetic field that exceeds the critical magnetic field (H_c)
- Critical Current is the maximum current a superconducting material can carry without losing superconductivity.
- This is because the current generates a self-induced magnetic field around the conductor, following Ampère's law:

$$B = \mu_0 H \quad \dots(4)$$

When this magnetic field exceeds the critical magnetic field (H_c), superconductivity breaks down.

- Equation for a Superconducting Ring:

$$I_c = 2\pi R H_c \quad \dots(5)$$

- Where:

I_c = Critical current

R = Radius of the superconducting ring

H_c = Critical magnetic field

- This relation shows that the critical current is directly proportional to both the radius of the superconductor and the critical magnetic field.



- Critical Current Density (J_c)

- The critical current density (J_c) is the current per unit cross-sectional area of the superconductor.
- It is defined as:

$$J_c = \frac{I_c}{A} \quad \dots(6)$$

Where:

J_c = Critical current density (A/m²)

I_c = Critical current (A)

A = Cross-sectional area of the superconductor (m²)

- J_c is an important parameter for thin films, wires, and coils, where the geometry influences current flow.

- Temperature Dependence of Critical Current

- Similar to the critical magnetic field, the critical current also decreases with increasing temperature and vanishes at the critical temperature (T_c). The approximate relation is:

$$I_c(T) = I_c(0) \left[1 - \left(\frac{T}{T_c} \right)^2 \right] \quad \dots(7)$$

Where:

$I_c(0)$ = Critical current at absolute zero

T = Temperature

T_c = Critical temperature

- As current flows through a superconductor, it generates a magnetic field around it. If the magnetic field at the surface exceeds H_c , Cooper pairs break apart, and the material returns to the normal state. Hence, the current itself can cause the breakdown of superconductivity even without an external magnetic field.

vi) Meissner Effect in Superconductors

- The Meissner Effect is one of the most fundamental and defining properties of superconductors. It refers to the complete expulsion of magnetic flux from the interior of a superconducting material when it is cooled below its critical temperature (T_c) in the presence of an external magnetic field.
- The Meissner Effect is the phenomenon where a superconductor expels magnetic field lines from its interior, becoming a perfect diamagnet when cooled below its critical temperature (T_c).
- Mathematically, the magnetic induction (B) inside the superconductor becomes zero:

$$B = 0 \quad \text{for} \quad T < T_c$$

- This effect occurs regardless of whether the magnetic field was present before or after the cooling process.
- Consider a superconducting material placed in an external magnetic field (H):
- **Above T_c (Normal State):** Magnetic field lines pass through the material freely. The material behaves like a normal conductor.
- **Below T_c (Superconducting State):** The magnetic field lines are expelled from the material's interior. The material shows perfect diamagnetism with $B = 0$ inside.

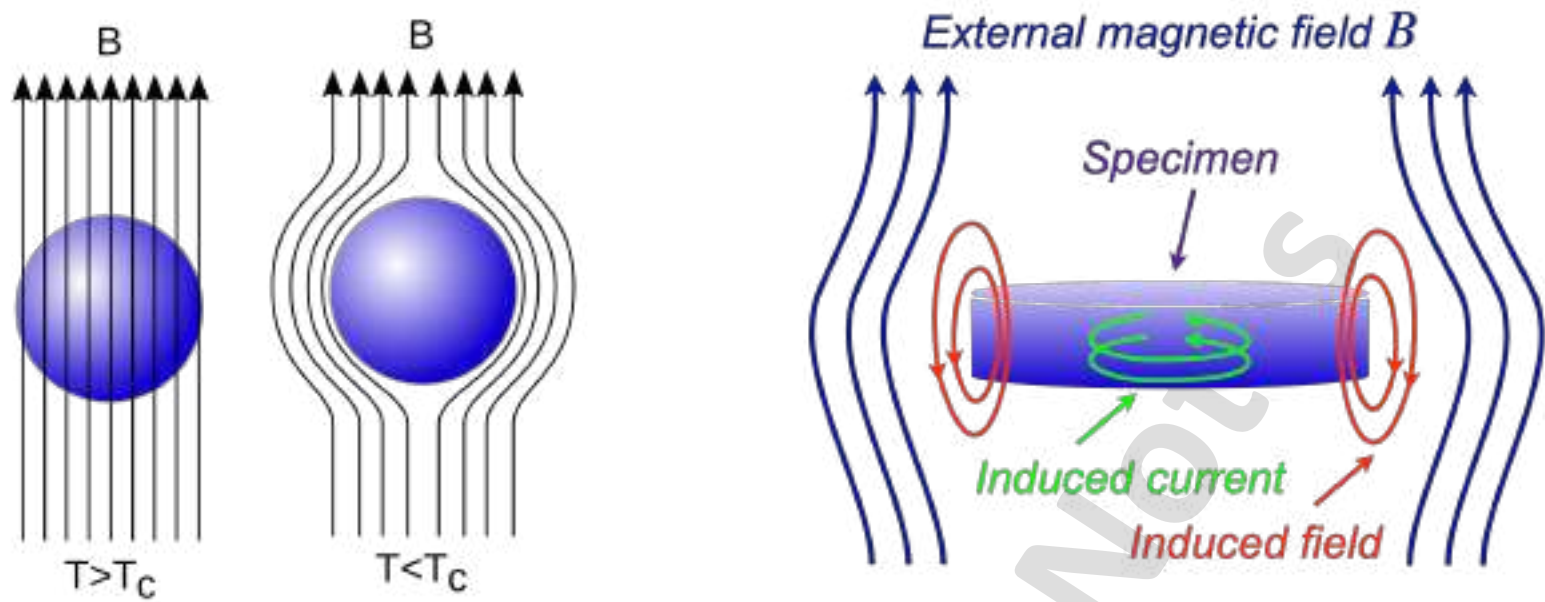


Fig. 8: Meissner Effect in Superconductors

- **At $T > T_c$:** The material is in normal conductor state and not a superconductor. When a magnetic field is applied to it, the it penetrates through the material. The magnetic induction inside the specimen (B) is given by;

$$B = \mu_0 (H + M).$$

- **At $T < T_c$:** The material turns a superconductor and as magnetic field is expelled out of superconductor. The magnetic induction inside the material is $B = 0$, hence;

$$0 = \mu_0 (H + M)$$

$$\therefore M = -H$$

- Magnetic susceptibility is the degree of magnetization of a material in response to an applied magnetic field.
- If magnetic susceptibility is negative the material is diamagnetic.
- For superconductors Magnetic Susceptibility of the material is;

$$\chi = \frac{M}{H} = \frac{-H}{H} = -1 \therefore \chi = -1 \quad \dots(8)$$

- This indicates that superconductors are **perfect diamagnetic**.

vii) Magnetic Penetration Depth or London Penetration Depth

- The magnetic penetration depth (λ) is a key parameter in the study of superconductivity. It describes how deep an external magnetic field can penetrate into a superconductor before being completely expelled due to the Meissner effect.
- When a magnetic field is applied to a superconductor, the applied field does not suddenly drops to zero at surface. Instead the field decays exponentially according to the formula;

$$H(x) = H(0) e^{-x/\lambda}$$

where $H(0)$ is the applied field at the surface at $x = 0$ and x is the distance from the surface.

Or Mathematically, the magnetic field

$$B(x) = B_0 e^{-x/\lambda}$$

Where: $B(x)$ = Magnetic field at depth x inside the superconductor

B_0 = Magnetic field at the surface ($x = 0$), λ = Magnetic penetration depth.

x = Distance from the surface into the material.

- The London penetration depth (λ_L or λ) characterises the distance to which a magnetic field penetrates into a superconductor. The temperature dependence of λ is given by relation;

$$\lambda(T) = \frac{\lambda(0)}{\sqrt{1 - \left(\frac{T}{T_c}\right)^4}} \quad \dots(9)$$

Where; $\lambda(T)$ and $\lambda(0)$ are the penetration depths at T and $0K$.

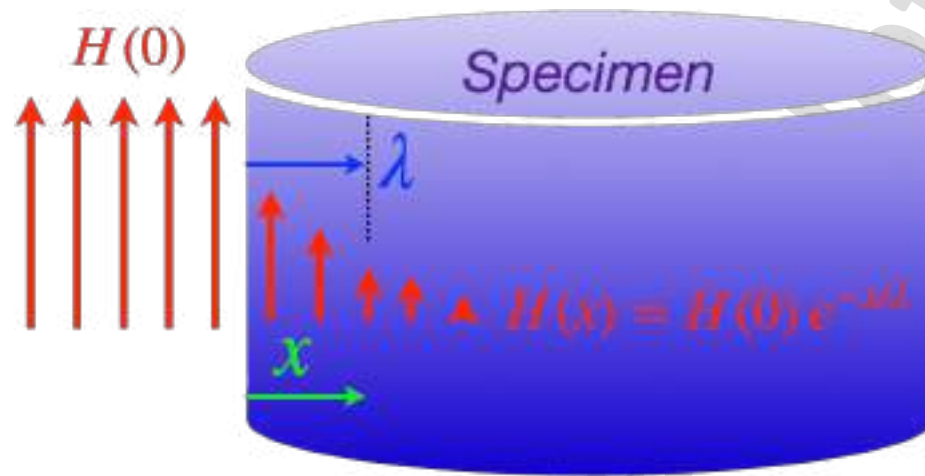


Fig. 9: Magnetic penetration depth.

viii) Flux Quantisation

- Flux quantization is a fundamental phenomenon observed in superconductors, where the magnetic flux passing through a superconducting loop is quantized, meaning it can only take on discrete values. This discovery was a key piece of evidence supporting the BCS theory of superconductivity.
- Flux quantization refers to the phenomenon where the magnetic flux (Φ) enclosed by a superconducting loop can only exist in discrete multiples of a fundamental unit known as the flux quantum (Φ_0).
- Mathematically, it is expressed as:

$$\Phi = n\Phi_0$$

- Where:

Φ = Magnetic flux through the loop

n = Integer ($n = 0, \pm 1, \pm 2, \pm 3, \dots$) representing the quantization number

Φ_0 = Flux quantum and is called **fluxon**, given by:

$$\Phi_0 = \frac{h}{2e} \quad \dots(10)$$

- Here:

h = Planck's constant (6.626×10^{-34} J·s)

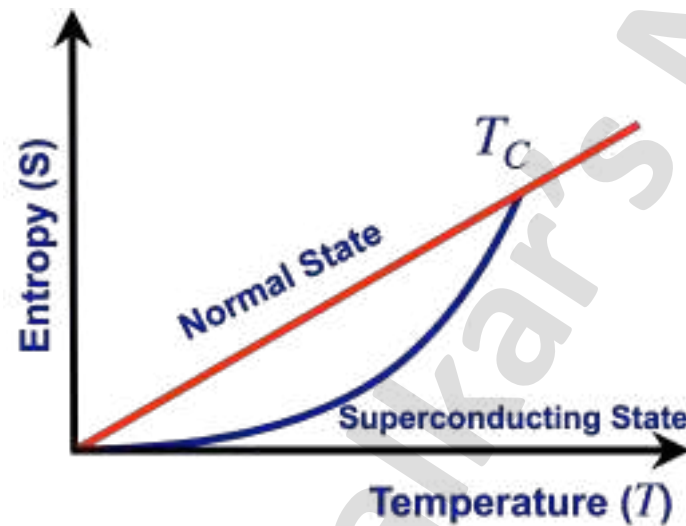
e = Elementary charge (1.602×10^{-19} C)

Numerical Value:

$$\Phi_0 \approx 2.0678 \times 10^{-15} \text{ Wb (Weber).}$$

ix) Entropy

- Entropy is a measure of the disorder or randomness in a system. In the context of superconductivity, entropy plays a crucial role in understanding the phase transition from the normal (resistive) state to the superconducting state.
- When a material is cooled below its critical temperature (T_c), it undergoes a phase transition from the normal conducting state to the superconducting state.
- During this transition: Entropy Decreases Significantly:
 $S_{\text{superconducting}} < S_{\text{normal}}$
- This decrease in entropy reflects a transition to a more ordered state.

**Fig. 10: Variation of entropy of aluminium****x) Isotope Effect**

- In all superconductors, the entropy decreases significantly on cooling below the critical temperature T_c . For aluminium, the change in entropy was observed to be small of the order of $10^{-14} \times k$ per atom, where k is the Boltzmann constant.
- The Isotope Effect is a key phenomenon that provided strong evidence for the BCS theory of superconductivity. It refers to the observation that the critical temperature (T_c) of a superconductor decreases as the isotopic mass of the material increases.
- The critical temperature (T_c) is the temperature below which a material becomes superconducting.
- When a superconductor's atoms are replaced by their heavier isotopes (same element, different atomic mass), T_c tends to decrease.
- This relationship is known as the **Isotope Effect**.

$$T_c \propto \frac{1}{\sqrt{M}} \quad \dots(11)$$

$$M^{-\alpha} \cdot T_c = \text{constant}$$

Where:

α is constant and is approximately equal to $\frac{1}{2}$.

T_c = Critical temperature.

M = Isotopic mass of the element.

4. Types of Superconductors

i) Type I Superconductors (Soft Superconductors)

- The metals which exhibit zero resistivity at low temperatures and have the property of excluding magnetic fields from the interior of the superconductor are called Type I superconductors.
- Type I superconductors are well described by the BCS theory and they are usually made of pure metal.
- The transition from superconducting state to normal state in presence of magnetic field occurs sharply at critical field H_c as shown in Fig. 11 (a).
- **Magnetic Behavior:**
Type I superconductors exhibit the complete Meissner effect, meaning that when exposed to an external magnetic field, they completely exclude the field from their interior, creating a perfect diamagnetic state.
- **Critical Magnetic Field:**
Type I superconductors have a single critical magnetic field, which is the maximum magnetic field strength that can be applied without destroying superconductivity. If the applied magnetic field exceeds, the material returns to its normal, resistive state.
- **Transition to Normal State:**
The transition from the superconducting state to the normal state occurs suddenly when the magnetic field exceeds H_c or when the temperature exceeds T_c . This results in an abrupt loss of superconductivity.
- **Critical Temperature:**
These superconductors have relatively low critical temperatures, typically below 10 K, making them less practical for many applications compared to Type II superconductors.
- **Examples of Type I Superconductors:**
 - Lead (Pb)
 - Mercury (Hg)
 - Aluminum (Al)
 - Tin (Sn)
 - Zinc (Zn)

ii) Type II Superconductors (Hard Superconductors)

- Type II superconductors are a broader class of superconducting materials that exhibit unique behaviors, particularly under high magnetic fields.
- They are often more practical for real-world applications than Type I superconductors due to their higher critical temperatures and greater tolerance to magnetic fields.
- The superconductors which have much higher critical fields and could carry much higher current densities while remaining in the superconducting state are called Type II superconductors.
- These superconductors are usually alloys and their diamagnetism is more complex. The transition from superconducting to normal state is gradual.
- At lower critical magnetic field (H_{c1}) external magnetic field enters into superconductor. It does not lose its superconductivity and exists in mixed or vortex state.
- If the value of external magnetic field is increased above upper magnetic field (H_{c2}), they lose their superconductivity as shown in Fig. 11(b).

- Partial Meissner Effect (Mixed State):

Unlike Type I superconductors, Type II superconductors do not completely expel magnetic fields. Instead, when exposed to a magnetic field, they exhibit a partial Meissner effect. Magnetic flux penetrates the superconductor in the form of quantized vortices between two critical magnetic field values, H_{c1} and H_{c2} .

- Two Critical Magnetic Fields:

- Lower Critical Field (H_{c1}):

Below this field, Type II superconductors exhibit complete Meissner effect, just like Type I superconductors. The material is in the superconducting state with no magnetic field inside.

- Upper Critical Field (H_{c2}):

When the external magnetic field exceeds H_{c2} , the superconductivity is completely destroyed, and the material returns to the normal state. Between H_{c1} and H_{c2} , the superconductor exists in a mixed state where magnetic flux partially penetrates.

- Mixed State (Vortex State):

In the range between H_{c1} and H_{c2} , magnetic flux penetrates the superconductor in the form of vortices or flux lines. These vortices are regions where the magnetic field exists inside the superconductor, surrounded by circulating supercurrents. The superconducting state persists, but the material is not in a perfect diamagnetic state.

- High Critical Temperature (T_c):

Type II superconductors typically have higher critical temperatures compared to Type I superconductors, often exceeding 20 K and sometimes reaching high-temperature superconductivity ranges (>77 K, the boiling point of liquid nitrogen).

- Examples of Type II Superconductors:

- Alloys and Composites:

- Niobium-titanium (NbTi)
- Niobium-tin (Nb_3Sn)
- Vanadium-silicon (V_3Si)

- High-Temperature Superconductors:

- Yttrium barium copper oxide (YBCO)
- Bismuth strontium calcium copper oxide (BSCCO)
- Magnesium diboride (MgB_2).

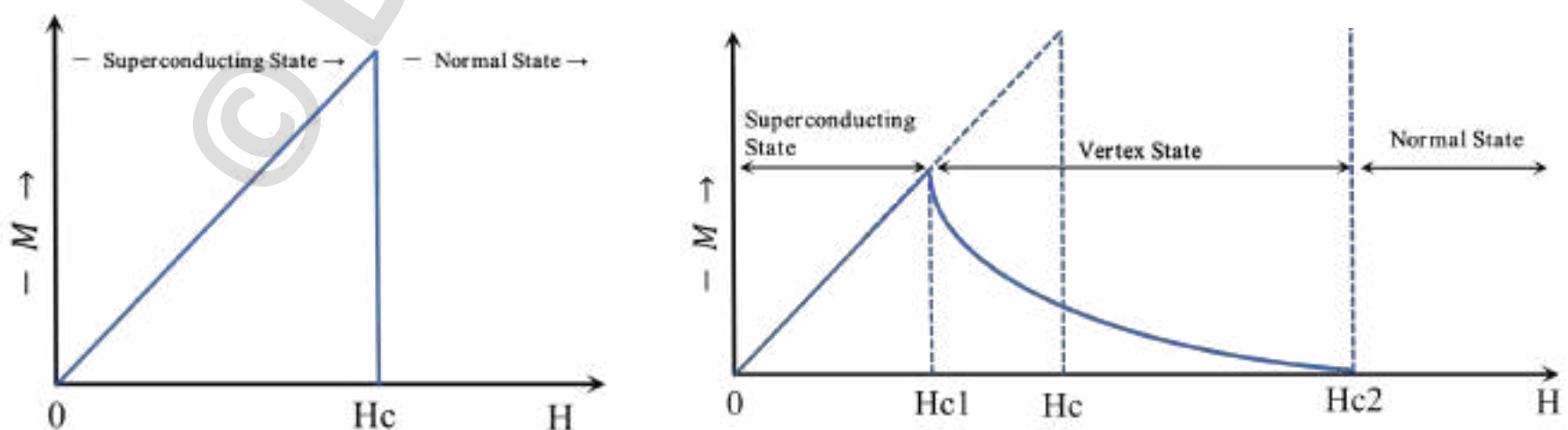


Fig. 11: a) Type I Superconductor b) Type II Superconductor



Comparison of Type-I and Type-II Superconductors

Property	Type-I Superconductors	Type-II Superconductors
Definition	Exhibit a complete Meissner effect and lose superconductivity abruptly beyond a critical field.	Allow partial magnetic field penetration (vortex state) and transition gradually from superconducting to normal state.
Type	They are known as soft superconductors	They are known as Hard superconductors
Magnetic Behavior	Perfect diamagnetism (Meissner effect).	Mixed state: Partial magnetic field penetration (vortex formation).
Critical Fields	Single critical field (H_c).	Two critical fields: Lower (H_{c1}) and Upper (H_{c2}).
Transition Behavior	Abrupt transition from superconducting to normal state.	Gradual transition with a mixed (vortex) state.
Critical Temperature (T_c)	Generally low ($< 10K$).	Can be high, ($T_c > 100K$ in high- T_c superconductors).
Superconducting State	Exists in pure elemental conductors.	Found in alloys, complex compounds, and high- T_c materials.
Magnetic Field Tolerance	Low – loses superconductivity quickly when exposed to external magnetic fields.	High – remains superconducting under strong magnetic fields.
Practical Applications	Limited due to low field tolerance and low T_c .	Widely used in advanced applications due to high H_{c2} and T_c .
Vortex Formation	No vortex state superconductivity vanishes at H_c .	Magnetic field penetrates as quantized vortices in the mixed state.
Energy Gap	Smaller energy gap.	Larger energy gap.
BCS Theory	Fully explained by BCS theory.	Some high- T_c superconductors do not strictly follow BCS theory.
Examples of High T_c	None all are low- T_c superconductors.	High- T_c superconductors like YBCO and BSCCO exist.
Meissner Effect	Exhibits Meissner Effect	Do not exhibits Meissner Effect
Cost & Availability	Usually inexpensive and easy to manufacture.	More expensive and complex to produce.
Diamagnetism	Exhibits perfect diamagnetism	Do not exhibits perfect diamagnetism
States of material	Material exists in two states for $T < T_c$ $H < H_c$: Superconductor $H > H_c$: Conductor	Material exists in three states for $T < T_c$ $H_c > H_{c1}$: Superconductor $H_{c1} < H_c < H_{c2}$: Mixed / Vortex $H_c < H_{c2}$: Conductor
Material Examples	Aluminium, lead, mercury, Tin (Sn) etc	Nb-Sn, Nb-Ti, Nb-Zr, Va-Ga, $YBa_2Cu_3O_7$, etc

5. Josephson effect (DC and AC)

- The Josephson Effect is the phenomenon of current flow across two weakly coupled superconductors, separated by a very thin insulating barrier. This setup is known as a Josephson Junction (JJ) as shown in Fig. 12 a).

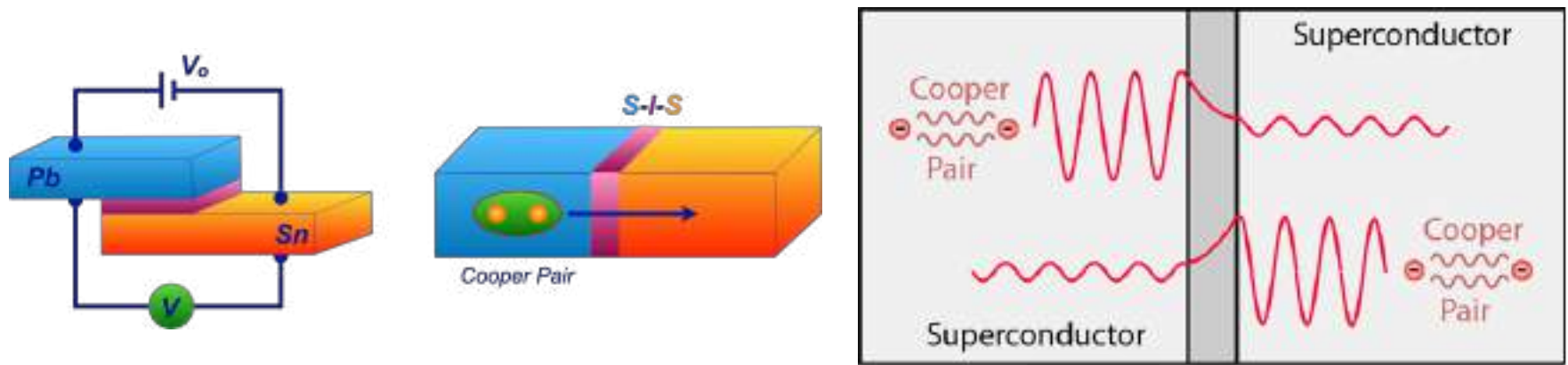


Fig. 12: a) Josephson Junction Superconductor–Insulator–Superconductor (S-I-S) structure with Pb and Sn
b) Phase difference and quantum tunneling of Cooper pairs

- The current that flows across the insulating barrier is called the **Josephson Current**. The junction is typically a Superconductor–Insulator–Superconductor (S-I-S) structure, where the insulating layer introduces a phase difference between the wave functions of Cooper pairs on opposite sides as shown in Fig. 12 b).
- Hence a **super-current** appears across the junction even though the applied voltage is zero.

- DC Josephson Effect

- Even when no external voltage is applied ($V=0$), a supercurrent can flow across the junction due to quantum tunneling of Cooper pairs. This is described by the equation:

$$I_S = I_C \sin \Phi \quad \dots(12)$$

where:

I_S = Supercurrent

I_C = Critical current (maximum supercurrent the junction can carry)

Φ = Phase difference between the two superconductors

- This effect demonstrates that superconductors can exhibit a persistent current without any voltage, a key feature in quantum computing and superconducting circuits.

- AC Josephson Effect

- If a DC voltage is applied across Josephson junction, it introduces an additional phase on the Cooper pairs during tunnelling. The DC voltage generates an **alternating current** I , given by,

$$I = I_C \sin \Phi + \Delta \Phi \quad \dots(13)$$

- Due to DC voltage, the energies of Cooper pairs on both sides of the barrier **differ in energy by $2eV$** . Cooper pair electrons contain **2 electrons** hence the **energy is $2eV$** . Using quantum mechanical calculations;

$$\Delta \Phi = 2\pi t \left(\frac{2eV}{\hbar} \right) \quad \dots(14)$$

where:

Φ = Phase difference between the superconductors, e = Elementary charge of an electron

\hbar = Reduced Planck's constant and V = Applied voltage

- Thus, the AC across the junction is given by,

$$I = I_C \sin \left(\Phi + 2\pi t \left(\frac{2eV}{h} \right) \right) \quad \dots(15)$$

Where; alternating current of frequency is; $\nu = \left(\frac{2eV}{h} \right)$ this frequency only depends on the applied voltage.

This effect is known as **AC Josephson effect**.

- The frequency of alternating currents does not depend on the dimensions of the superconductors, properties of superconductors such as critical temperature and chemical composition.
- Oscillating Supercurrent: Unlike the DC effect, where the current is steady, here the current oscillates with frequency ν .
- Voltage-to-Frequency Relationship: The frequency of oscillation is directly proportional to the applied voltage.
- Application in Metrology: This effect is used in Josephson voltage standards to precisely define the volt.

6. Superconducting Quantum Interference Devices (SQUIDs)

- A Superconducting Quantum Interference Device (SQUID) is an extremely sensitive magnetometer used to measure extremely weak magnetic fields, down to the order of 10^{-15} T (femtotesla). SQUIDs operate based on the Josephson Effect and quantum interference in superconducting loops.
- Principle of Operation
- SQUIDs consist of a superconducting loop with one or two Josephson Junctions (JJs). When a magnetic field is applied, the phase difference in the Josephson junctions changes, leading to variations in the supercurrent through the loop. This results in quantum interference, which allows precise measurement of magnetic flux.
- The device works based on the concept that the magnetic flux through a superconducting loop is quantized in discrete units of magnetic flux quantum (Φ_0), given by:

$$\Phi_0 = \frac{h}{2e} \approx 2.07 \times 10^{-15} \text{ Wb} \quad \dots(16)$$

where:

h = Planck's constant

e = Charge of an electron

- A small change in the external magnetic field causes a change in the phase of the wave function in the superconducting loop, leading to measurable voltage oscillations.
- **Construction and Working of SQUID**
- A Superconducting Quantum Interference Device (SQUID) consists of a superconducting loop containing one or more Josephson Junctions (JJs). It operates based on the principles of flux quantization and the Josephson Effect, making it one of the most sensitive magnetometers available.
- Superconducting Loop – A closed superconducting circuit made of materials like niobium (Nb) or YBCO (Yttrium Barium Copper Oxide) as shown in Fig. 13. a). The tunnel barrier is oxidised onto lead or niobium surface. It consists of two Josephson junctions arranged in parallel.
- When a weak external magnetic field (B) is applied, it induces a magnetic flux (Φ) through the superconducting loop. Since the loop is superconducting, the total flux is quantized in multiples of Φ_0 . This changes the phase difference across the Josephson junctions, leading to oscillations in the superconducting

current. The resulting voltage oscillations are measured and converted into a corresponding magnetic field value. A constant dc super-current is applied to the SQUID as shown in Fig. 13. b).

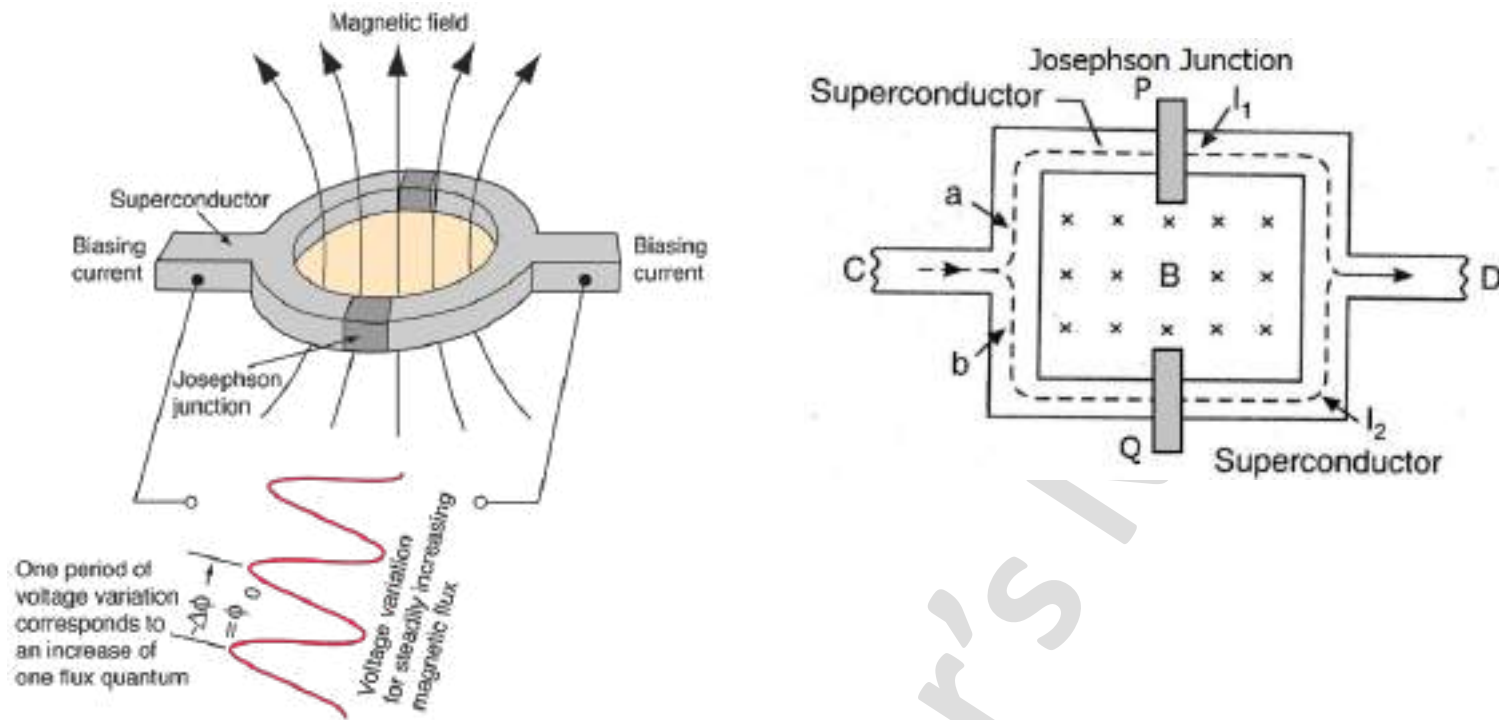


Fig. 13. a) Superconducting Loop. b) DC Josephson junctions P and Q

- I_1 and I_2 are currents tunnelling through **Josephson junctions**. The wave function experiences **a phase shift** at the Josephson junctions P and Q.
- **In absence of magnetic field:** Phase difference across P and Q = 0.
- **In presence of magnetic field:** It changes the **quantum mechanical phase difference** across each of the two junctions. This **phase difference** δ_ϕ between reuniting currents is **directly proportional to the magnetic flux** Φ through the ring.
- Total current (I_T) through parallel DC Josephson junctions is,

$$I_T = 2 (I_0 \sin \delta_\phi) \cos \frac{e\Phi}{\hbar} \quad \dots(17)$$

Where;

I_T = Total supercurrent in the SQUID loop

I_0 = Maximum supercurrent (critical current of a single Josephson junction)

δ_ϕ = Phase difference across the Josephson junction.

Φ = Magnetic flux through the SQUID loop.

e = Charge of an electron.

\hbar = Reduced Planck's constant.

- Applications of SQUID

- Medical Imaging – Used in Magnetoencephalography (MEG) and Magnetic Resonance Imaging (MRI) to detect tiny magnetic signals from the brain and heart.
- Geophysics – Detects weak geomagnetic field variations for mineral exploration.
- Quantum Computing – Used in superconducting qubits.
- Fundamental Physics – Helps in gravitational wave detection and dark matter research.
- Non-Destructive Testing (NDT) – Finds small defects in materials.

7. Applications of Superconductors: MagLev Trains (Magnetic Levitation Trains)

- MagLev trains, short for Magnetic Levitation Trains, are an advanced form of transportation that uses superconducting materials to achieve frictionless motion. These trains "float" above the tracks, reducing friction, enabling faster speeds, and offering smooth and efficient travel.
- **Working Principle of MagLev Trains**
- MagLev technology utilizes the Meissner Effect (the expulsion of magnetic fields from a superconductor) and electromagnetic levitation to achieve levitation and propulsion.

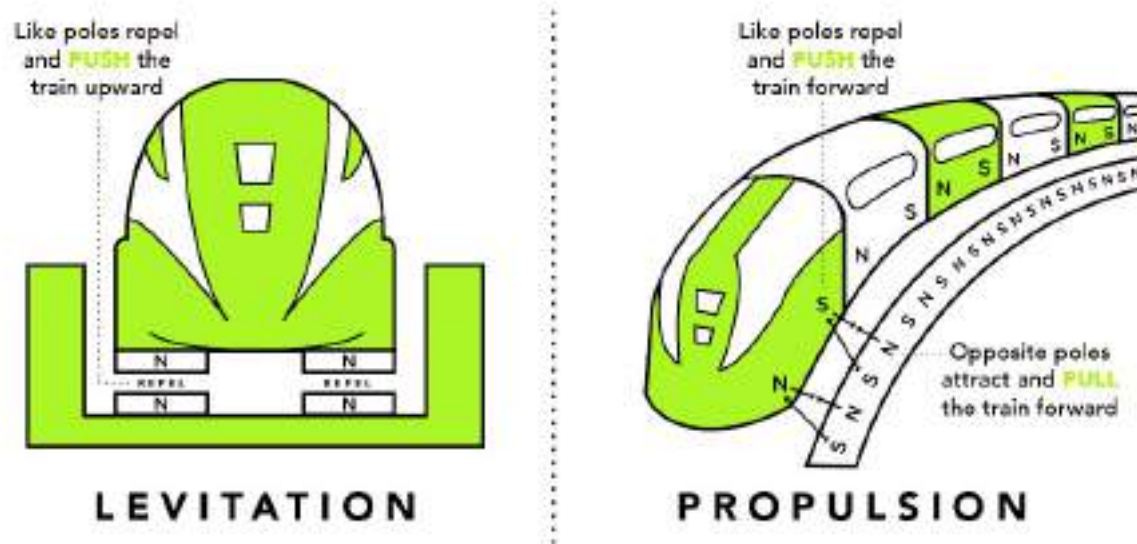


Fig. 14: Magnetic Levitation Train

i) Levitation:

- MagLev trains use superconducting magnets on the train's underside and electromagnetic coils on the track (or vice versa) to create a powerful repulsive force.
- This results in the train levitating several centimeters above the track, eliminating friction and reducing energy loss.

ii) Propulsion:

- Superconducting magnets on the train interact with the track's magnetic field, creating a moving magnetic field that pushes the train forward (like a linear motor).
- This method allows the train to accelerate smoothly without the need for mechanical wheels or engines.
- Superconductors, particularly high-temperature superconductors (HTS), are commonly used in the construction of the levitation and propulsion systems due to their ability to conduct electricity without resistance.
- YBCO (Yttrium Barium Copper Oxide) is one of the most popular high- T_c superconductors used in MagLev trains because it remains superconducting at higher temperatures (around 77K, which can be achieved using liquid nitrogen cooling). The Meissner Effect ensures that the superconductors expel magnetic fields, allowing the train to levitate.
- A levitation electromagnet is an electromagnet used to produce a magnetic field that can suspend an object, typically using electromagnetic levitation. For MagLev (Magnetic Levitation) trains, levitation electromagnets are used to generate magnetic forces that counteract gravity, allowing a train to float above a surface without physical contact as shown in Fig. 15.
- Levitation electromagnets play a vital role in MagLev transportation systems, contactless handling, and other advanced technologies. By harnessing electromagnetic forces, these systems can achieve frictionless motion, offering significant advantages in terms of speed, energy efficiency, and smoothness.

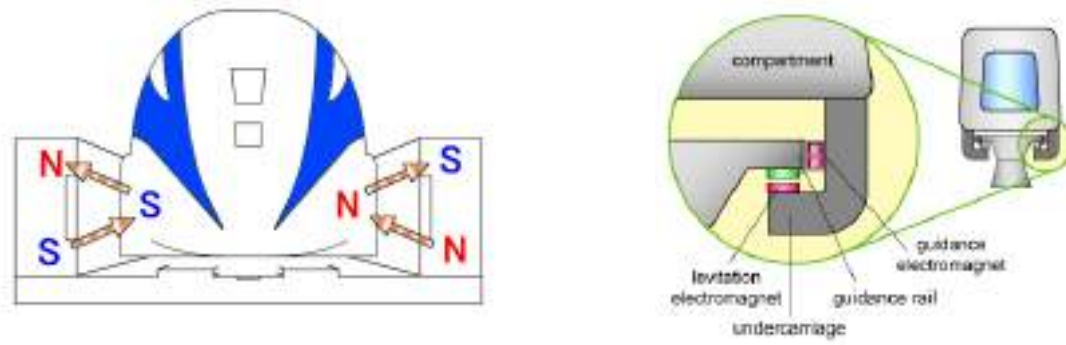


Fig. 15: Levitation electromagnet

- Advantages of MagLev Trains Using Superconductors

Frictionless Motion: Superconducting materials create magnetic fields that allow the train to float above the track, significantly reducing friction. This enables high speed and smoothness during travel, making it possible to reach speeds over 600 km/h (373 mph) in some test models.

High Speed: MagLev trains can travel faster than traditional trains due to the absence of mechanical contact with tracks, which allows them to achieve speeds of up to 500 km/h (310 mph) or higher. This makes them highly competitive for inter-city travel.

Energy Efficiency: Reduced friction means less energy is lost in overcoming resistance, making the trains more energy-efficient compared to conventional rail systems.

Low Maintenance: Since the train does not physically touch the track, wear and tear are minimized, leading to lower maintenance costs.

Quiet Operation: MagLev trains are quieter than traditional trains, as there is no friction between the wheels and the track, which often causes noise in conventional rail systems.

- Challenges of MagLev Trains

While MagLev technology offers many benefits, it also faces some challenges:

Infrastructure Cost: The construction of MagLev tracks is expensive because it requires specialized materials, superconducting magnets, and complex track designs. The infrastructure cost of MagLev systems can be higher than traditional rail systems.

Cooling Requirements: Superconducting materials used for levitation require cryogenic cooling (often using liquid nitrogen or helium), which can add complexity and cost. However, advancements in high-temperature superconductors (HTS) are helping reduce these requirements.

Limited Track Availability: MagLev trains require dedicated tracks, and the lack of infrastructure means that they cannot easily be integrated into existing railway systems.

**Problems with Solution:****Magnetism**

Problem 1: A magnetic material has a magnetisation of 2300 A/m and produces a flux density of 0.00314 Wb/m². Calculate magnetising force and relative permeability of the material.

Solution:

Magnetic Force $B = \mu_0(H + M)$

$$H = \frac{B}{\mu_0} - M = \frac{0.00314 \text{ Wb/m}^2}{12.57 \times 10^{-7} \text{ H/m}} - 2300 \text{ A/m} \therefore H = 198 \text{ A/m}$$

$$\text{Relative Permeability } \mu_r = \frac{B}{\mu_0 H} \text{ hence } \mu_r = \frac{0.00314 \text{ Wb/m}^2}{12.57 \times 10^{-7} \text{ H/m} \times 198 \text{ A/m}} \therefore \mu_r = 12.56$$

Problem 2: A diamagnetic material Al₂O₃ is subjected an external magnetic field of 10⁵ A/m. Evaluate magnetisation and magnetic flux density in Al₂O₃. Given: Susceptibility of Al₂O₃ is -5×10^{-5} .

Solution:

$$\text{Magnetisation } M = \chi H \therefore M = -5 \times 10^{-5} \times 10^5 \text{ A/m} \therefore M = -5 \text{ A/m}$$

Magnetic flux density

$$B = \mu_0(H + M) \therefore B = 12.57 \times 10^{-7} \text{ H/m} \times (10^5 \text{ A/m} - 5 \text{ A/m}) \therefore B = 0.126 \text{ Wb/m}^2$$

Problem 3: Find the relative permeability of ferromagnetic material if a magnetic field of strength 220 A/m produces magnetisation of 3300 A/m in it.

Solution:

$$\text{Relative permeability } \mu_r = (1 + \chi) \therefore \mu_r = \left(1 + \frac{M}{H}\right) \therefore \mu_r = \left(1 + \frac{3300 \text{ A/m}}{220 \text{ A/m}}\right) \therefore \mu_r = 16$$

Problem 4: The susceptibility of paramagnetic FeCl₃ is 3.7×10^{-3} at 27°C. What will be the value of its relative permeability at 200°K and 500°K?

Solution:

$$\text{Curie constant } C = \chi T = 3.7 \times 10^{-3} \times 300 \text{ K} = 1.11 \text{ K}$$

$$\chi_{200 \text{ K}} = \frac{C}{T} = \frac{1.11 \text{ K}}{200 \text{ K}} = 5.55 \times 10^{-3}$$

$$\chi_{500 \text{ K}} = \frac{C}{T} = \frac{1.11 \text{ K}}{500 \text{ K}} = 2.22 \times 10^{-3}$$

Problem 5: A field strength of 300 A/m produces a magnetization of 4400 A/m in a ferromagnetic material. What is the relative permeability of the material?

Solution:

$$\text{The relative permeability } \mu_r = 1 + \chi = 1 + \frac{M}{H} = 1 + \frac{4400 \text{ A/m}}{300 \text{ A/m}} = 15.67$$



Problem 6: The magnetic field in a diamagnetic material is 10000 A/m. Calculate the magnetization and flux density of the material if its susceptibility is -0.4×10^{-5} .

Solution:

$$\text{Magnetization } M = \chi H = -0.4 \times 10^{-5} \times 10000 \text{ A/m} = -0.04 \text{ A/m}$$

$$\text{Flux density } B = \mu_0 (H + M) = (4\pi \times 10^{-7} \text{ T m/A}) (10000 - 0.04) \text{ A/m} = \mathbf{0.0126 \text{ T}}$$

Superconductivity

Problem 7: The area of hysteresis loop drawn between B and H is 100m². Each unit space along the vertical axis represent 0.01Wb/m² and each unit space along the horizontal axis represents 40 A/m. Determine the hysteresis loss per cycle.

Solution:

The hysteresis loss per cycle = Area of hysteresis loop \times Value of unit length along B-axis \times Value of unit length along H-axis.

$$\text{The hysteresis loss per cycle} = 100 \text{ m}^2 \times 0.01 \text{ Wb/m}^2 \times 40 \text{ A/m}.$$

$$\text{The hysteresis loss per cycle} = \mathbf{40 \text{ J/m}^3}.$$

Problem 8: The transition temperature of Pb is 7.2K. However, at 5K it loses the superconductivity property if subjected to the magnetic field of 3.3×10^4 A/m. Find the maximum value of H which will allow the metal to retain its superconductivity at 0K.

Solution:

We have a formula;

$$H_c(T) = H_c(0) \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

$$H_c(0) = \frac{H_c(T)}{1 - \frac{T^2}{T_c^2}} = \frac{3.3 \times 10^4 \text{ A/m}}{1 - \frac{5^2}{7.2^2}} = \mathbf{6.37 \times 10^4 \text{ A/m}}$$

Problem 9: The critical field of niobium is 1×10^5 A/m at 8K and 2×10^5 A/m at 0K. Calculate the transition temperature of niobium.

Solution:

We have a formula;

$$H_c(T) = H_c(0) \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

$$T_c = \frac{T}{\left[1 - \frac{H_c(T)}{H_c(0)} \right]^{1/2}} = \frac{8 \text{ K}}{\left[1 - \frac{1 \times 10^5 \text{ A/m}}{2 \times 10^5 \text{ A/m}} \right]^{1/2}} = \mathbf{11.3 \text{ K}}$$



Problem 10: The critical magnetic field at 5K is 2×10^3 A/m in a superconductor ring of radius 0.02m. Find the value of critical current.

Solution:

We have a formula; Critical Current; $I_C = 2\pi R H_C$

$$I_C = 2 \times 3.143 \times 0.02 \text{ m} \times 2 \times 10^3 \text{ A/m} = \mathbf{251.4A}$$

Problem 11: Calculate the critical current for a wire of lead (Pb) having a diameter of 1mm at 4.2K. The critical temperature for lead is 7.18K and $H_C = 6.5 \times 10^4$ A/m.

Solution:

We have a formula;

$$H_c(T) = H_C(0) \left[1 - \left(\frac{T}{T_C} \right)^2 \right] = 6.5 \times 10^4 \text{ A/m} \left[1 - \left(\frac{4.2K}{7.18K} \right)^2 \right] = \mathbf{4.28 \times 10^4 \text{ A/m}}$$

The critical current;

$$I_C = 2\pi R H_C = \pi d H_C = 3.14 \times 1 \times 10^{-3} \text{ m} \times 4.28 \times 10^4 \text{ A/m} = \mathbf{134.5A}$$

Problem 12: In a superconducting material, the isotopic mass is 199.5 amu and the critical temperature is 5K. Calculate isotopic mass at 5.1K.

Solution:

We have a formula;

$$T_C \propto \frac{1}{\sqrt{M}} \quad \therefore T_1 \sqrt{M_1} = T_2 \sqrt{M_2} \quad \text{hence, } M_2 = M_1 \left[\frac{T_1}{T_2} \right]^2; M_2 = 199.5 \text{ amu} \left[\frac{5K}{5.1K} \right]^2$$

Therefore isotopic mass at 5.1K is; $M_2 = \mathbf{191.68 \text{ amu}}$

Problem 13: A Josephson junction with a voltage difference of $650 \mu V$ radiates electromagnetic radiation. Calculate its frequency.

Solution:

We have a formula;

$$\nu = \frac{2eV}{h} \quad \text{therefore } \nu = \frac{2 \times 1.6 \times 10^{-19} \times 650 \times 10^{-6}}{6.63 \times 10^{-34}} \quad \text{hence } \nu = \mathbf{3.13 \times 10^{11} \text{ Hz}}$$

Problem 14: Calculate the voltage required to produce a frequency of 2×10^{11} Hz across the Josephson junction.

Solution:

We have a formula;

$$\nu = \frac{2eV}{h} \quad \text{therefore } V = \frac{\nu h}{2e} = \frac{2 \times 10^{11} \times 6.63 \times 10^{-34}}{2 \times 1.6 \times 10^{-19}} = \mathbf{414.38 \mu V}$$



Q. No.	Questions
1	With neat labelled diagram, explain the phenomenon of Meissner effect in superconductors and also prove that the superconductors exhibit diamagnetic nature.
2	With neat labelled diagram, explain the construction and working of the DC-SQUID.
3	What is magneto-caloric effect? With neat labelled diagram explain the adiabatic demagnetization method to achieve low temperature.
4	Explain the phenomenon of Giant magneto resistance (GMR) with graph and write formula for Giant magnetic resistance.
5	Explain BCS theory of superconductors.
6	Explain four probe resistivity method to characterize the zero resistance in superconductors.
7	Explain ac and dc Josephson's effect.
8	With neat diagram of SQUID, explain that SQUID is very sensitive magnetometer
9	What is the importance of isotope effect in superconductivity?
10	Explain in detail, any four properties of superconducting materials.
11	How superconductivity in materials can be confirmed using resistance and magnetization measurements?
12	Define critical field. The critical temperature of Hg with isotopic mass 199.5 amu is 4.185 K. What will be its critical temperature when its isotopic mass is increased to 203.4 amu.
13	With neat labelled M-H curve explain the hysteresis behaviour of the ferromagnetic materials.
14	Explain in short the properties of superconductors: i) critical field ii) critical temperature iii) Isotope effect iv) persistent current
15	Give difference between Type I and Type II superconductors
16	The transition temperature for Pb is 7.2 K. However, at 5 K it loses the superconducting property if subjected to magnetic field of 3.3×10^4 A/m. Find the maximum value of H which will allow the metal to retain its superconductivity at 0 K.
17	The critical field of niobium is 1×10^5 A/m at 8 K and 2×10^5 A/m at 0 K. Calculate the transition temperature of the element
18	The transition temperature for lead is 7.26 K. The maximum critical field for the material is 8×10^5 A/m. Lead has to be used as a superconductor subjected to a magnetic field of 4×10^4 A/m. What precaution will have to be taken?
19	In a superconducting material isotopic mass is 199.5 amu and critical temperature is 5K. Calculate isotopic mass at 5.1 K.
20	Explain phenomenon of dc Josephson effect.
21	Explain phenomenon of ac Josephson effect.
22	Explain with neat diagram, the working of MagLev Trains
23	For a certain metal the critical magnetic field is 5×10^3 A/m at 6K and 2×10^4 A/m at 0K. Determine its transition temperature.
24	Write a short note on Critical field of superconductor.
25	What are Cooper pairs? Write their properties?



26	Give any five applications of superconductors
27	A Josephson junction has a voltage of 8.5 mV across its terminals. Calculate the frequency of the e.m. waves generated by it.
28	A Josephson junction with a voltage difference of 650 mV radiates electromagnetic radiation. Calculate its frequency.
29	A long thin superconducting wire of a metal produces a magnetic field of $105 \times 10^3 \text{ A/m}$ on its surface due to the current through it at a certain temperature T. The critical magnetic field of the metal is $150 \times 10^3 \text{ A/m}$ at 0K. The critical temperature T_C of the metal is 9.2 K. What is the value of T?
30	The transition temperature of mercury with an average atomic mass of 200.59 amu is 4.153 K. Determine the transition temperature of one of its isotopes $^{80}\text{Hg}_{204}$
31	The critical temperature of a superconductor at zero magnetic field is T_C . Determine the temperature at which the critical field becomes half of its value at 0K.
32	Write short notes on DC-SQUIDS.
33	Write the relation between isotopic mass and transition temperature.
34	State Meissner effect and isotope effect.
35	Describe the properties of cooper pairs.
36	What is phenomenon of Superconductivity?
37	Describe the properties of cooper pairs.
38	Describe the phenomenon of Superconductivity?
39	Write the expression & Draw labeled diagram showing the relation between critical magnetic field and Temperature.
40	Write short note on persistent current in superconductors.
41	List any four applications of superconductors.



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UNIT 4: INTRODUCTION TO NANOSCIENCE

1. Introduction

- History of Nanoscience and Nanotechnology

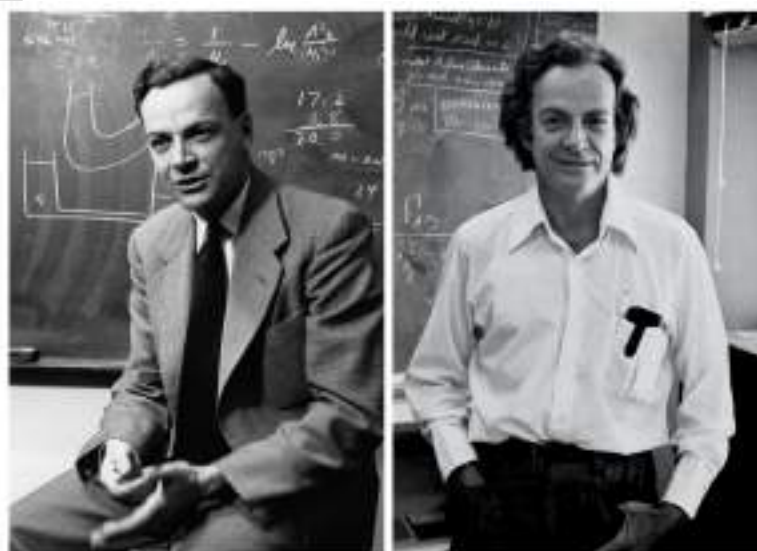
- The Greek word "nano" (meaning dwarf) refers to a reduction of size, or time, by 10^{-9} , which is one thousand times smaller than a micron. One nanometer (nm) is one billionth of a meter and it is also equivalent to ten Angstroms. As such a nanometer is 10^{-9} meter and it is 10,000 times smaller than the diameter of a human hair. A human hair diameter is about 50 micron (i.e., $50 \times 10^{-6}m$) in size, meaning that a 50 nanometer object is about $1/1000^{\text{th}}$ of the thickness of a hair. One cubic nanometer (nm^3) is roughly 20 times the volume of an individual atom. A nano-sized particle compares to a basketball like a basketball to the size of the earth. To understand "nano" world, definition and history of nanotechnology is needed.

- Nanoscience and Nanotechnology

- Nanotechnology is a known field of research since last century. Nanotechnology is the study of phenomena and finetuning of materials at atomic, molecular and macromolecular scales, where properties differ significantly from those at a larger scale. Products based on nanotechnology are already in use and analysts expect markets to grow by hundreds of billions of euros during this decade.
- Nanoscience is the study of systems in nanoscale and nanotechnology is the ability to systematically organise and manipulate properties and behaviour of matter in the atomic and molecular levels. Through nanoscience and nanotechnology it has become possible to study and develop very useful functional devices, materials, and systems at nanoscale.
- Holding nanoscale science, engineering and technology, nanotechnology involves imaging, measuring, modelling, and manipulating matter at this length scale.
- Many fields are contributing to nanotechnology, including molecular physics, materials science, chemistry, biology, computer science, electrical engineering, and mechanical engineering.

- How 'Nano' Started?

- The ideas and concepts behind nanoscience and nanotechnology started with a talk entitled ***"There's Plenty of Room at the Bottom"*** by physicist Richard Feynman at an American Physical Society meeting at the California Institute of Technology (CalTech) on December 29, 1959, long before the term nanotechnology was used. In his talk, Feynman described a process in which scientists would be able to manipulate and control individual atoms and molecules.



Physicist Richard Feynman, the father of nanotechnology



- The Japanese scientist, Norio Taniguchi, Tokyo University of Science was first to use the term "nano-technology" in a 1974 conference, to describe semiconductor processes such as thin film deposition and ion beam milling exhibiting characteristic control on the order of a nanometer. His definition was, "'Nano-technology' mainly consists of the processing of, separation, consolidation, and deformation of materials by one atom or one molecule."
- However, the term was not used again until 1981 when Eric Drexler, who was unaware of Taniguchi's prior use of the term, published his first paper on nanotechnology in 1981. The development of nanotechnology based on experimental research and advances in past. In nanoelectronics, nanoscale thickness was demonstrated in the gate oxide and thin films used in transistors as early as the 1960s, but it was not until the late 1990s that MOSFETs (metal–oxide–semiconductor field-effect transistors) with nanoscale gate length were demonstrated.
- Nanotechnology and nanoscience got a boost in the early 1980s with two major developments: the birth of cluster science and the invention of the scanning tunneling microscope (STM).
- These developments led to the discovery of fullerenes in 1985 and the structural assignment of carbon nanotubes (CNT) discovered by Sumio Iijima of Nippon Electric Company, Limited (NEC) in 1991. The development of FET in the 1990s also laid the foundations for modern nanoelectronic semiconductor device fabrication.
- In a timeframe of approximately half a century, at present nanotechnology has become the foundation for remarkable industrial applications and exponential growth.
- The term Nanotechnology covers the basic understanding, physics of nanomaterials which can be classified into different classes based on their properties, shapes or sizes.
- The different groups include fullerenes, metal NPs, ceramic NPs, and polymeric NPs. NPs possess unique physical and chemical properties due to their high surface area and nanoscale size.
- It wasn't until 1981, with the development of the scanning tunneling microscope that could "see" individual atoms, that modern nanotechnology began.
- ***Nanoscience and nanotechnology involve the ability to see and to control individual atoms and molecules.***
- Everything on Earth is made up of atoms—the food we eat, the clothes we wear, the buildings and houses we live in, and our own bodies. But something as small as an atom is impossible to see with the naked eye. In fact, it's impossible to see with the microscopes typically used in a high school science classes. The microscopes needed to see things at the nanoscale were invented in the early 1980s.
- Once scientists had the right tools, such as the scanning tunneling microscope (STM) and the atomic force microscope (AFM), the age of nanotechnology was born.
- Although modern nanoscience and nanotechnology are quite new, nanoscale materials were used for centuries. Alternate-sized gold and silver particles created colors in the stained glass windows of medieval churches hundreds of years ago.
- The artists back then just didn't know that the process they used to create these beautiful works of art actually led to changes in the composition of the materials they were working with. Today's scientists and engineers are finding a wide variety of ways to deliberately make materials at the nanoscale to take advantage of their enhanced properties such as higher strength, lighter weight, increased control of light spectrum, and greater chemical reactivity than their larger-scale counterparts.
- Here is one example: Medieval stained glass windows are an example of how nanotechnology was used in the pre-modern era.



Fig. 1: Medieval stained glass windows

2. Comparison of Nanomaterial sizes

- Just how small is “nano?” In the International System of Units, the prefix "nano" means one-billionth, or 10^{-9} ; therefore one nanometer is one-billionth of a meter.
- It's difficult to imagine just how small that is, so here are some examples: A strand of human DNA is 2.5 nanometers in diameter. A human hair is approximately 80,000 — 100,000 nanometers wide.
- One nanometer is about as long as your fingernail grows in one second.
- The illustration shown in Fig. 2 has examples of the size and the scale of nanotechnology, showing just how small things at the nanoscale actually are.

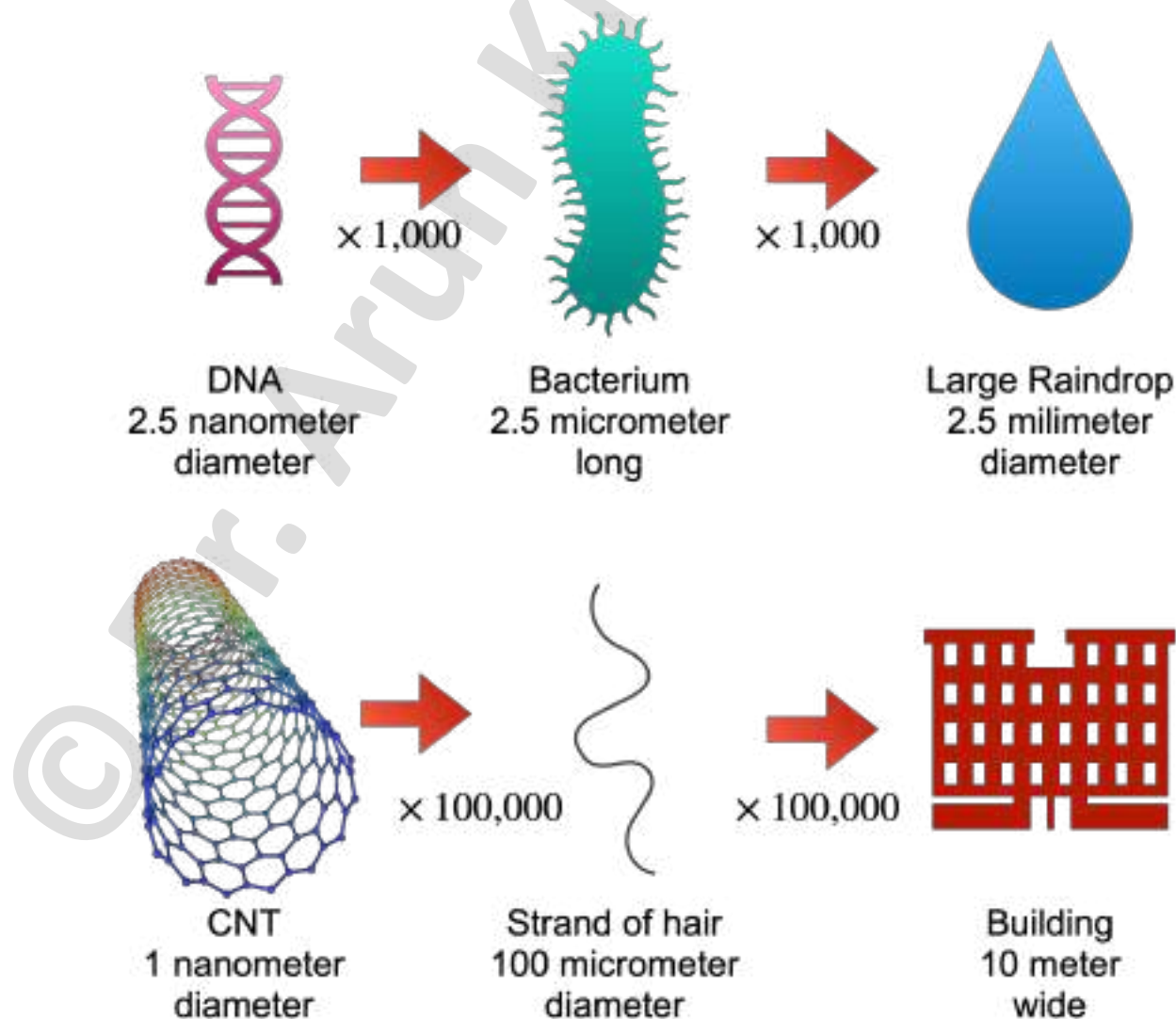


Fig. 2: The Scale of Things

- The scale of a human hand skin to it's DNA molecule are shown in Fig. 3 with the scale of 10cm to 1nm.

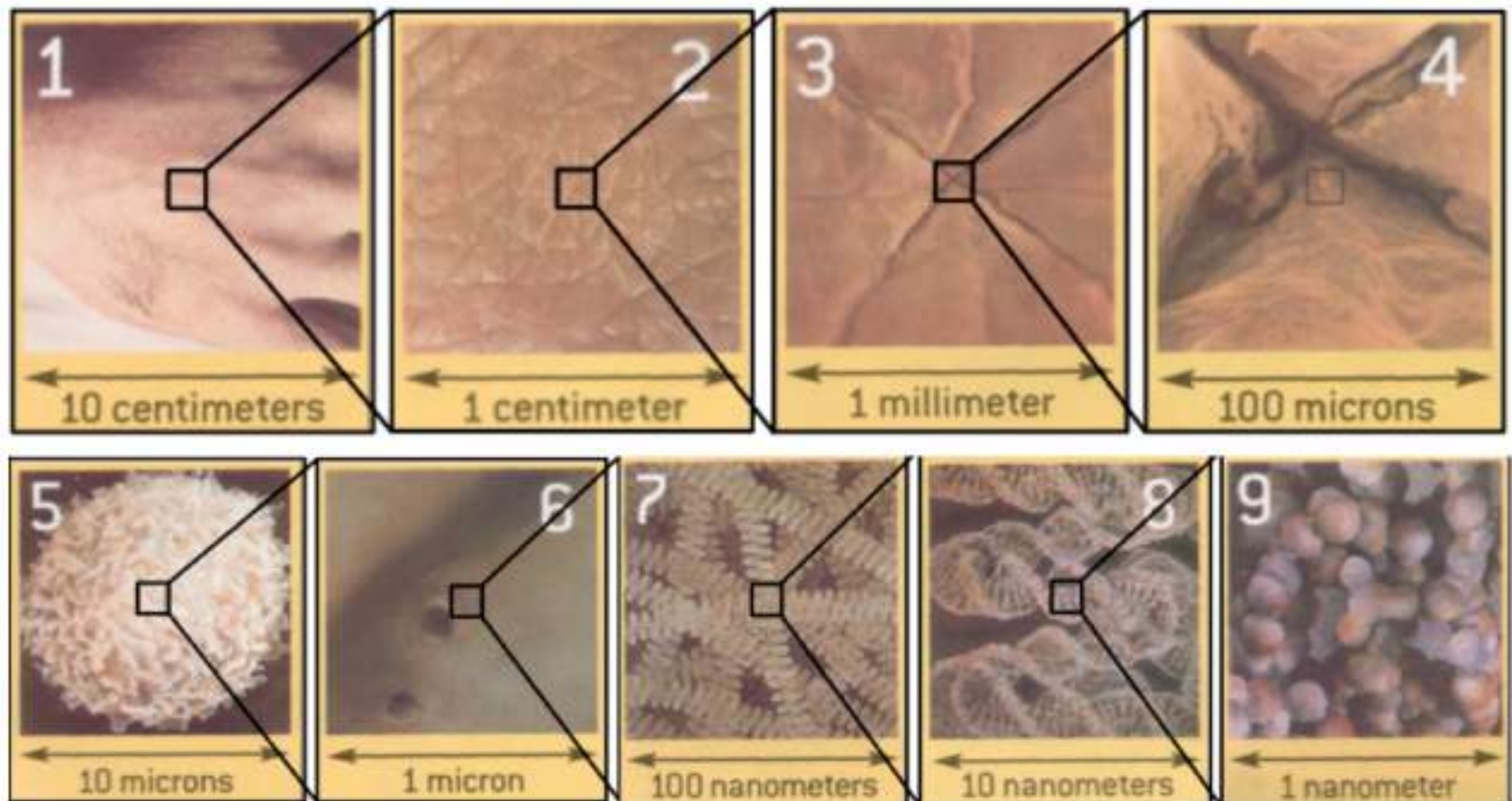


Fig. 3: The scale of skin to DNA molecule

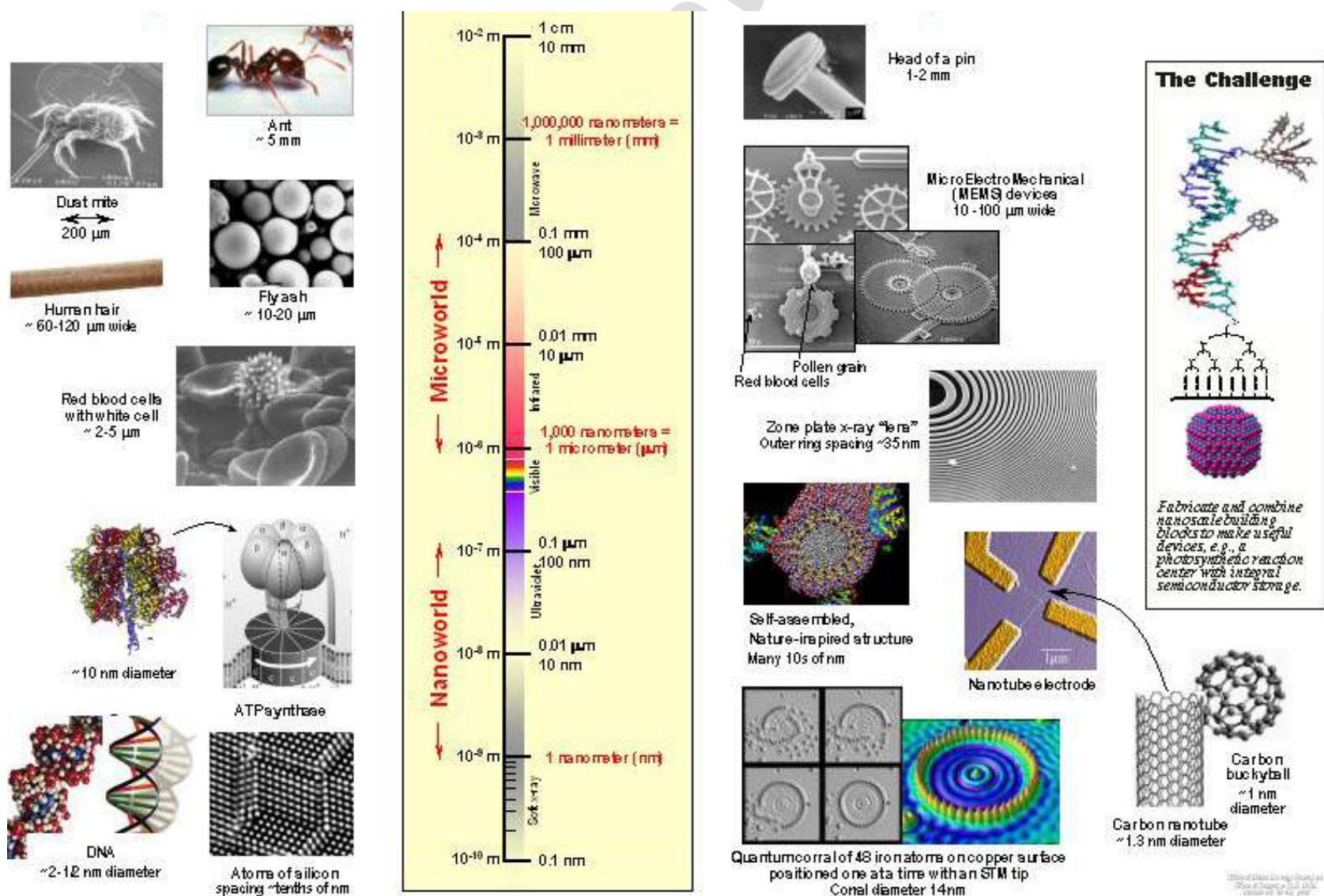


Fig. 4: Comparison of Nanomaterials Sizes

- The size of nanoscale objects and phenomena compared with the size of small everyday objects are shown in this picture. It provides some sense of how this scale relates to more familiar, everyday scales.

3. Cause of change in properties of nanomaterials

- In the last two decades, researchers began developing the ability to manipulate matter at the level of single atoms and small groups of atoms and to characterise the properties of materials and systems at that scale.
- This capability has led to the surprising discovery that clusters of small numbers of atoms or molecules—nanoscale clusters—often have properties that are significantly different from the properties of the same matter at either the single-molecule scale or the bulk scale.
- The properties like optical, physical, chemical, electrical etc of materials changes drastically when the material get reduced to nanoscale. What has happened with the properties of material when reduced to the nanoscale? The reasons to change the property of nanomaterials are;
- Surface to volume ratio
- Small size effect (Quantum confinement),
- Discrete energy levels (large energy band gap).
- **Surface to volume ratio**
- Surface area to volume ratio in nanoparticles has a significant effect on the nanoparticles properties. Nanoparticles have a relative larger surface area when compared to the same volume of the material.

- Example 1:

Consider the example of Rubik's cube which has 6 surfaces as shown in Fig. 5.

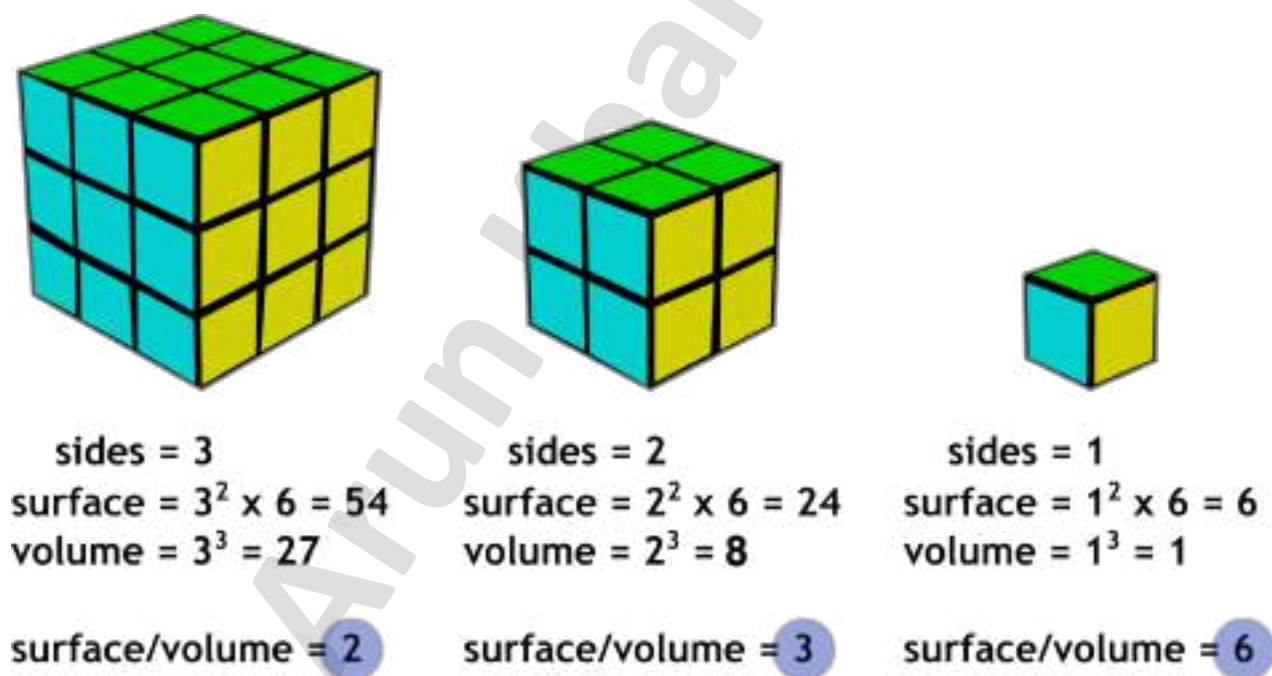


Fig. 5: Surface area to volume ratio in nanoparticles

Consider 3 sides of cube;

$$\text{Surface} = 3^2 \times 6 = 54; \text{Volume} = 3^3 = 27, \text{ Therefore surface to volume ratio} = \frac{54}{27} = 2.$$

Now; Consider 2 sides of cube;

$$\text{Surface} = 2^2 \times 6 = 24; \text{Volume} = 2^3 = 8, \text{ Therefore surface to volume ratio} = \frac{24}{8} = 3,$$

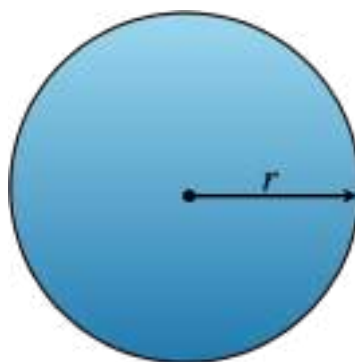
Now finally; consider 1 side of cube;

$$\text{Surface} = 1^2 \times 6 = 6; \text{Volume} = 1^3 = 1, \text{ Therefore surface to volume ratio} = \frac{6}{1} = 6$$

Hence as particle size gets smaller, the surface area to volume ratio gets larger.

- Example 2:

One more example, let us consider a sphere of radius r :



The surface area of the sphere $S = 4\pi r^2$, if $r = 1$ then $S = 4\pi$

The volume of the sphere $V = \frac{4}{3}\pi r^3$, if $r = 1$ then $V = \frac{4}{3}\pi$

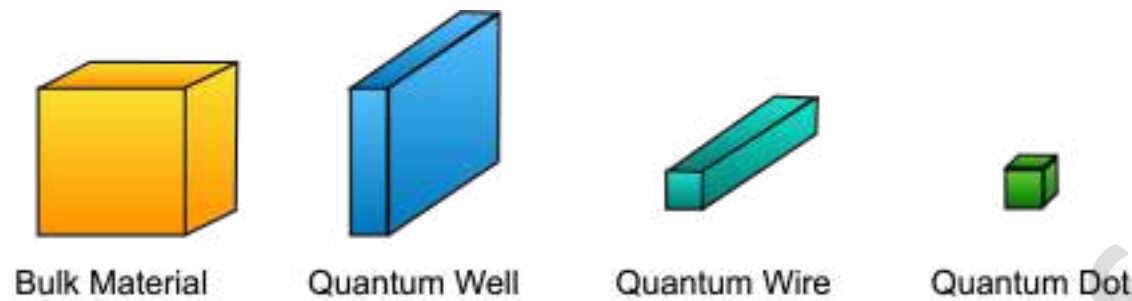
Therefore the surface area to the volume ratio $\frac{V}{S} = \frac{4\pi}{4\pi \times 3} = \frac{1}{3}$.

The ratio of the volume and surface area of a sphere is 1:3.

- It means that the surface area to volume ratio increases with the decrease in radius of the sphere and vice versa.
- It can also be conclude here that when given volume is divided into smaller piece, the surface area increases. Therefore as particle size decreases, a greater portion of the atoms are found at the surface compared to those inside.
- For example, a particle of size 3 nm has 50% of its atoms on its surface, at 10 nm 20% of its atoms and at 30 nm has 5% of its atoms on its surface. Therefore nanoparticles have a much greater surface area per unit volume compared with the larger particles.
- It leads to nanoparticles more chemically reactive. As growth and catalytic chemical reaction occurs at surfaces, therefore a given mass of nanomaterial will be much more reactive than the same mass of material made up of large particles. It is also found that materials which are inert in their bulk form are reactive when produced in their nanoscale form. It can improve their properties.

4. Quantum Confinement Effect and Discrete Energy Levels:

- When the dimension of the material is reduced to only a few tens of nanometer energy levels of electrons can no longer remain continuous. But these energy levels now become discrete with a small and finite separation. This situation of discrete energy levels is known as quantum confinement.
- This effect can change optical, electrical, magnetic and mechanical behavior of materials in nanometer regime. In nanometer range specific behavior of individual atom dominates. The behavior of individual atom is very different from behavior of atoms in bulk material. Nanosystems that exploit quantum size confinement effect include quantum well, quantum wire, quantum dots etc.
- When the systems are quantum defined only in one dimension to nanoscale, while the other two dimensions remain large (as in thin films, layers) then the system is quantum well.
- Here electrons are free to move in two dimensions and restricted along third direction. If two dimensions are quantum confined to nanoscale and third dimension remains large then the resulting system is quantum wire.
- When all three dimensions are quantum confined into nanoscale regime, then the resulting system is quantum dot. The key feature of nanoparticles is the fine control available over their band gap due to quantum size confinement.



- In a bulk material, the number of atoms is very large and the overlap of this high number of atomic orbital creates a continuum of closely spaced 'molecular' orbital which form the valence and conduction bands.
- However, if the material is reduced to a nanoscale size the situation changes. There are fewer atomic orbital overlapping and the valence and conduction bands are no longer continuous and are instead formed of discrete energy levels, and more importantly the band gap between the valence and conduction bands becomes wider which is known as quantum confinement as shown in Fig. 6.
- Nanoparticles that are small enough to have their band gap influenced by quantum confinement are known as quantum dots and by precisely controlling the size of the quantum dots during synthesis the photoluminescence emission and absorption wavelengths can be finely tuned, which is ideal for optoelectronic applications.

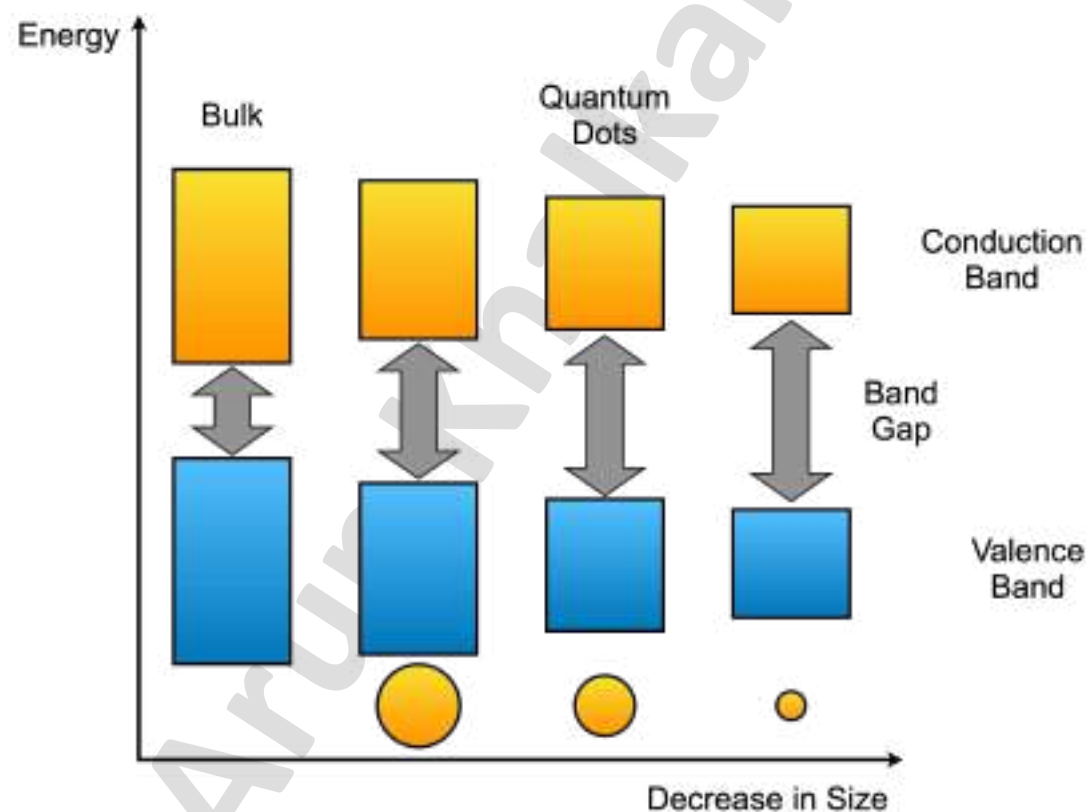


Fig. 6: The influence of particle size on the band gap of quantum dots due to quantum confinement

5. Seeing at the Nanoscale

- How do scientists see what's going on in the extremely small world of nanotechnology? The microscopes that are typically used in high school and college won't do the job. Nanoscientists use high-powered microscopes that use unique methods to allow them to see the surface features on the atomic scale, effectively opening the door to modern nanotechnology.
- **Exploring the World through Microscopes**
- Beginning as early as the 1930s, scientists were able to see at the nanoscale using instruments such as the scanning electron microscope, the transmission electron microscope, and the field ion microscope. The most recent and notable developments in microscopy are the scanning tunneling microscope and the atomic force microscope.
- The electron microscope, first developed by German engineers Ernst Ruska and Max Knoll in the 1930s, uses a particle beam of electrons to illuminate a specimen and create a highly magnified image. Electron microscopes

yield much greater resolution than the older light microscopes; they can obtain magnifications of up to 1 million times, while the best light microscopes can magnify an image only about 1,500 times.

- The scanning tunneling microscope (STM) is among a number of instruments that allows scientists to view and manipulate nanoscale particles, atoms, and small molecules. Its development earned its inventors, Gerd Binig and Heinrich Rohrer, the Nobel Prize in Physics in 1986.
- Atomic force microscopes (AFMs) gather information by "feeling" the surface with a mechanical probe. Gerd Binig, along with Calvin Quate and Christoph Gerber, developed the first AFM in 1986.
- Quantum dots: the color of fluorescence is determined by the size of particles and the type of materials. STM images of material, AFM images of material, Quantum Dots: The colour of fluorescence is determined by the size of particles and the type of materials.

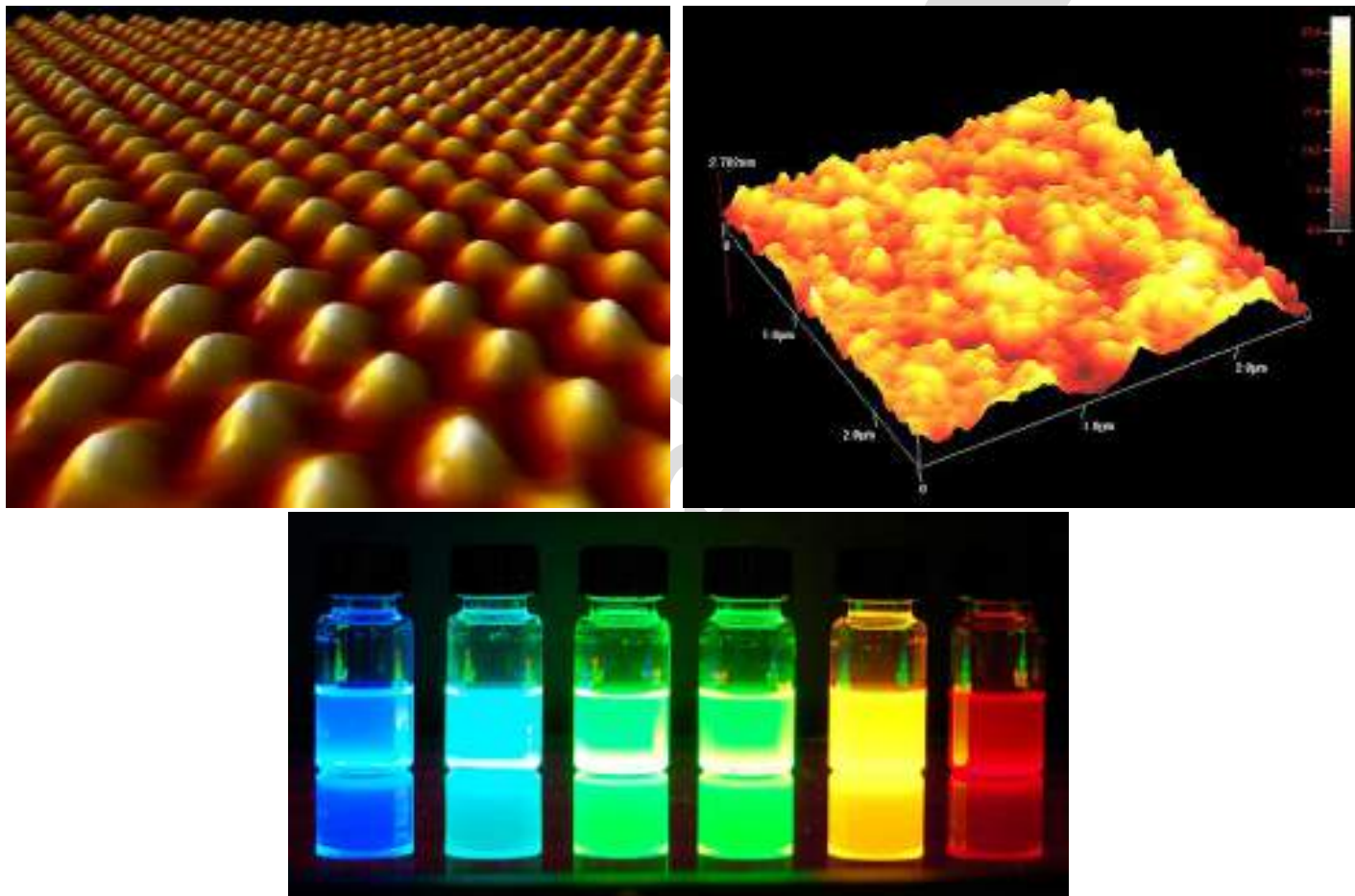


Fig. 7: STM, AFM and Quantum Dots

6. Various Nanoparticles

- A nanoparticle or ultrafine particle is usually defined as a particle of matter that is between 1 and 100 nanometres (nm) in diameter.
- The term is sometimes used for larger particles, up to 500 nm, or fibers and tubes that are less than 100 nm in only two directions.
- At the lowest range, metal particles smaller than 1 nm are usually called atom clusters instead.
- Nanoparticles are usually distinguished from microparticles (1-1000 μm), "fine particles" (sized between 100 and 2500 nm), and "coarse particles" (ranging from 2500 to 10,000 nm), because their smaller size drives very different physical or chemical properties, like colloidal properties and optical or electric properties.
- Nanoparticles occur in a great variety of shapes, which have been given many formal and informal names such as nanotubes, nanowires, nanosheets, nanospheres, nanorods, nanochains, nanostars, nanoflowers, nanoreefs, nanowhiskers, nanofibers, nanoprisms, nanobars, nanocubes, nanopyramids, nanorice, quantum dots etc.
- Here are few examples are shown in Fig. 8.

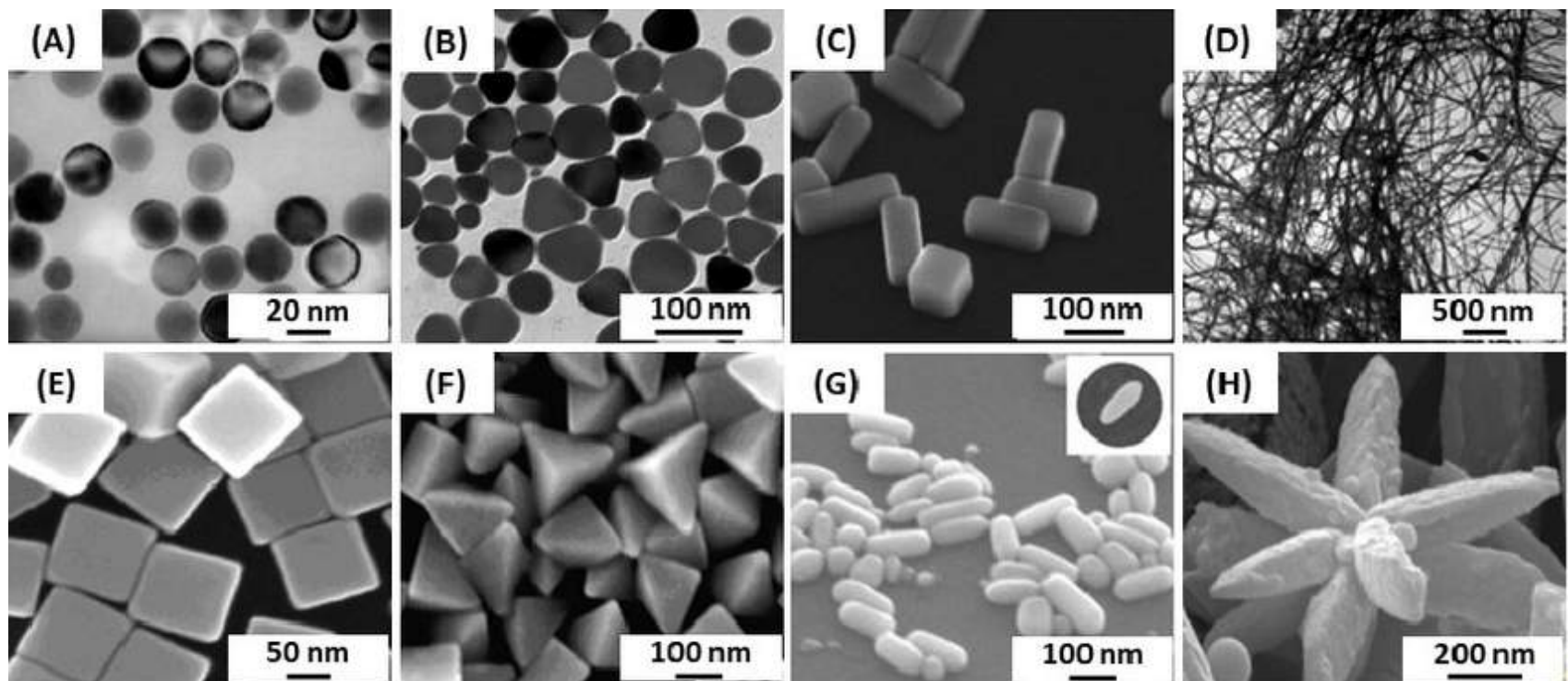


Fig. 8: TEM images of silver nanoparticles with different shapes

(A) nanospheres, (B) nanoprisms, (C) nanobars and (D) nanowires, (E) nanocubes, (F) pyramids, (G) nanorice and (H) nanoflowers. [Image source: DOI:10.3390/bios9020078].

- Different types of nanoparticles

- Carbon-Based Nanoparticles: CNT, C60, Graphene etc.
- Ceramic Nanoparticles: oxides, carbides, carbonates, phosphates etc.
- Metal Nanoparticles: gold, silver, aluminium etc.
- Semiconductor Nanoparticles: GaN, GaP, InP, InAs, ZnO, ZnS, CdS, CdSe, CdTe etc.
- Polymeric Nanoparticles: Rapamycin, Hyperforin, Fenofibrate, Coumarin-6 etc.
- Lipid-Based Nanoparticles; liposomes, polyethylene glycol etc.

- Carbon allotropes

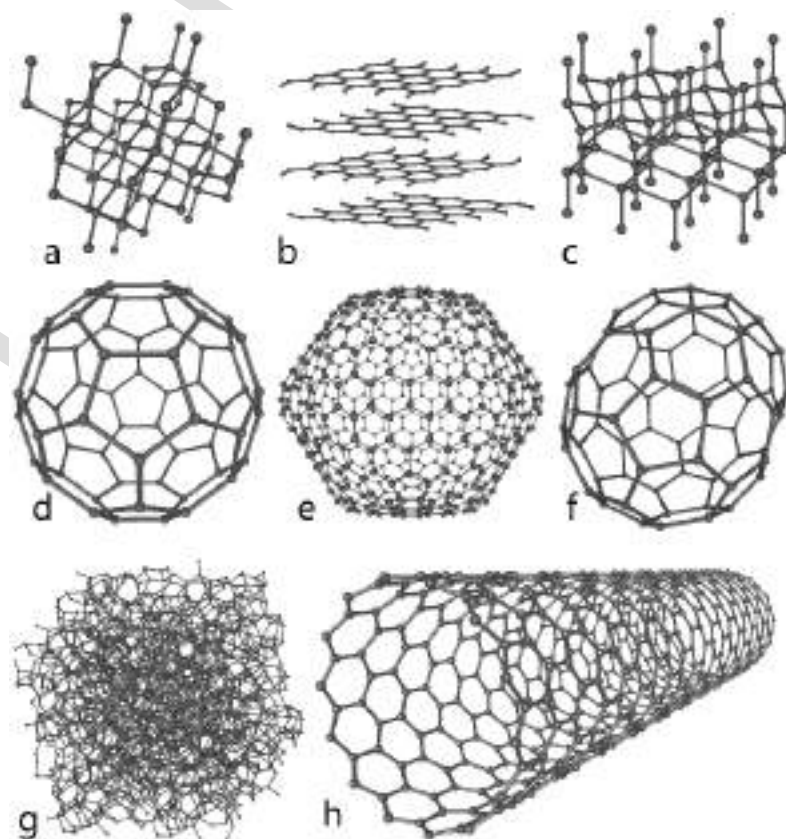


Fig. 9: Schematic representation of carbon allotropes

a) Diamond, b) Graphite, c) Lonsdaleite, d) C60, e) C540, f) C70, g) Amorphous carbon, h) SWNT.

7. Properties of nanoparticles

- The various properties of nanoparticles play a very crucial role for emerging applications in various fields. Following properties are important to study the nanoparticles.

- Optical properties
- Electrical properties
- Magnetic properties
- Mechanical properties

Let study all above properties one by one.

A) Optical properties

- One of the most fascinating and useful aspects of nanomaterials is their optical properties. The properties like colour and transparency are considered as optical properties. These properties are observed to change at nanoscale level. It is one of the most useful features of nanoparticles. It has a wide range of applications in visual science.
- Nanoparticles are helpful in the optical experiment. Thus, used in the manufacturing of various optical detectors, laser beam, sensor, and imaging. Applications in the display, solar cell, photo catalysis and photo electrochemistry are also very prevalent.
- For example bulk gold appears yellow in colour while in nanosize gold appears red in colour. The optical properties of nanomaterials depend on parameters such as size, shape, surface characteristics, and other variables including doping and interaction with the surrounding environment or other nanostructures.
- The main reason for change in optical properties at nanoscale level is that nanoparticles are so small that electrons in them are not as free to move as in case of bulk material.
- Due to this restricted movement of electrons, nanoparticles react differently with light as compared to bulk material. Colour can arise from various mechanisms as outlined shown in Fig.10.



Fig. 10: Various mechanisms of optical properties

- Nanomaterials exhibit a variety of unusual and interesting optical properties that can differ significantly from the properties exhibited by the same bulk material. By carefully controlling the size, shape and surface functionality of nanoparticles a wide range of optical effects can be generated with many useful applications.
- An optical response in a nanomaterial can be created through several different mechanisms, depending on the nanomaterial size, composition and arrangement, and each method may provide certain benefits depending on the target application.

i) Scattering, Absorption and Extinction:

- When light is incident on a nanoparticle, it can be scattered or absorbed, the sum of scattering and absorption is referred to as extinction. Nanoparticles are in the size regime where the fraction of light that is scattered or absorbed can vary greatly depending on the particle diameter.
- At diameters less than 20 nm, nearly all of the extinction is due to absorption. At sizes above 100 nm, the extinction is mostly due to scattering. By designing a particle with a larger or smaller diameter, the optimal amount of scattering and absorption can be achieved.
- The sum of *scattering & absorption* is called as **extinction**.
- Diameters $<20\text{ nm}$, the *extinction* is due to **absorption**.
- Diameters $>100\text{ nm}$, the *extinction* is due to **scattering**.
- A particle with a *larger or smaller diameter*, the optimal amount of *scattering and absorption* can be achieved.
- Another byproduct of this relationship between size and absorption/scattering is that aggregation can increase the effective size of a nanoparticle resulting in an increase in scattering. This is why 20 nm diameter silica particles are clear in solution but re-suspensions of dried 20 nm silica particles (aggregated) will be a milky white colour.



Fig. 11: A 20 nm diameter silica particles with milky white colour.

ii) Optical Properties of Metallic Nanoparticles

- Surface Plasmons (SP) are the origin of the colour of metal nanomaterials. In case of metals as the size of particles decreases, the oscillations of electron gas on the surface of nanoparticle is observed. These oscillations are called as **surface plasmons (SP)**.
- So, if nanoparticles are exposed to electromagnetic wave (light) having a wavelength comparable or greater than the size of the nanoparticles and light has a frequency close to that of SP then SP will absorb energy.
- Thus nanoparticles start exhibiting different colours as their size changes and frequency of SP changes with it. The frequency of the SP depends on the dielectric constant of the nanomaterial, the shape of the nanoparticle and specific geometrical shape that the particle has.
- Nanoscale structures made of metals such as gold, silver and aluminium can support *surface plasmon modes* where the free electrons in the material naturally resonate at a frequency that depends on the composition, size and shape of the particle.
- When the wavelength of incident light matches the oscillation frequency, the particles can strongly absorb or scatter the light resulting in a strongly coloured particle.
- By tuning the size and shape, the peak resonance wavelength can be shifted across the visible and into the infrared region of the spectrum allowing for a wide range of colour tunability.
- In addition to metal nanoparticles, there have been recent examples of metal oxide nanoparticles doped with other metal atoms that show strong and tunable plasmon resonances. By changing the particle size, dopant and dopant concentration, plasmon resonances in the near-infrared (NIR) and short-wavelength infrared (SWIR) can

been fabricated. Gold nanoparticles with different sizes show different colours as shown in Fig. 12. Metallic nanoparticles (MNPs) exhibit unique optical properties due to Localized Surface Plasmon Resonance (LSPR), size-dependent absorption and scattering, and nonlinear optical effects. These properties make them useful in sensing, imaging, catalysis, and photonic applications.

- LSPR occurs when conduction electrons in metallic nanoparticles oscillate collectively in response to incident light, leading to strong absorption and scattering.
- Gold (Au) and Silver (Ag) nanoparticles show tunable LSPR peaks in the visible to near-infrared range. Gold nanoparticles (AuNPs) appear red at small sizes (~10 nm) but turn blue when aggregated due to plasmon coupling.

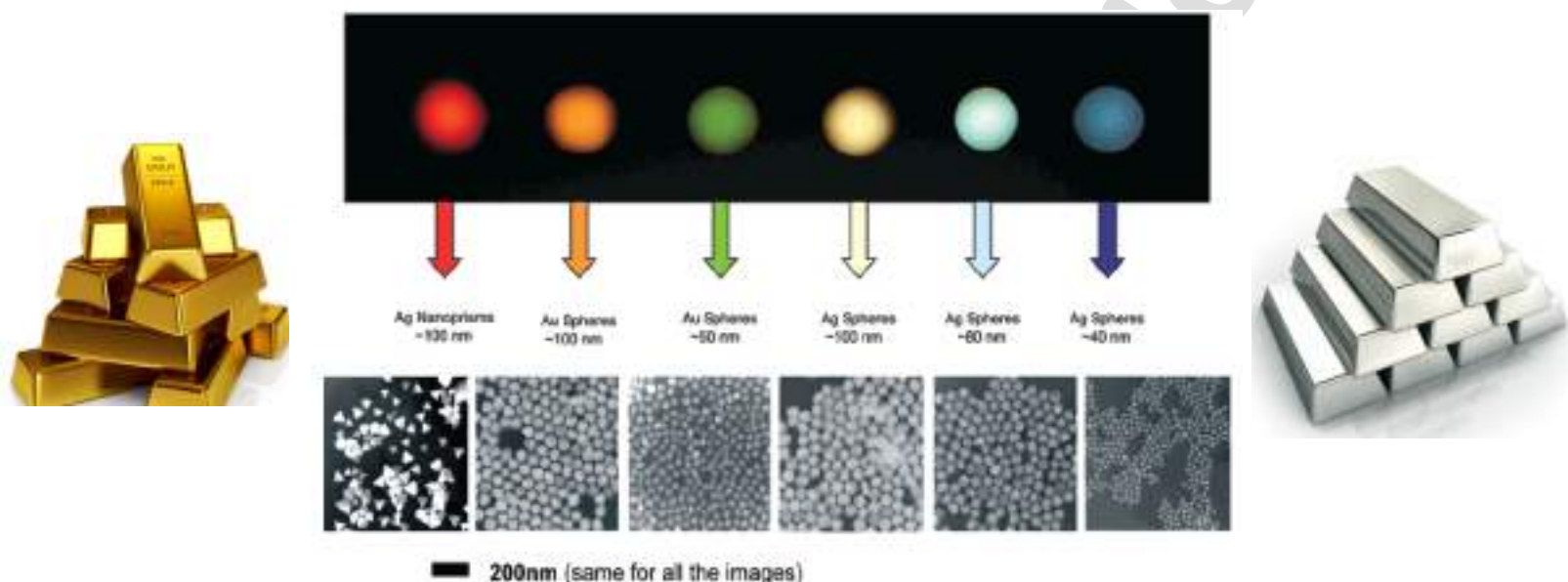


Fig. 12: Gold and Silver nanoparticles with different sizes show different colours.

iii) G. Mie theory for change in optical properties

- Gustav Mie Theory (Mie Scattering Theory) is a mathematical framework used to describe the interaction of light with spherical particles, including metallic nanoparticles. It explains how the optical properties of nanoparticles such as absorption, scattering, and plasmon resonance change based on size, composition, and surrounding medium.
- G. Mie explained the phenomenon using Maxwell's equation in 1908. According to Mie theory, when electromagnetic radiation incident on uniform sized spherical nanoparticles embedded in a medium, intensity gets reduced. It is necessary to consider mainly the dielectric constant of medium in which the particles float and the dielectric constant of particles.
- It provides a full analytical solution for:
 - Extinction cross-section (σ_{ext}): The total energy loss due to absorption and scattering.
 - Absorption cross-section (σ_{abs}): Energy absorbed by the nanoparticle.
 - Scattering cross-section (σ_{sca}): Energy scattered by the nanoparticle.
- For nanoparticles much smaller than the incident wavelength (λ), the quasi-static approximation of Mie Theory simplifies to the well-known plasmon resonance condition, leading to localized surface plasmon resonance (LSPR) in metallic nanoparticles. A beam of electromagnetic radiation of intensity I_0 and wavelength λ passes through a medium having dielectric constant E_m as shown in Fig. 13.
- When electromagnetic radiation incident on spherical particles of uniform size a part of the radiation is absorbed and a part is scattered.

- Thus the intensity of transmitted light changes. If the particles are embedded uniformly in medium then intensity of transmitted light is given by ;

$$I = I_0 e^{-\mu x}$$

where,

$$\mu = \frac{N}{V} C_{ext}$$

N is number of particles in medium,

V is Volume of colloidal particles,

C_{ext} is extinction cross section of a particle.

- At nanoscale, as size of the nanoparticles change, there is change in the length of medium and thus the values of μ and x changes.
- This changes the intensity of transmitted light and it depends on the wavelength of incident light. This changes the colour of nanoparticles at different nanoscale region.
- G. Mie theory successfully explained absorption of light of visible wavelength for nano- particles, but for particle size less than ~ 10 nm, there is need to consider dielectric constant which depends also on particle size.

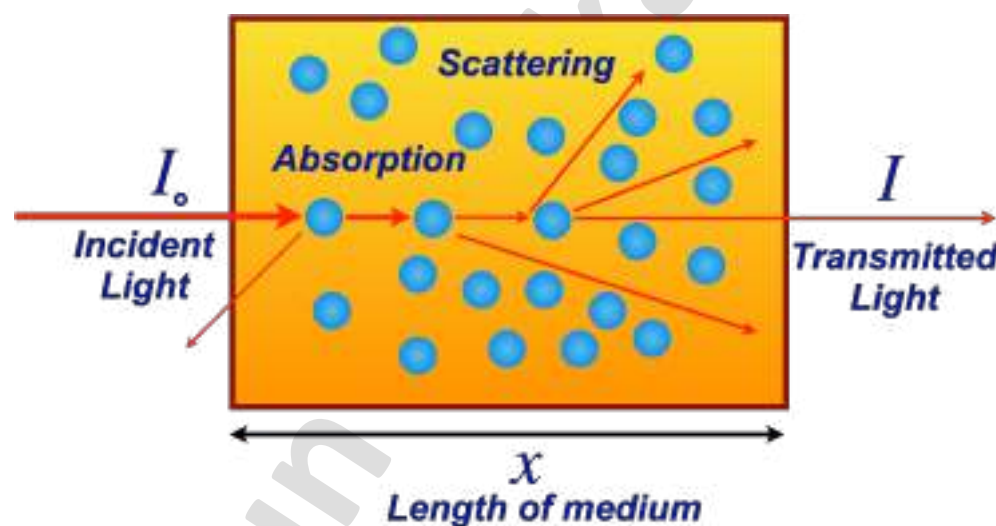


Fig. 13: Incident radiation I_0 passes through a medium of thickness x .

iv) Optical Properties of Semiconductor Nanoparticles

- The most striking property of nanoparticles made of semiconducting elements is the pronounced changes in their optical properties compared to those of the bulk material. When size of material reduced, then electron gets confined to the particle (confinement effects) leading to:
 - increase in bandgap energy and
 - band levels get quantized (discrete).
- Surface states (trap states), which lie in the bandgap become important and changes the optical properties of nanocrystals. The energy level spacing increases with decreasing particle size due to Quantum Size Confinement Effect. The simplest experiment to determine the size dependence in semiconductor nanoparticles is to study absorption spectrum of the material as a function of wavelength of incident photons.
- When photons are incident on semiconductor material they will be absorbed only when the minimum energy of photons is enough to excite an electron from the valence band to conduction band, i.e. when the photon energy equals the energy gap of the semiconductor. If lower energy photons are incident, there cannot be any absorption. Therefore there is a sudden rise in absorption when the photon energy is same as the energy gap. This is the onset of absorption.

- If the energy gap increases there should be a shift in the onset of absorption towards the shorter wavelength. The variation of energy gap with particles size is represented in Fig. It is observed that one expects a blue shift with absorption in smaller and smaller particles, which is indicative of increasing energy gap.
- For every small particle, one often uses the terminology borrowed from chemistry, viz. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) instead of top of valence band and bottom of conduction band used in case of extended solid.

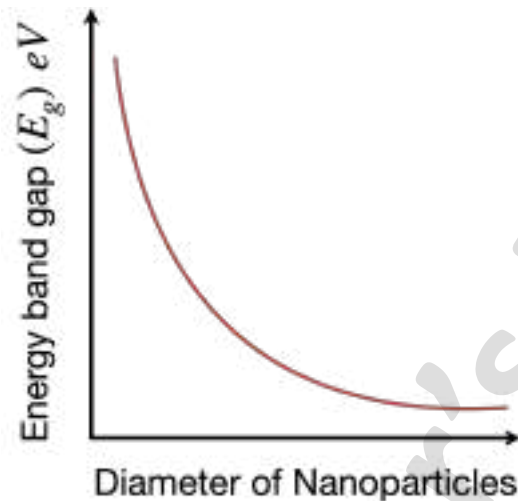


Fig. 14: Variation of Energy gap with particle size

- Exciton:

- There is significant shift in the optical absorption spectra toward the blue (shorter wavelength) as the particle size is reduced. In a bulk semiconductor a bound electron-hole pair, called an **exciton**, can be produced by a photon having energy greater than that of the band gap of the material.
- The band gap is the energy separation between the top filled energy level of the valence band and the nearest unfilled level in the conduction band above it.
- The photon excites an electron from the filled band to the unfilled band above. The result is a hole in the otherwise filled valence band, which corresponds to an electron with an effective positive charge.
- Because of the Columb attraction between the positive hole and the negative electron, a bound pair, called an exciton, is formed that can move through the lattice. The separation between the hole and the electron is many lattice parameters. The existence of the exciton has a strong influence on the electronic properties of the semiconductor and its optical absorption.
- An exciton can move in the crystal whose center of mass motion is quantized. Different kinds of excitons are identified in a variety of materials. When the electron-hole pair is tightly bound with distance between electron and hole comparable to lattice constant then it is called Frenkel exciton.
- At the other extreme, one may have an exciton with electron-hole separation much larger compared to lattice constant. Such a weakly bound electron-hole pair is called Mott-Wannier exciton.
- For example, Cd_2P_2 is a dark brown semiconductor with energy gap of approximately 0.5 eV. When its particles are made, it progressively passes through a series of colours like brown, red, yellow and white with particle size changing from 30\AA to 15\AA . For 15\AA particles the band gap increases to 4 eV.
- The same is true for CdS. The bulk semiconductor with energy gap of 2.42 eV is orange in colour. As the particles become smaller and energy gap increases it becomes yellowish and ultimately white.

- Quantum Dots

- Nanoparticles made of semiconductor materials, often referred to as quantum dots (QD), absorb and emit light at certain wavelengths that depend strongly on particle size and shape due to quantum confinement effects.

- By changing the size and composition of the quantum dots, their emission wavelengths can be tuned from the UV through the visible to the near infrared regions of the spectrum.
- For example, by tuning the size of CdSe QDs from 2 nm to 4.2 nm in diameter, the emission wavelength can be shifted across the visible spectrum, with the smaller particles emitting in the blue and the larger particles emitting red light.

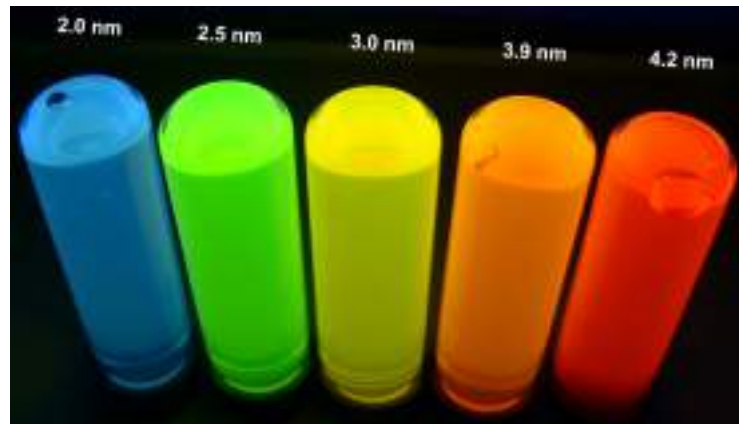


Fig. 15: CdSe QDs from 2 nm to 4.2 nm in diameter

- As fluorescent materials, quantum dots offer a number of advantages over organic fluorescent dyes: in addition to the ability to easily tune optical properties by varying particle size, the QDs are less likely to photobleach under high intensity illumination, offer comparable or larger quantum yields than organic dyes, and can be excited much further away from their emission peak, giving them a large effective Stokes shift and allowing more flexibility with imaging or choosing excitation sources to avoid auto-fluorescence in biological samples.
- QDs are used in a variety of applications including photodetectors, solar cells, light emitting diodes (LEDs), televisions, and for medical imaging. At nano composites we use QDs as components of multi-functional particles – typically for diagnostics and imaging.
- An example is a metal cored quantum dot composite particle that is used in lateral flow diagnostic devices.
- **Photonic Crystals**
- Photonic Crystals are periodic dielectric structures that are designed to form the energy band structure for photons, which either allows or forbids the propagation of electromagnetic waves of certain frequency ranges, making them ideal for light-harvesting applications.
- A photonic crystal is a periodic optical nanostructure that affects the motion of photons in much the same way that ionic lattices affect electrons in solids. Photonic crystals occur in nature in the form of structural coloration and animal reflectors, and, in different forms.
- This type of “structural colour” has many examples in nature, such as the iridescent blue appearance of a morpho butterfly wing, which is due to nanoscale periodic structures that reflect only blue wavelengths of light.
- Structural colour gives rise to the multi-colored iridescence of opal gemstones, which are made from highly ordered assemblies of silica particles. Highly monodisperse nanoparticles can be used for the assembly of colloidal crystals where dried particles will organize into a periodic assembly that can diffract light.
- Structural colour assemblies can also be created dynamically in solution using magnetically responsive particles, such as the particles shown below which align into ordered structures in the presence of a magnetic field.

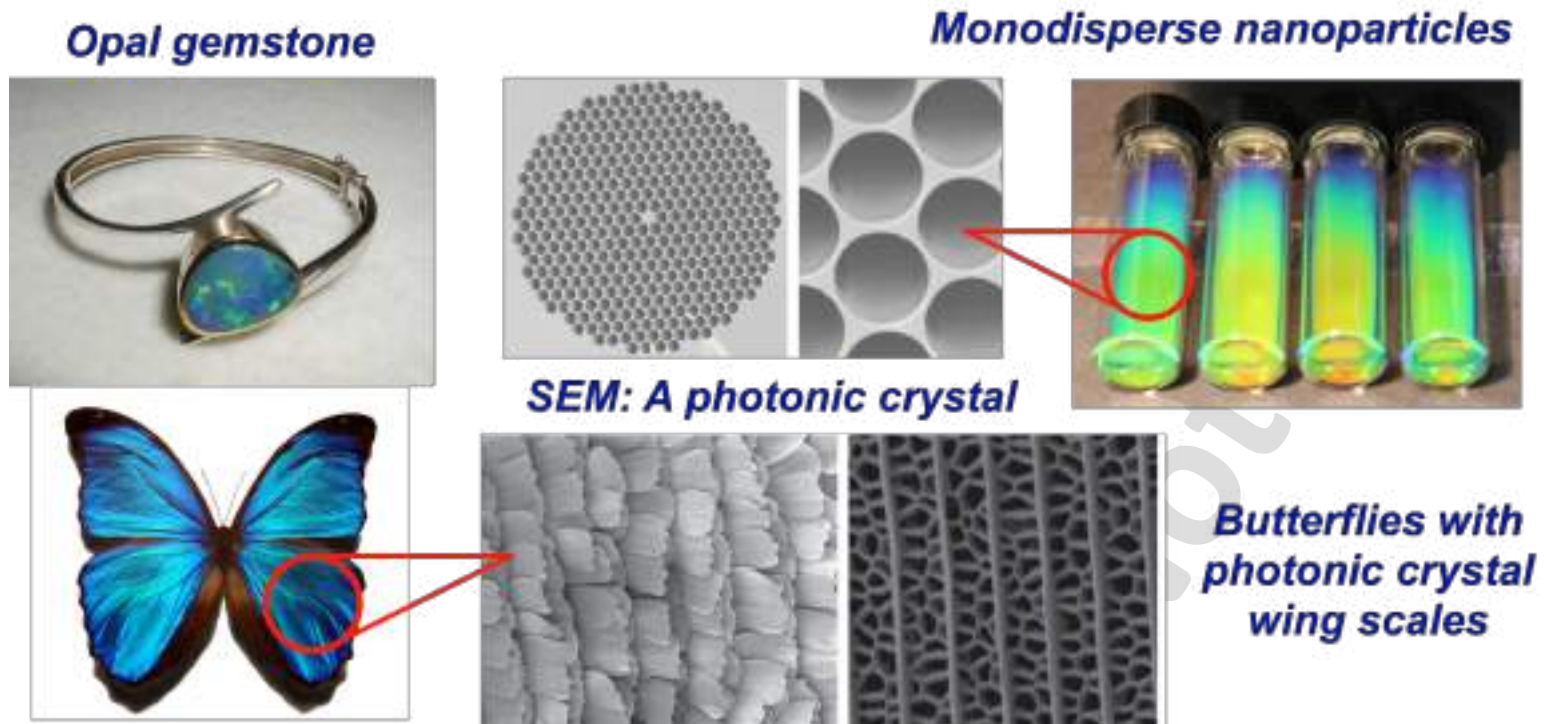


Fig. 16: Photonic Crystals

- Optical Properties of Zinc Oxide (ZnO) Nanoparticles

- Zinc Oxide (ZnO) is a wide-bandgap semiconductor with unique optical properties that make it useful in applications such as UV-blocking materials, sensors, optoelectronics, and photocatalysis.
- UV-Visible Absorption: ZnO has a direct bandgap of ~ 3.37 eV (at room temperature), allowing it to strongly absorb ultraviolet (UV) light. ZnO nanoparticles absorb photons in the 200–400 nm range, making them effective UV-blocking agents in sunscreens and optical coatings.
- Photoluminescence (PL): ZnO exhibits strong photoluminescence, with two main emissions. Near-band-edge (NBE) emission in the UV region (~ 380 nm) due to exciton recombination. Visible emission (green, yellow, or orange) caused by intrinsic defects such as oxygen vacancies and zinc interstitials.
- Quantum Confinement Effect: In ZnO nanoparticles, reducing particle size to the nanometer scale leads to a blue shift in optical absorption due to quantum confinement effects, which influence electronic band structure. In bulk ZnO, the exciton Bohr radius is ~ 2 nm. When ZnO nanoparticles are smaller than 5 nm, the bandgap increases due to quantum confinement, shifting absorption towards shorter wavelengths (blue shift). Example: Bulk ZnO absorbs at ~ 370 nm, but nanosized ZnO (< 5 nm) absorbs at 340 nm or lower.
- Refractive Index and Transparency: ZnO is highly transparent in the visible region with a high refractive index (~ 2.0), making it useful in optical coatings, sensors, and transparent conductive films.
- Nonlinear Optical Properties: ZnO exhibits strong nonlinear optical behavior, including second-harmonic generation (SHG) and multiphoton absorption, making it applicable in laser technology and optical switching.
- Photocatalytic Activity: ZnO nanoparticles efficiently absorb UV light, generating electron-hole pairs that drive photocatalytic reactions, making them valuable in environmental remediation and solar energy applications.
- These optical properties contribute to the extensive use of ZnO nanoparticles in UV-blocking materials, LEDs, photodetectors, biosensors, and solar cells.
- The large size ZnO particles blocks UV light and have ability to scatter visible light. Hence they appear white.
- Where as, nanosized ZnO particles also blocks the UV light but they are so small as compared to the wavelength of visible light that they don't scatter it. Hence it appears clear. Here is a SEM image of ZnO nanoparticles is shown which is used in sunscreen cream.



Fig. 17: optical properties of Zinc Oxide

- **Analysis of ZnO Nanoparticles in Sunscreen (Based on SEM Image)**
- The SEM (Scanning Electron Microscope) image provided shows Zinc Oxide (ZnO) nanoparticles, which are used as UV-blocking agents in sunscreen creams. Below are key observations based on the image:
- **Particle Morphology & Size:** The ZnO nanoparticles exhibit irregular, rod-like and plate-like structures. The scale bar (500 nm) indicates that most ZnO particles are in the 100–300 nm range, which is suitable for effective UV absorption while maintaining transparency in visible light.
- **Optical Properties & UV Protection:** ZnO is a wide-bandgap semiconductor (~ 3.37 eV, ~ 370 nm absorption) that effectively blocks both UVA and UVB radiation. The nanosized ZnO particles prevent whitening effects, making the sunscreen transparent on the skin while still offering strong UV protection.
- **Agglomeration & Dispersion:** The image shows some degree of particle agglomeration, which can affect the even distribution of ZnO in sunscreen formulations. Proper surface functionalization (e.g., coatings or dispersants) is used to prevent excessive clumping and improve spreadability on the skin.
- **Benefits of Nano-ZnO in Sunscreen:** Broad-spectrum UV protection (absorbs UV rays while being transparent in the visible range). Non-toxic and photostable, unlike organic UV filters, which can degrade under sunlight. Hypoallergenic and suitable for sensitive skin.

B) Electrical properties

- Nanoparticles (NPs) exhibit unique electrical properties due to their high surface-to-volume ratio, quantum confinement effects, and electron transport characteristics. These properties make them highly valuable in nanoelectronics, sensors, photovoltaics, and energy storage devices.
- Materials are often classified according to their ability to let current flow through them. The resistivity (or conductivity) in solids can be measured in principle by connecting electrically conducting wires to solid material of known geometry, applying a voltage difference across it and measuring the current flowing through it.
- Current flowing through it is given by Ohm's law. The resistivity in bulk material is mainly due to scattering of electrons by ions and crystal defects.
- In nanostructures the resistivity mainly depends on scattering from boundaries of nanoparticles when particle size becomes less than mean free path between collisions.
- Thus smaller particle size increases resistivity. Various types of defects in the lattice also increase the resistivity by limiting mean free path but nanoparticles are too small to have internal defects.

- Energy band gap with respect to size of nanoparticles

- We know that every particle has some electrostatic property. Thus, nanoparticles also show a wealth of conduction differently. This electrical conductivity plays a significant role in nanoparticles such as nano rods, carbon nanotubes etc.
- Inside the nanoparticles, its energy band structure and charge carrier density can also influence the bulk particles differently.
- For example, high-density electron storage is possible using quantum dot devices that use lasers and light-emitting diodes (LED).
- The spacing of the electronic levels and the band gap increases with decreasing particle size. This is because the electron hole pairs are now much closer together and the Coulombic interaction between them can no longer be neglected giving an overall higher kinetic energy.
- This increase in band gap can be observed experimentally by the blue-shift in the absorption spectrum or sometimes even visually by the colour of the samples.
- A larger band gap means that more energy is required to excite an electron from the valance band to the conduction band and hence light of a higher frequency and lower wavelength would be absorbed. Hence the band gap of nanoparticles increases with decrease in size as shown in Fig. 18.

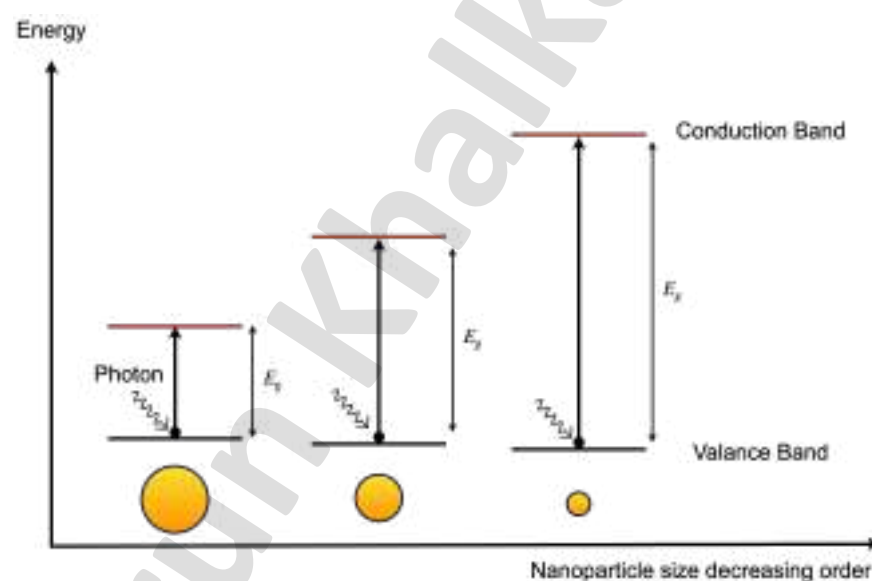


Fig. 18: Band gap increases as size of nanoparticles decreases.

- I-V Characteristics of bulk conductor and Nanomaterials

- Electrical properties are characterised by the mean free path of electron which is path of the electron collision due to atoms or ions. The mean free path changes at nanoscale due to collision and tunneling within the conductor.
- The I-V characteristics of bulk conductors and nanomaterials show distinct differences due to quantum effects like Coulomb blockade and electron tunneling in nanostructures.

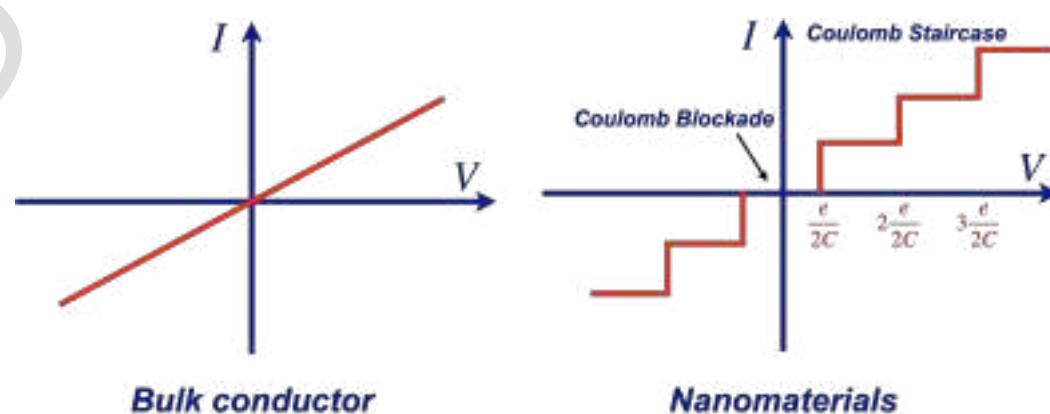


Fig. 19: I-V Characteristics of bulk conductor and Nanomaterials



- **I-V Characteristics of bulk conductor:** When voltage V is applied across the conductor, current I flowing through it is governed by Ohm's Law and has a linear variation. The current increases linearly with voltage. Electrons experience scattering with atoms or phonons, leading to resistance.
- **I-V Characteristics at nanoscale:**
 - Coulomb Blockade: At very small scales ($\sim 1-10$ nm), charging energy prevents current flow until voltage reaches a threshold.
 - Coulomb Staircase: As voltage increases, current steps up in discrete levels due to the quantized transfer of electrons (one-by-one).
 - Tunneling Effect: If the nanomaterial is a quantum dot or nanoparticle, electrons can tunnel through thin insulating barriers. The repeated tunneling of single electron produces '*Coulomb staircase*'.
 - The mean free path of electrons is modified due to increased surface scattering and confinement effects.
 - If dimensions of conductor are in nanoscale (1-100 nm), there appears a region around zero voltage for which there is no current. A single electron is transferred by tunneling when the voltage is $\pm e/2C$.
 - Therefore, when the voltage is less than this electron cannot be transferred. This gives a region of zero current at low bias voltage and is known as '*Coulomb blockade region*'. The electrons are transferred when the voltage is $\pm e/2C$.
- **Electrical resistivity:** The materials of nano-sized grains have larger number of grain boundaries than corresponding polycrystalline materials. Electrical resistivity of materials having nano-sized grain is larger than the polycrystalline materials due to scattering of electrons at grain boundaries.

C) Magnetic properties

- Magnetic properties of nanoparticles (NPs) differ significantly from their bulk counterparts due to quantum size effects, surface effects, and finite-size effects.
- These properties are highly dependent on factors such as composition, size, shape, and the surrounding environment.
- Material shows magnetic properties due to orbital and spin motions of electrons. Electron has *spin and orbital magnetic moment*. The vector sum of all the moments of electrons gives the total *moment of the atom*. Iron, cobalt and manganese, have a *net magnetic moment*.
- Crystals of these atoms become *ferromagnetic* in which magnetic moments aligned in the *same direction*.
- **Hysteresis B-H curve for bulk and nanoparticles**
 - The hysteresis loop (B-H curve) represents the magnetic response of a material when subjected to an external magnetic field. The behavior of bulk materials and nanoparticles differs significantly due to quantum confinement, surface effects, and finite-size effects.
 - In bulk ferromagnetic materials, the magnetic moment is less than the moment in the bulk material. Presence of '*domains*' in one direction but moments of different domains are in different directions.
 - When bulk ferromagnetic materials are subjected to alternating magnetic fields, they show hysteresis for which the B-H curve is as shown in Fig.20(a).
 - In nano sized ferromagnetic particles, essentially consisting of a single domain there is no hysteresis and the B-H curve, as shown in Fig.20(b).
 - This variation in the magnetisation is due to change in cohesive forces between the atoms when material is in the nano particle form.

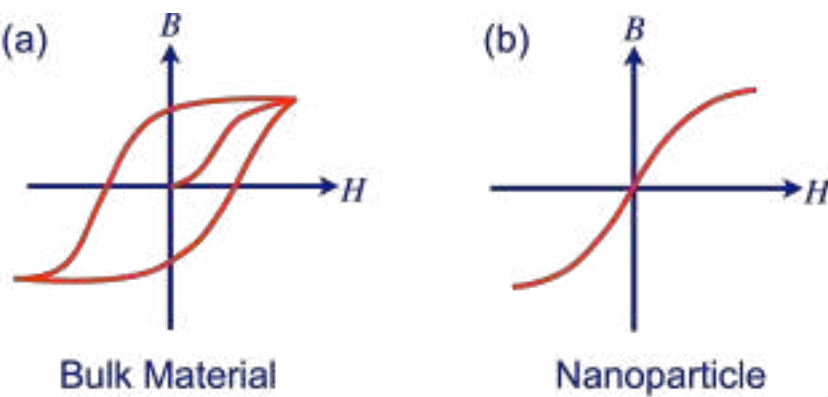


Fig.20: Hysteresis B-H curve for bulk and nanoparticles

- **Dependence of magnetic moment on the dimension**
- There is an increase in magnetic moment per atom as we decrease the dimensionality of the system. In small systems, a large fraction of atoms is at surface. Surface atoms have lower coordination number than bulk atoms.
- Fig. 21 shows dependance of magnetic moment on coordination number. As coordination number increases the magnetic moment decreases. Small clusters have lower coordination number hence magnetic moment of a very small cluster is more than bulk material.
- This is indicative of fundamental differences in magnetic behaviour between nano structures and bulk materials.
- This effect is important as surface spins are usually not ordered along the same directions as the spins in the interior of the material, thus we expect nano crystals with more surface to have less μ_B per atom than bulk materials purely based on surface effect.

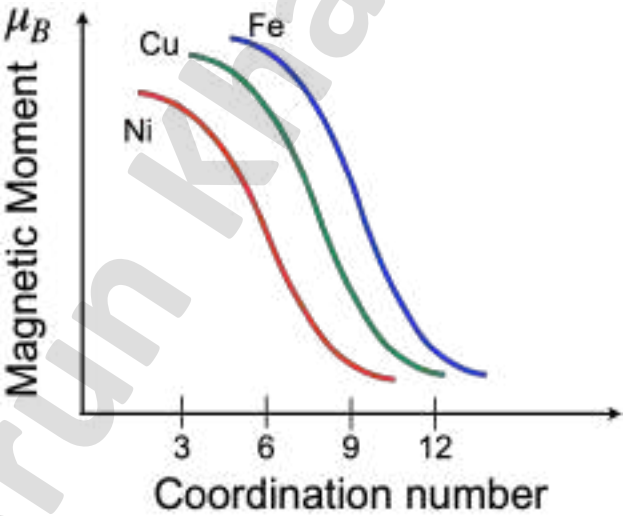


Fig. 21: Magnetic moment Vs Coordination number

- Fe can have a maximum possible moment of $6\mu_B$ per atom ($3\mu_B$ orbital + $3\mu_B$ spin) this implies that in 0D nano crystals very little of the orbital magnetic moment is quenched.
- The values of magnetic moment which dependent on the dimensionality are shown in the table.

Material / Size	Magnetic Moment (μ_B / atom)			
	0D	1D	2D	Bulk
Ni	2.0	1.1	0.68	0.56
Fe	4.0	3.3	2.96	2.27

← Increasing magnetic moment / atom

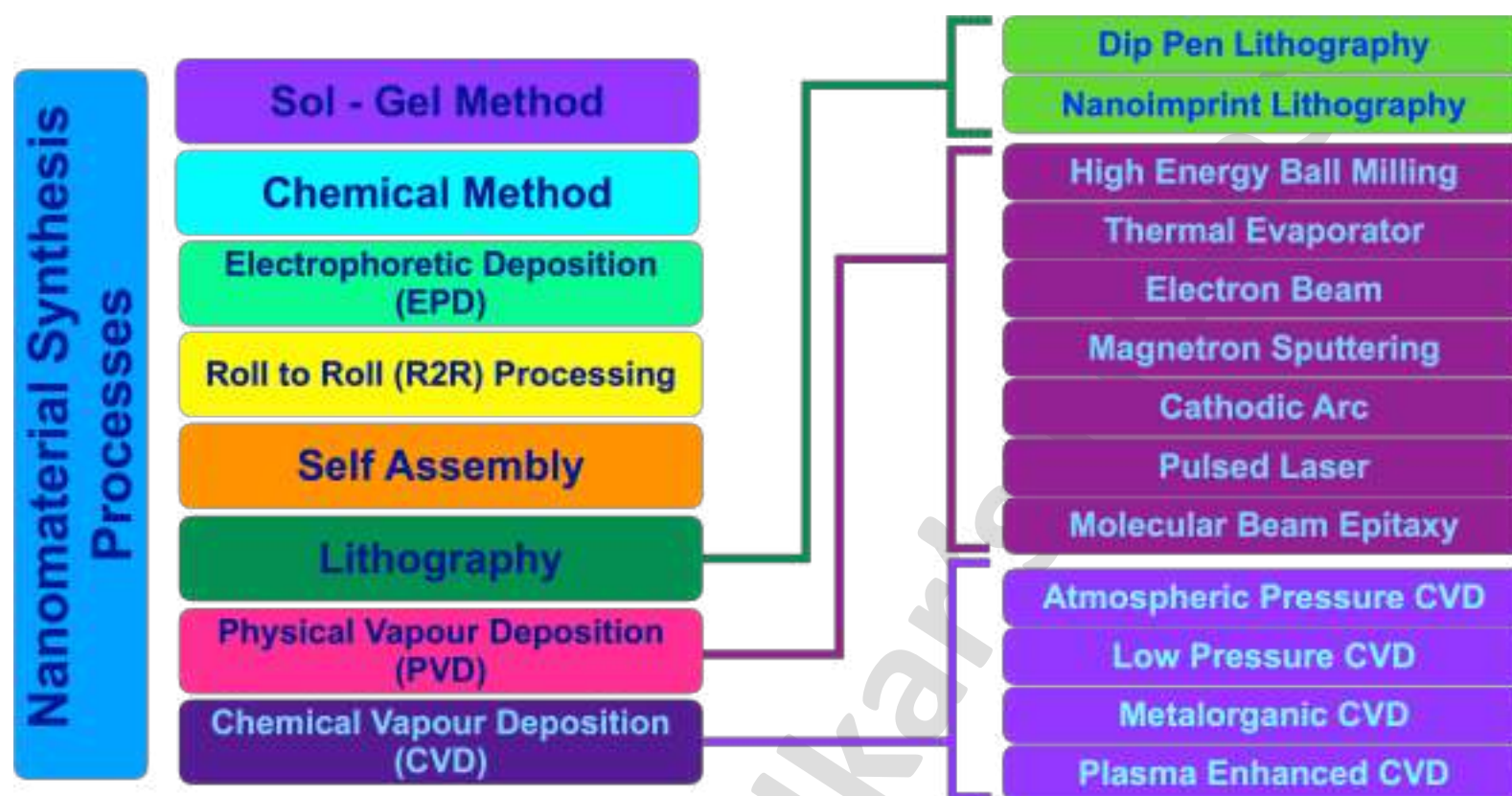
Dependence of magnetic moment on the dimensionality

**D) Mechanical properties**

- Mechanical properties describe how materials respond to different external forces such as tension, compression, shear, and impact. Nanoparticles (NPs) exhibit unique mechanical behaviors compared to bulk materials due to their size effects, high surface-area-to-volume ratio, and quantum effects.
- As for the traditional materials, the mechanical properties of metals generally consist of ten parts, which are brittleness, strength, plasticity, hardness, toughness, fatigue strength, elasticity, ductility, rigidity and yield stress.
- Most inorganic non-metallic materials are brittle materials, which do not have properties such as plasticity, toughness, elasticity, ductility and so on.
- Besides, some organic materials are flexible materials, which do not have properties such as brittleness and rigidity. Nanomaterials have excellent mechanical properties due to the volume, surface and quantum effects of nanoparticles.
- As nanoparticles are added to a common material, these particles will refine the grain to a certain extent, forming an intra-granular structure or an inter-granular structure, thereby improving the grain boundary and promoting the mechanical properties of materials.
- Hardness, elasticity and ductility depend upon the bonds between atoms.
- Highly pure materials show different mechanical properties than the bulk material.
- Young's modulus decreases in metallic nano crystals with decrease in particle size.
- Yield stress increases with the decrease in grain size in bulk materials with nano sized grains.
- Stronger materials can be produced by making materials with nano sized grains.
- The carbon nanotubes are estimated to be about 20 times stronger than steel.

8. Methods of preparation of nanomaterials

- Following are the various methods by which we can synthesis various nanomaterials and nanoparticles for various applications.



- Manufacturing at the nanoscale is known as nanomanufacturing.
- Nanomanufacturing involves scaled-up, reliable, and cost-effective manufacturing of nanoscale materials, structures, devices, and systems. It also includes research, development, and integration of top-down processes and increasingly complex bottom-up or self-assembly processes.
- In more simple terms, nanomanufacturing leads to the production of improved materials and new products. As mentioned above, there are two basic approaches to nanomanufacturing, either top-down or bottom-up.
- **Top-down approach**
 - It involves the breaking down of the bulk material into nanosized structures or particles. Top-down synthesis techniques are extension of those that have been used for producing micron sized particles.
 - Top-down approaches are inherently simpler and depend either on removal or division of bulk material or on miniaturization of bulk fabrication processes to produce the desired structure with appropriate properties.
 - The biggest problem with the top-down approach is the imperfection of surface structure.
- **Bottom-up approach:**
 - The alternative approach is the 'bottom- up', which has the potential of creating less waste and hence the more economical.
 - Bottom-up approach refers to the build up of a material from the bottom: atom-by-atom, molecule-by-molecule, or cluster-by cluster.
 - Many of these techniques are still under development or are just beginning to be used for commercial production of nanopowders.

i) Here are two examples of heritage sites,

- **Top-down approach:** Ellora Caves is a UNESCO World Heritage Site located in the Sambhajinagar (Formerly Aurangabad) district of Maharashtra, India. It is one of the largest rock-cut monastery-temple cave complexes in the world. The construction type is similar to top down approach.

- **Bottom-up approach:** The Kalaram Temple is an old Hindu shrine dedicated to Rama in the Panchavati area of Nashik city in Maharashtra, India, which was constructed using cubes of stones. The construction type is similar to bottom up approach.



Top Down Approach: Ellora Caves; Bottom Up Approach: Kalaram Temple

- In a similar way Bottom-up and the top-down approaches in synthesis of carbon-based nanomaterials is shown in Fig. 22 as an example.

ii) Synthesis of carbon-based nanomaterials:

- **Top-down approach:** A bulk material of carbon let's say a chunk is transformed to a smaller fragments like powder. Furthermore it is exfoliation of multilayer to monolayer of carbon material is produced or synthesised.
- **Bottom-up approach:** A precursor containing carbon molecules is used. High energy is applied in the form of ionisation to condensate and formation of carbon clusters. The final product by both approaches are the allotropes of carbon like fullerenes, CNTs, graphene or artificial diamond.

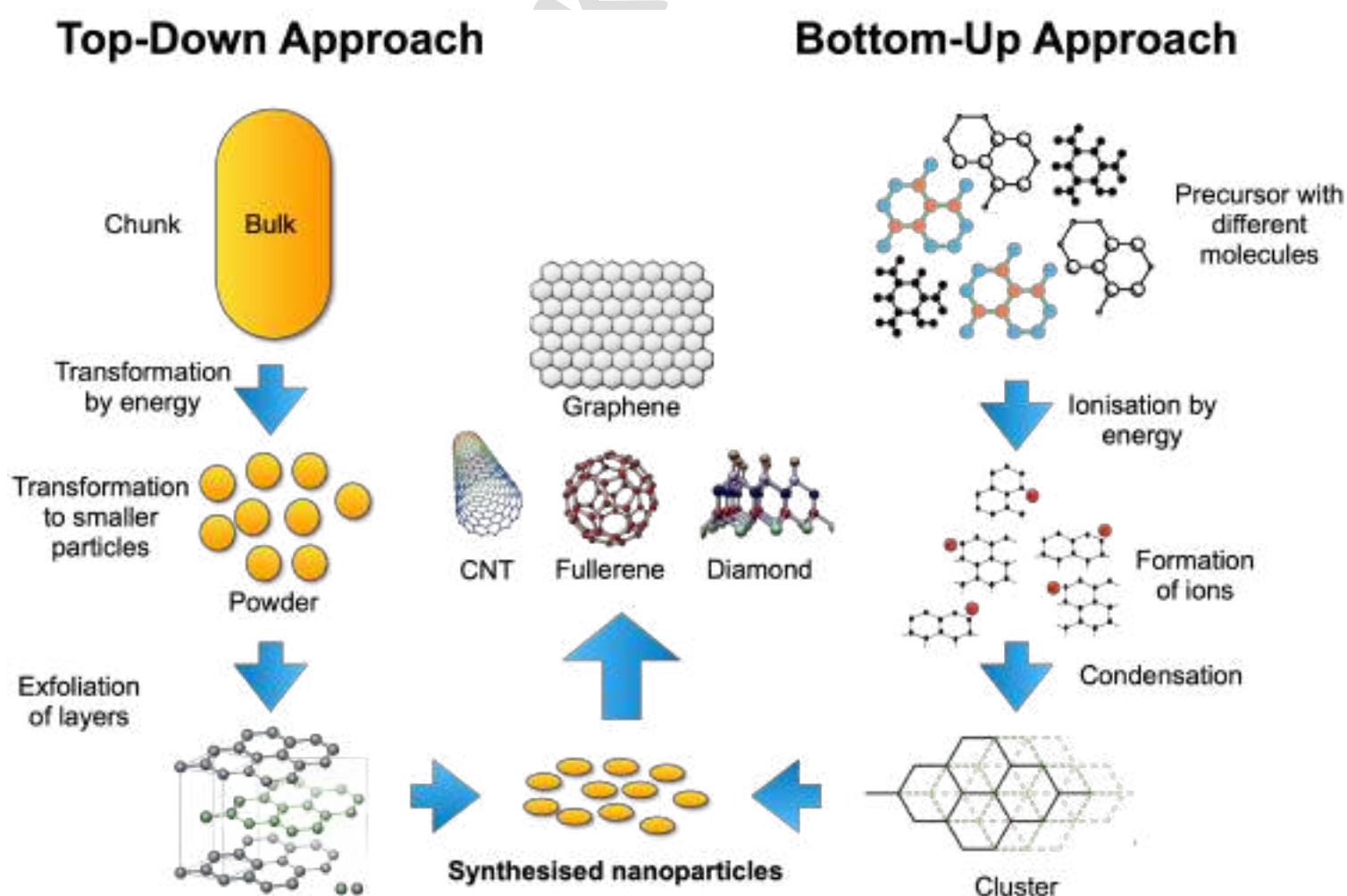


Fig. 22: Synthesis of carbon-based nanomaterials

[Image recreated from source: Gerardo Morell et. al. DOI: 10.13140/RG.2.2.16446.28483]

**- Nano-manufacturing**

- Within the top-down and bottom-up categories of nano-manufacturing, there are a growing number of new processes that enable nano-manufacturing.
- Among these are:
- Chemical Vapour Deposition (CVD),
- Physical Vapour Deposition (PVD),
- Sol – Gel method,
- Chemical method,
- Electrophoretic deposition (EPD),
- Roll-to-roll processing (R2R),
- Self-assembly,
- Lithography etc.

A) Physical vapour deposition (PVD)**i) Introduction**

- As the name suggests, PVD is a technique that uses primarily physical means to deposit a thin layer of material. PVD involves a number of steps performed under high-temperature vacuum conditions.
- PVD is characterised by a process in which the material goes from a condensed phase to a vapour phase and then back to a thin film condensed phase. The most common PVD processes are high energy ball milling, sputtering and evaporation.
- PVD is used in the manufacture of items which require thin films for mechanical, optical, chemical or electronic functions. First, a solid precursor material is gasified, typically through the use of high-power electricity or laser.
- The gasified atoms are then moved into a reacting chamber where the coating substrate is located. Source material atoms then stick to the substrate, forming a thin coat. PVD is used as the deposition method to produce an extremely hard, corrosion-resistant coating.
- Thin films made with PVD have a high-temperature tolerance and superior ablation resistance. PVD is also considered an environmentally-friendly process.
- The process does have a few drawbacks. One of the main drawbacks is its high cost, due in part to the intense heating and cooling that is required.
- PVD is also a 'line of sight' technique, which means it is not ideal for coating non-visible surfaces. The process is also considered to be relatively slow.
- The analogy for PVD, let's consider a burning candle in which initially wax is in solid phase, due to temperature of flame it gets melt and converts into liquid phase, furthermore, it turns into gaseous phase. If we hold any object like paper over the candle flame then black pigment or lamp black gets deposited on it. In this process wax is converted into the lamp black. Both have different phases and properties.
- Scientifically Heat from the flame melts the wax by radiation and conduction, capillary action draws the wax up the wick, molten wax is vaporised, chemical reactions produce the flame, heated solid carbon particles glow, and convection currents sweep away the products of combustion. This technique is used in PVD.

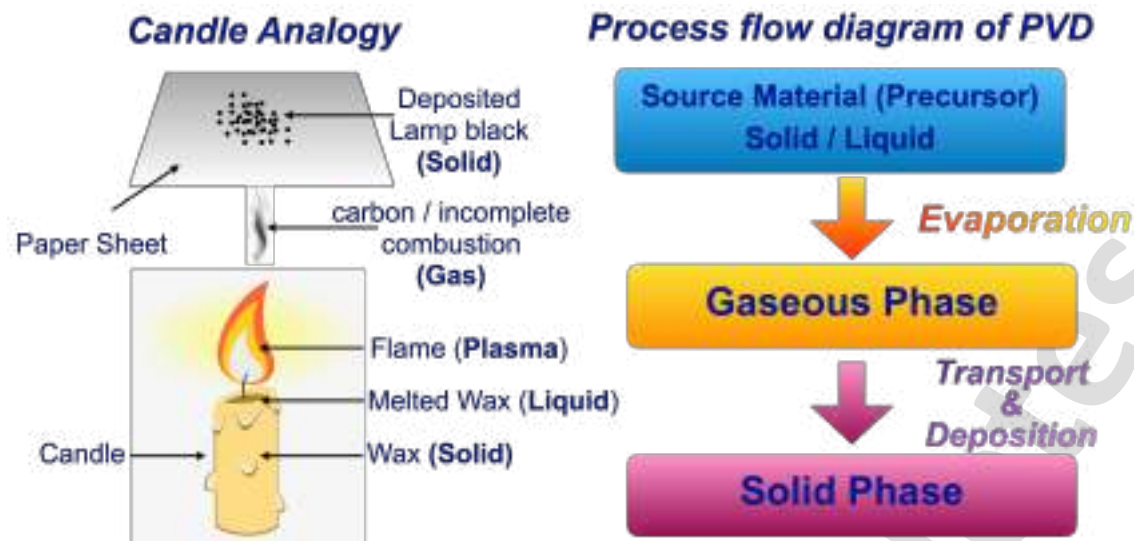


Fig. 23: Process flow for PVD

ii) Physical vapour deposition (PVD) Process

- The process flow diagram of PVD is shown in Fig.24
- In this method the material is evaporated & then blown towards a cold finger (a cool cylinder) where the particles are deposited.
- The set up is as shown in figure. The material is kept in crucibles. It is evaporated. As the density of vapour is high close to crucibles, the small particles start interacting to form larger particles.
- To avoid formation of large particles, an inert gas is used to blow the particles away from crucibles towards the cold finger. The particles condense on cold finger.
- The particles grow while travelling from the crucibles to the cold finger. Hence the particle size can be controlled by changing the distance between the crucibles & the cold finger & by changing the pressure of inert gas. The particles collected on the cold finger are scraped off using scrapers.
- The particles fall into the funnel. A piston anvil arrangement is used to compact the nano particle in pellet form.

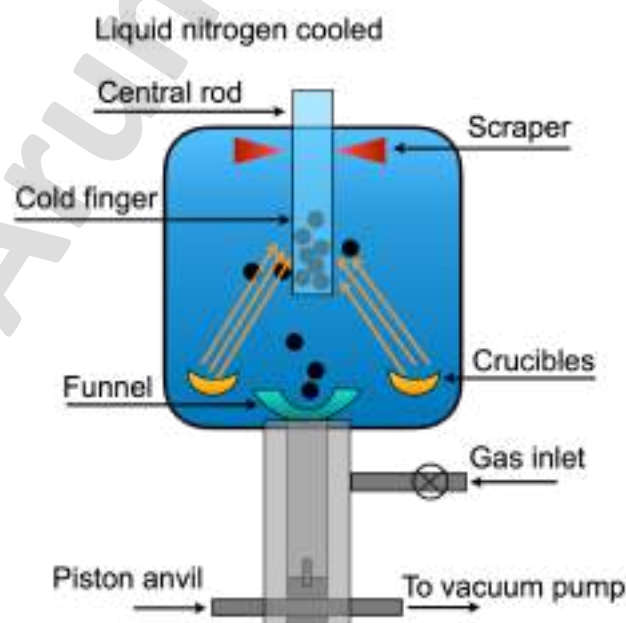


Fig. 24: Schematic of nanoparticle synthesis by PVD method

- Physical vapour deposition involves the transfer of a material on an atomic level, which has important benefits in several field.
- Which includes source generally called as precursor which get sputtered evaporated in to gaseous phase and then deposited on the substrate which is again in solid phase.
- In this process the physical morphology changes from precursor.

- In this process the material that is going to be deposited onto a surface starts out in the solid form, gets broken down to the atomic level and deposited in the gas phase, and afterward becomes a solid again.
- The atoms of the deposition material will react with the gas during the transport stage.
- Almost any type of inorganic and a small range of organic materials can be applied via the physical vapour deposition method.

iii) Thermal Evaporator

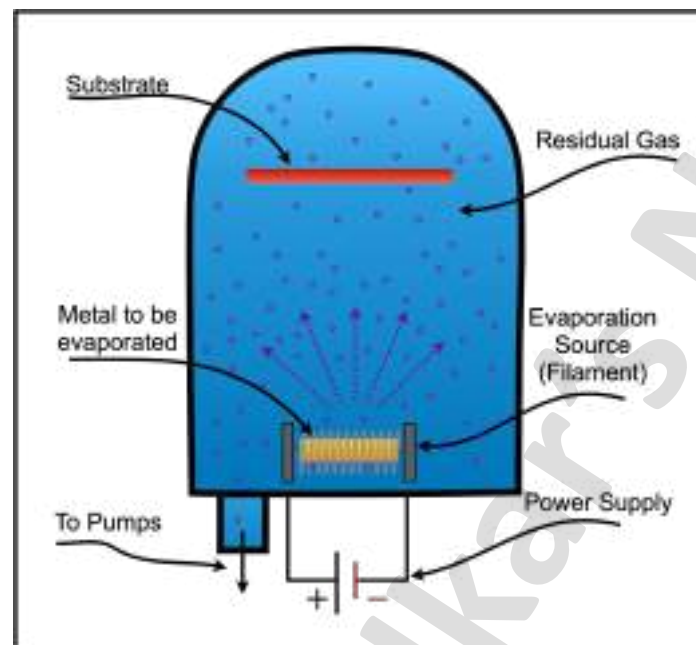


Fig. 25: Schematic of thermal evaporator

- A schematic of thermal evaporator is shown in Fig. 25. A thermal evaporator uses an electric resistance heater to melt the material and raise its vapour pressure to a useful range.
- This is done in a high vacuum, both to allow the vapour to reach the substrate without reacting with or scattering against other gas phase atoms in the chamber and reduce the incorporation of impurities from the residual gas in the vacuum chamber. Thermal evaporation is the simplest way of depositing material onto a substrate.
- **Optimization:**
 - Purity of the film depends on the purity of the source material and the quality of the vacuum.
 - Thicknesses of the film vary due to the geometry of the chamber.
 - Collision with the residual gases aggravates non uniformity of the thickness.
- **Limitations:**
 - Limited to low melting point metals ex: Al, Au, Ni Cr etc.
 - Dielectric material Evaporation is difficult. Filament limits the amount of material that can be deposited. Density and Adhesion is poor compared to the sputtered films. Step coverage is more difficult to improve.
- **Advantages:**
 - It is simple and cheap.
 - Less substrate surface damage.
 - Excellent purity of films.
- **Disadvantages:**
 - Limited to low melting point metals. It's not possible to evaporate the Dielectric materials.
 - Filament limits the amount of material that can be deposited. Density is poor. Adhesion is poor.
 - Step coverage is more difficult to improve.

iv) High Energy Ball Milling

- Ball milling is the simplest method to preparation of nanoparticles in the form of powder. The schematic of ball milling is shown in Fig. 26. Ball milling process where a powder mixture placed in the ball mill is subjected to high-energy collision from the balls. The ball mill contains a stainless steel container and many small iron, hardened steel, silicon carbide, or tungsten carbide balls are made to rotate inside a mill (drum). The container may be filled with inert or air gas. The powder of a material is taken inside the steel container. This powder will be made into nanosize using the ball milling technique. A magnet is placed outside the container to provide the pulling force to the material and this magnetic force increases the milling energy when milling container or chamber rotates the metal balls.
- The turn disc rotates in one direction while the bowls rotate in the opposite direction. The centrifugal forces, created by the rotation of the bowl around its own axis together with the rotation of the turn disc, are applied to the powder mixture and milling balls in the bowl. The powder mixture is fractured and cold welded under high energy impact. Since the rotation directions of the bowl and turn disc are opposite, the centrifugal forces are alternately synchronised. Thus friction resulted from the hardened milling balls and the powder mixture being ground alternately rolling on the inner wall of the bowl and striking the opposite wall. Various types of mills used in this method as planetary, Vibratory, Rod, Tumbler. The ball to material mass ratio is normally maintained at 2:1. These silicon carbide balls provide very large amount of energy to the material powder and the powder then get crushed.
- This process of ball milling is done approximately 100 to 150 hrs to get uniform fine powder. Ball milling is a mechanical process and thus all the structural and chemical changes are produced by mechanical energy. Control the speed of rotation and duration of milling grind material to fine powder (few nm to few tens of nm). Some materials like Co, Cr, W, Al-Fe, Ag-Fe etc are made nanocrystalline using ball mill.

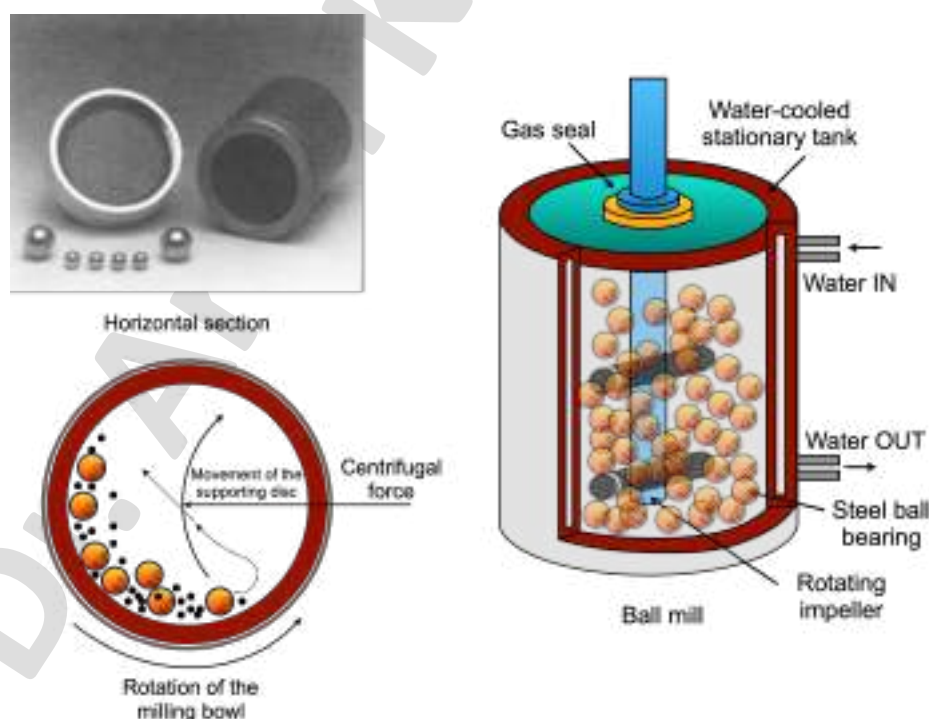


Fig. 26: Schematic of ball milling

- **Advantages:**
 - Nanopowders of 2 to 20 nm in size can be produced.
 - The size of nanopowder also depends upon the speed of the rotation of the balls.
 - It is an inexpensive and easy process.
- **Disadvantages:**
 - As the process is not so sophisticated, therefore the shape of the nanomaterial is irregular.
 - There may be contaminants inserted from ball and milling additives.
 - This method produces crystal defects.

B) Chemical Vapour Deposition (CVD)

i) Introduction

- Chemical vapor deposition (CVD) is parent to a family of processes whereby a solid material is deposited from a vapor by a chemical reaction occurring on or in the vicinity of a normally heated substrate surface. The resulting solid material is in the form of a thin film, powder, or single crystal.
- By varying experimental conditions, including substrate material, substrate temperature, and composition of the reaction gas mixture, total pressure gas flows, etc., materials with a wide range of physical, tribological, and chemical properties can be grown.
- A characteristic feature of the CVD technique is its excellent throwing power, enabling the production of coatings of uniform thickness and properties with a low porosity even on substrates of complicated shape.
- Another important feature is the capability of localized, or selective deposition, on patterned substrates.
- CVD and related processes are employed in many thin film applications, including dielectrics, conductors, passivation layers, oxidation barriers, conductive oxides, tribological and corrosion-resistant coatings, heat-resistant coatings, and epitaxial layers for microelectronics.
- Other CVD applications are the preparation of high-temperature materials such as tungsten, ceramics, etc.
- Similarly the production of solar cells, high-temperature fiber composites and particles of well-defined sizes can also be prepared.
- Recently, high T_c superconductors, and more recently carbon nanotubes, have also been made by this technique.
- Since oxygen activity in the vapor can be precisely controlled during the deposition, no annealing in oxygen is needed to achieve superconductivity. A simplified concept diagram of CVD is shown as Fig. 27.
- A typical CVD system consists of sources and feed lines for gases; mass flow controllers for metering the gases into the system; a reaction chamber or reactor; a system for heating up the wafer on which the film is to be deposited; temperature sensors.
- A CVD is consists of a reaction chembar made of quartz tube surrounded by heating coils which is embedded in furnace. Sample loading door and gas inlet and outlet are attached to the ends of quartz tube. Pressure sensor is provided to monitor the pressor inside the quartz tube.
- In typical CVD, the wafer (substrate) is exposed to one or more volatile precursors, which react and/or decompose on the substrate surface to produce the desired deposit. Frequently, volatile by-products are also produced, which are removed by gas flow through the reaction chamber.
- Chemical vapour deposition (CVD) results from the chemical reaction of gaseous precursor(s) at a heated substrate to yield a fully dense deposit.

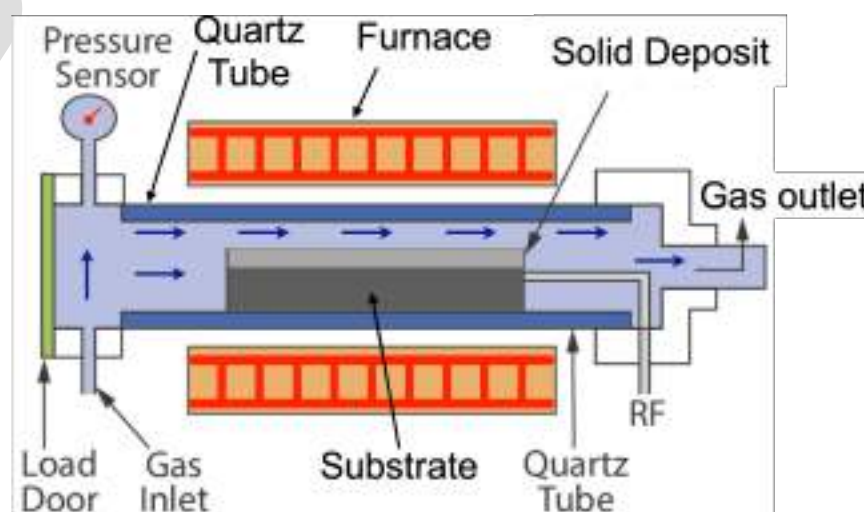


Fig. 27: Schematic of Chemical vapour deposition (CVD) system

ii) Growth Mechanism

- A basic CVD process consists of the following steps as illustrated in Fig. 28. A predefined mix of reactant gases and diluent inert gases are introduced at a specified flow rate into the reaction chamber; the gas species move to the substrate; the reactants get adsorbed on the surface of the substrate; the reactants undergo chemical reactions with the substrate to form the film; and the gaseous by-products of the reactions are desorbed and evacuated from the reaction chamber.

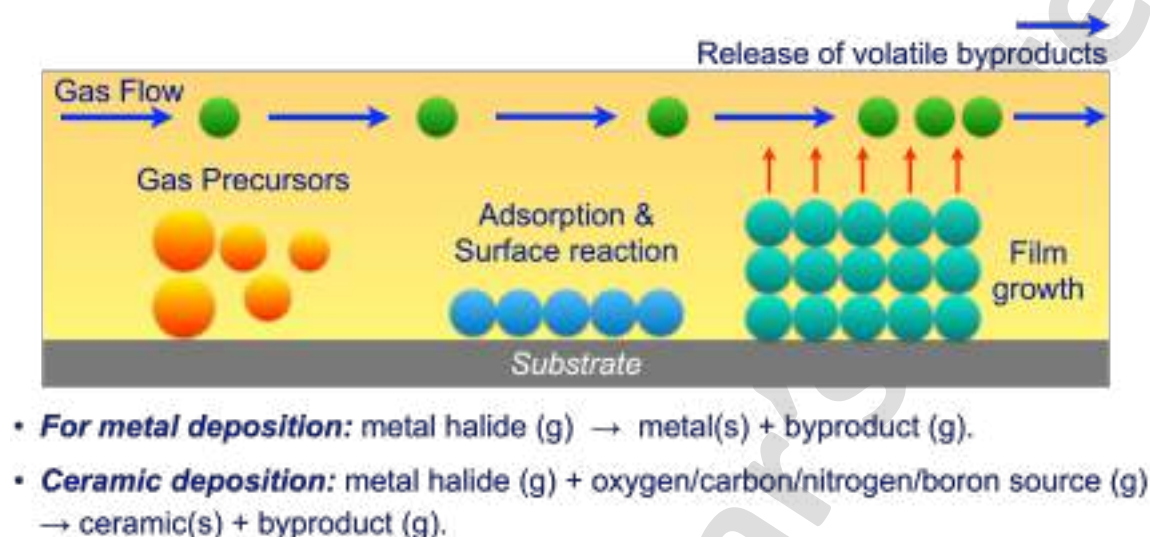


Fig. 28: Growth mechanism of CVD

iii) Chemical Method

- Chemical methods use colloidal solutions of nanoparticles which are filtered or centrifuged and dried.
- Colloids contain two or more phases, out of the three phases solid, liquid and gas, coexist. Colloids can contain two or more phases of the same or different materials. Nanoparticles of metals are generally insoluble in organic or inorganic solvents but they can be prepared in colloidal form.
- Colloidal dispersions in organic liquids are called organosols and dispersions in water are called hydrosols. Nanoparticles of nearly the same size can be obtained by controlling the concentration of reactants in the solution. Fig. 29 shows experimental set up to synthesize colloidal solution in which 3 neck flask is used which is rested on a hot plate embeded with magnetic stirrer.
- It is a nice reaction chamber with a round bottom and angled necks allows you to connect three components for complex chemical reactions. The 3 necks of flask are used to insert thermometer, pipette and inlet/outlet for inert gas. Magnetic stirrer is used to mix the solution well to carried out chemical reaction properly. The rpm of stirrer and temperature can be controlled with the help of control panel. During chemical reaction, larger particles have smaller surface energy hence particles keep growing to larger sizes. This is called 'Ostwald ripening'.

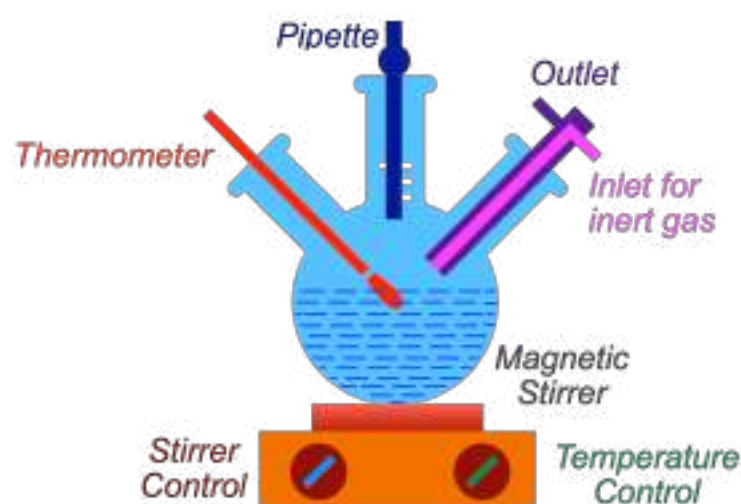


Fig. 29: Schematic of Synthesis of colloids

iv) Ostwald ripening

- Ostwald ripening is a phenomenon observed in solid solutions or liquid sols that describes the change of an inhomogeneous structure over time, i.e., small crystals or sol particles dissolve, and redeposit onto larger crystals or sol particles. Dissolution of small crystals or sol particles and the redeposition of the dissolved species on the surfaces of larger crystals or sol particles was first described by Wilhelm Ostwald in 1896.
- Ostwald ripening is generally found in water-in-oil emulsions, while flocculation is found in oil-in-water emulsions. The surface energy is also reduced when some particles come together to form an aggregate.
- In Ostwald ripening, the particle size increases whereas in aggregation, particles come together without increase in the individual particle size as shown in Fig. 30.

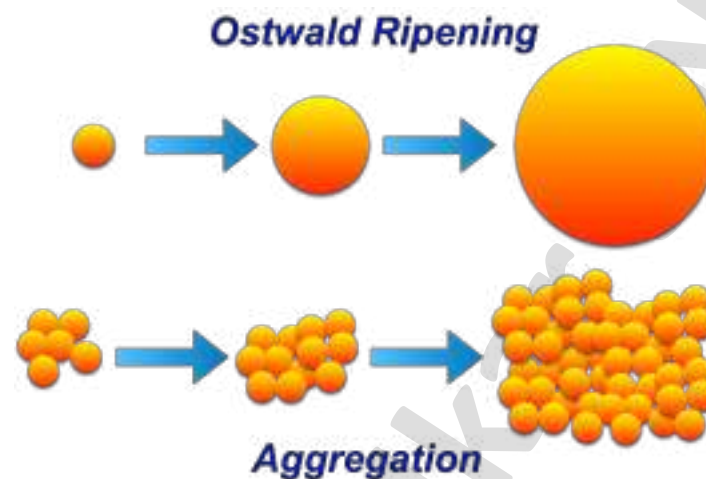


Fig. 30: Schematic of Ostwald ripening and aggregation nanoparticles

v) Growth mechanism of nanoparticles using Lamer diagram

- The correlation between the nucleation and the growth of the generated nuclei, the LaMer diagram suggested by LaMer could clarify how mono dispersed particles are obtained in a homogeneous solution. LaMer theory competently describes the kinetic formation of particles which are controlled by diffusion of elements (particles, ions, etc).
- The effect of concentration on particle size can be understood using the Lamer diagram shown in Fig. 31. At the beginning the saturation concentration is maintained C_S before the reaction starts. The formation of nuclei begins when a certain concentration C_0 is reached. The nucleation increases upto a concentration C_N above which there is super saturation. The rate of nucleation is maximum when the concentration is C_N .
- The rate of nucleation decreases when concentration decreases from C_N to C_0 . As the concentration falls below C_0 , no new nuclei are formed but the nuclei grow in size. The concentration has to be adjusted so that new nuclei are not formed during the growth of nuclei as the different nuclei will be in different stages of their growth and hence be of different sizes.

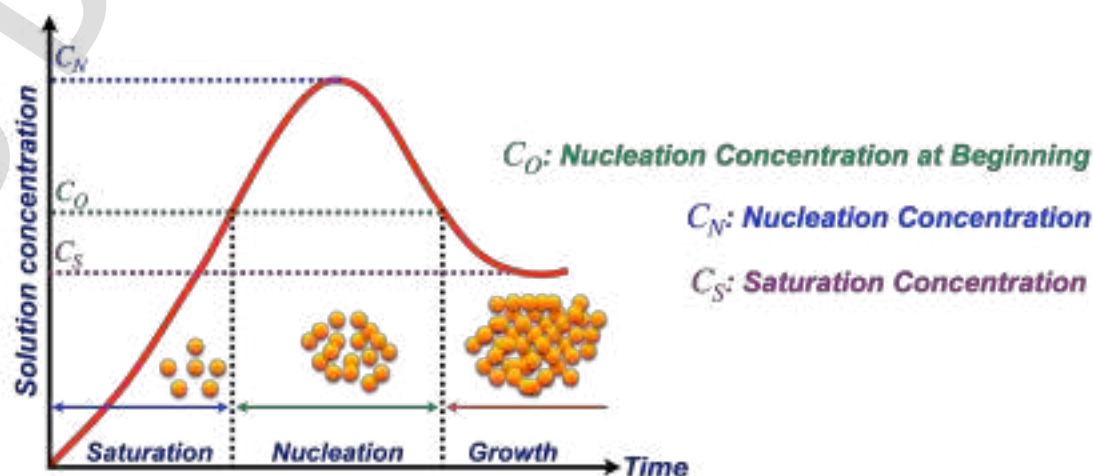


Fig. 31: Schematic of Lamer diagram

vi) Example: Synthesis of Au nanoparticles by colloidal route

- Colloidal metal nanoparticles can be produced by reduction of metal salt or acid.
- Highly stable gold nanoparticles are obtained by reducing Chloroauric Acid (HAuCl_4) with trisodium citrate ($\text{Na}_3\text{C}_6\text{H}_5\text{O}_7$). Gold nanoparticles are formed by nucleation and condensation. The particles grow by reduction of Au^+ on the surface. The particles are stabilized by oppositely charged citrate ions by Coulomb force.
- The formation of gold nanoparticles is shown in Fig. 32.

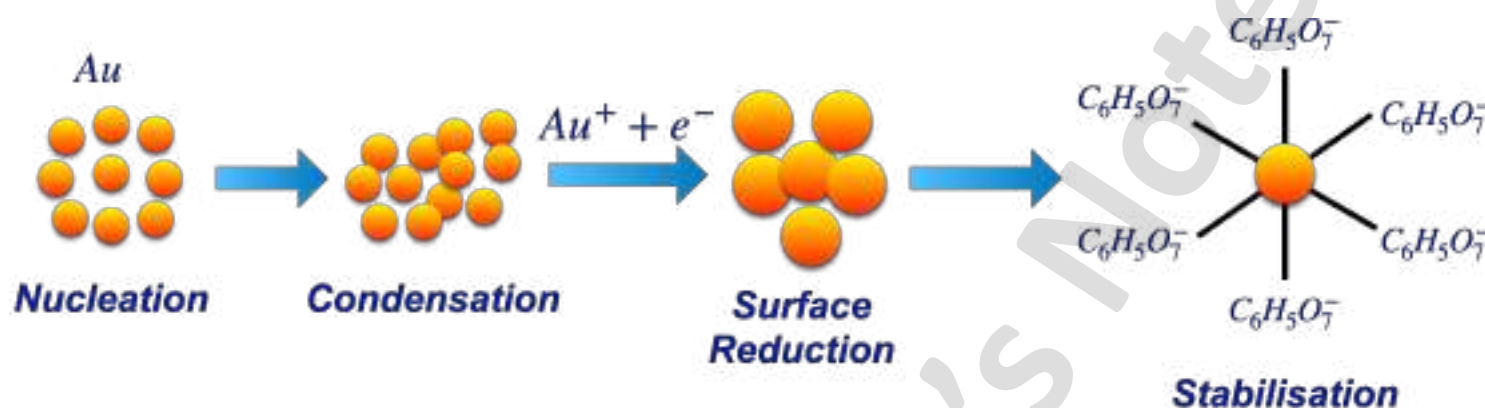


Fig. 32: Synthesis of Gold nano particles

9. Aerogels

i) Introduction of Aerogels

- Aerogels are highly porous materials having ultra-low density. These monolithic materials are formed by interconnection of particles of nanometer size, to form a nanoporous solid.
- The pores themselves are usually nonuniform with sizes from 10 to 100 nm. Aerogels are synthesized by sol-gel method and dried by special procedures to retain their porous structure.
- Aerogels were first synthesized by an American scientist Samuel Kistler in 1930s.
- Aerogels can be made of a wide variety of substances, including: Silica, transition metal oxides (for example, iron oxide),
- Lanthanide and actinide metal oxides (for example, praseodymium oxide),
- Several metal oxides (for example, tin oxide), Semiconductor nanostructures (such as cadmium selenide quantum dots, titanium dioxide), Carbon, Carbon nanotubes, Metals (such as copper and gold).

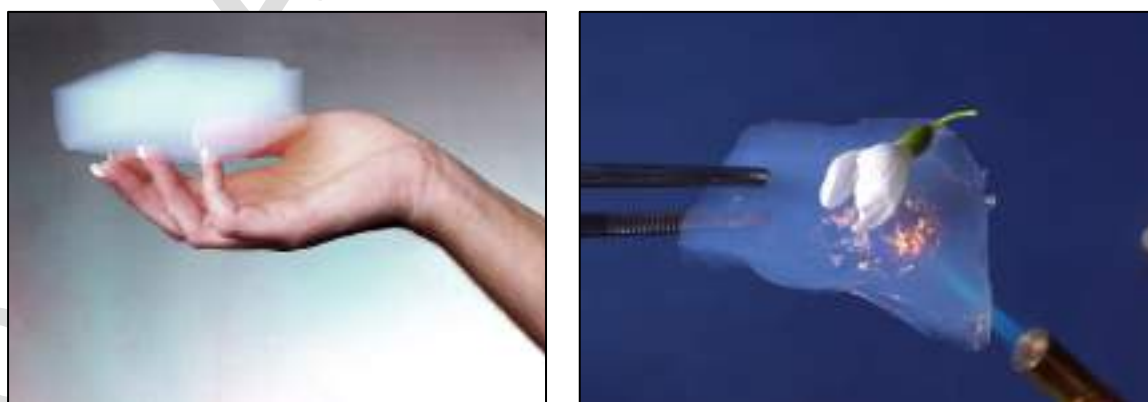


Fig. 33: Aerogel is transparent, highly insulating material

ii) Types of Aerogels

- The three most common types of aerogels are silica, carbon and metal oxides, but it's silica that is most often used experimentally and in practical applications.
- Silica aerogel is the primary type in use or study. It is silica-based and can be derived from silica gel or by a modified Stober process.

- Silica aerogel also has a high optical transmission of $\sim 99\%$ and a low refractive index of ~ 1.05 .
- It is very robust with respect to high power input beam in continuous wave regime and does not show any boiling or melting phenomena.
- This property permits to study high intensity nonlinear waves in the presence of disorder in regimes typically inaccessible by liquid materials, making it promising material for nonlinear optics.
- It has remarkable thermal insulative properties, having an extremely low thermal conductivity. Due to these remarkable properties, silica aerogels have been explored a lot due to their immense applications in various fields.

iii) Properties of Aerogels

- One of the best known and most useful physical properties of aerogel is its incredible lightness—it typically has a density between 0.0011 to 0.5 g cm^{-3} , with a typical average of around 0.020 g cm^{-3} . It is possible to have very high porosity ($80\text{--}90\%$), very low density and high surface area ($500\text{--}1,500 \text{ m}^2/\text{g}$) for these aerogels. They have very low index of refraction ($1\text{--}1.05$) and very low speed of sound through them (20 m/s).
- Young's modulus in these materials is quite low ($10^6\text{--}10^7 \text{ N/m}^2$). Very low value of thermal conductivity (0.003 W/m.K) which is lower than most commonly used insulators make them best available thermal insulator. It can be transparent or opaque or can be coloured.



Fig. 34: Silica Aerogels used as thermal insulator

iv) Applications of Aerogels

- It was assumed in last decades that use of aerogel is difficult commercially because of number of reasons like risky supercritical drying process, expensive synthesis procedure and their low fracture toughness etc.
- It is progressive development of cost effective synthesis routes and technological development and demands, interest in aerogels is increasing.
- Applications of aerogels are based on their properties. They are nontoxic and biodegradable making them eco-friendly.
- Their unique properties such as very low thermal conductivity makes them best thermal insulators for various applications such as insulation of space vehicles, automobile engines etc.
- Aerogels have been commercially used in jackets and blankets to be used under extreme low temperature conditions.
- Large windows of aerogels are being used in houses and buildings in some places to control the temperature in the interior. The transparency and heat insulation properties are used.
- Indeed it is possible to make aerogel-textile composites so as to make blankets, coats etc. by making them rollable. They can be obtained in the form of thin films, molds and tiny balls.

10. Applications of Nanomaterials

i) Medical

- Advancement in nanotechnology have helped to change medical norms in disease prevention, diagnosis, and treatment.
- The traditional drug delivery system, the drug is distributed to the affected tissues or organs of the patient's body as well as to the healthy tissues or organs.
- This leads to the side effects. In the targeted drug delivery system, the drug is dissolved, entrapped, encapsulated or attached to a nano particle.
- The system is then embedded in a capsule which is guided towards the affected part of the body.
- The capsule is opening at the specific tissues or organs controlled by externally applied magnetic field or infrared light or physiologically.
- Then drug can be delivered in controlled manner.
- Cancer therapy is one of the most common uses of nanotechnology for many people.
- There have been many new advances in nanotechnology for screening and treatment to remove colon and prostate cancer.
- The goal is to use tiny molecules (nanoparticles) to transport drugs within cancer cells, allowing direct treatment of these cells, without compromising healthy cells and tissues.
- However, this is just one of many ways nanotechnology can be used to eliminate cancer.

ii) Medicine (targeted drug delivery)

- The traditional drug delivery system, the drug is distributed to the affected tissues or organs of the patient's body as well as to the healthy tissues or organs.
- This leads to the side effects. In the targeted drug delivery system, the drug is dissolved, entrapped, encapsulated or attached to a nano particle.
- The system is then embedded in a capsule which is guided towards the affected part of the body.
- The capsule is opening at the specific tissues or organs controlled by externally applied magnetic field or infrared light or physiologically.
- Then drug can be delivered in controlled manner.

iii) Space and Defence

- Nanotechnology has a wide range of applications in space defence.
- Nanomaterials in various forms are used for reduction of weights of space vehicles, improving efficiency of solar cell, insulation of space vehicle, ignitior and propellents, etc.
- A few of them are listed below:
- High efficiency light weight solar cells:
Satellites or spacecrafts are mainly powered by solar energy. Currently solar cells have reached an efficiency of 30 - 40 %. Using luminescent dye sensitized nanoparticle based or nanoparticle-based solar cell arrays have potential to reduce the weight of solar cells as well as increase in efficiency.
- Insulation for space vehicles:
- Space vehicles should withstand harsh and extreme environments during launching and in space. Materials should also sustain high or low temperature and high or low pressure. Use of silica fibers and nanoparticles provide insulation in solid rocket motors and also they are better radiation protectors.

- Better ignitors and propellants:
- Nanocrystalline materials such as alumina particles are better propellants than conventional one. A nanocomposite of Fe_2O_3 and aluminium burns much faster and is more sensitive than conventional thermites.
- Fatigue resistant materials:
- Fatigue strength in aircraft usually decreases with time. Some nanomaterials have better fatigue strength and life is increased by 200–300 %.
- Detection of biological weapons:
- Biological weapons may use dangerous microbes or viruses as weapons. Some nanoparticle oxides like CaO , Al_2O_3 and MgO interact with such chemicals much faster than microparticles and are ideally suited for fast decomposition of warfare chemicals.

iv) Electronics

- In the spin-electronic devices, the spin property of electrons (instead of charge) is taken into consideration.
- Advantage with spin is that it cannot be easily destroyed by scattering from collisions with other charges, impurities or defects. The electronic devices with typical dimensions of few nanometers in either of three directions display unique properties. Such devices are fast, compact, and relatively cheap. Such devices are typically known as spin-electronic (spin-electronic) devices.
- Few applications are listed as below:
- **Single electron transistor (SET)**
- The single electron transistor is a switching device in which a quantum dot is placed between the source and the drain. It uses controlled electron tunneling to amplify current. They offer low power consumption and high operating speed.
- **Spin valves**
- Spin values are commercially used in computer read heads. Their use has enabled to increase the data storage capacity of magnetic memory devices due to their ability to detect small magnetic fields.
- **Giant Magneto Resistance (GMR)**
- GMR effect is the change in magnetic field of certain materials after application of magnetic field. This is very effective in observing small changes in the magnetic field and useful as a read device of the magnetically stored data. The data storing and reading in computer hard disks is the direct application of GMR.
- **Spin polarized Field Effect Transistor (S-FET)**
- In S-FET Polarized beam of light was used to obtain spin polarized electrons from the source. It is expected that this will help in faster and efficient data processing.
- **Nanophotonics**
- In nanophotonics, nanostructures (quantum dots, nanowires or 2-D thin films) or nanocomposites are used to produce light or detect light. They can be used for light production, propagation, manipulation like amplification, filter, detection etc.
- **Display technologies for TV and monitor**
- The flat panel television or computer monitors are products of nanotechnology. Even the coatings used on screens of TV or monitors can be of nanoparticles, which have better properties in terms of color quality and resolution than micro particle coatings.

**v) Automobiles**

- Nanotechnology has a wide range of applications in automobiles. Nanomaterials in various forms are used for designing sturdy structural parts, smooth and non-scratch paints, self-cleaning windows, better tires, reduction of harmful emission, etc.
- A few of them are listed below:
- **Sturdy structural parts**
 - Various body parts of vehicles are made up of steel, some alloys, rubbers, plastics etc. Nanotube composites have mechanical strength better than steel.
- **Smooth and non-scratch Paints**
 - Cars are spray painted with fine particles. Nanoparticle paints provide smooth, non-scratch thin attractive coating.
- **Self cleaning glass for windows**
 - Self cleaning glass can be made by dissolving small amount of titania (TiO_2) nanoparticles while manufacturing glass. Titania is able to dissociate organic dust in presence of UV light available in the sunlight. Drops of waters on glass give hazy look, but TiO_2 -containing glass can spread water evenly giving clear sight.
- **Small motor parts**
 - Small motors are needed in vehicle (such as wipers, window glass movements, etc). Very powerful electric motors are made using shape memory alloys using nanoparticles of materials like Ni-Ti. They require less power and gives better performance.
- **Better tires**
 - Tires of vehicles undergo wear and tear with use and also increase its weight. By using nanoparticle clay, better, light weight, less rubber consuming thinner tires are possible that can reduce the overall weight, increase in fuel consumption and speed.
- **Controlling harmful emission**
 - Use of efficient nanomaterial catalysts is one solution to convert harmful emission into less harmful gases. Large surface area of nanoparticles is useful to produce better catalysts. They are capable of absorbing emission of particles and poisonous gases like CO and NO from vehicle exhausts.
- **Hydrogen fuel**
 - Instead of using conventional petro fuels, there are numerous advantages of using hydrogen as a fuel. When hydrogen fuel is burned it can only produce harmless water vapor. Hydrogen gas is normally stored in a metal cylinder under high pressure.
 - Nanocylinders of carbon nanotubes have potential to store hydrogen in very small space.
- Introduction to Quantum Computing
 - Classical computing relies on principles of Boolean algebra and logic gates. Data is processed in binary system that is, either 0 (off / false) or 1 (on / true) that are called as bits.
 - The transistors and capacitors in CPU can only be in one state at any point either in 0 or 1. For more processing power, we need small dimensional transistors in large density on chip of the processor.
 - Thus, we need to reach very smaller dimension of materials in the range of few nanometers. At this nano scale, a threshold is reached and quantum mechanical effects such tunneling, uncertainty principle comes becomes dominant.
 - Hence, there is limit to the size of transistors at nano level and also on its processing power.

vi) Qubit

- A qubit (quantum bit) is the fundamental unit of quantum information in quantum computing. Unlike classical bits, which can be either 0 or 1, a qubit can exist in a superposition of both states simultaneously, thanks to the principles of quantum mechanics.
- Quantum computing applies the properties of quantum physics to process information. A number of elemental particles such as electrons or photons can be used for storing the information. Either the charge of particles or polarization acts as a representation of 0 and/or 1. Each of these particles is known as a quantum bit, or qubit.
- A qubit is a unit of quantum information. Quantum computer uses mainly two principles of quantum mechanics superposition and entanglement.
- **Principle of quantum computing**
- **Superposition**
- A qubit can be in a state of 0, 1, or both (0 and 1) at the same time until it is measured. This property allows quantum computers to perform multiple calculations simultaneously, exponentially increasing processing power. Thus, at one time the number of computations possible in a quantum computer is 2^n , where n is the number of qubits used. For example, a quantum computer consisting of 500 qubits has a potential to perform 2500 calculations in a single step.
- **Entanglement**
- When two or more qubits become entangled, their states become interdependent, meaning the state of one qubit is instantly correlated with the state of another, no matter how far apart they are. Entanglement enables ultrafast data processing and secure quantum communication.
- Entanglement is correlation between particles acting as q-bits such as photons, electrons. By knowing the spin state of one entangled particle (up or down) we can know the spin of its correlated particle.
- Quantum entanglement allows qubits separated by distances to interact with each other instantaneously. When multiple qubits act coherently, they can process multiple operations simultaneously. Thus, large information is processed within a fraction of the time.

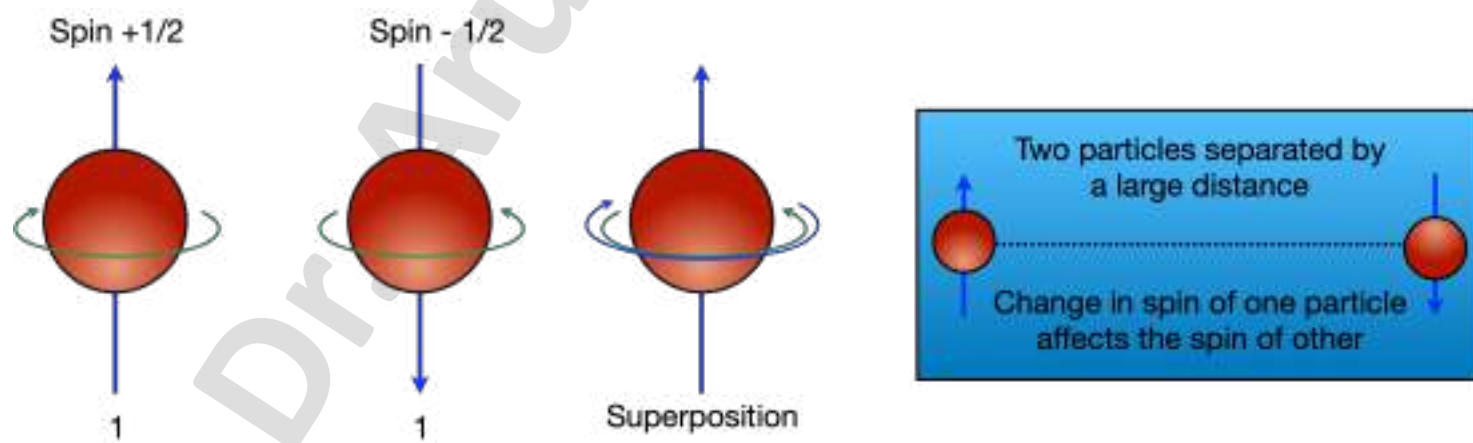


Fig. 35: Entanglement

- Quantum Interference

- Quantum interference is a fundamental principle of quantum mechanics that plays a crucial role in the efficiency of quantum computing. It occurs when quantum states overlap and interact, reinforcing or canceling each other, much like waves in physics. Quantum states can interfere with each other, allowing quantum algorithms to amplify correct solutions while canceling incorrect ones, leading to highly efficient problem-solving.

**vii) Quantum Computer**

- A quantum computer is an advanced computing device that leverages the principles of quantum mechanics to perform complex calculations at unprecedented speeds.
- Unlike classical computers, which use bits (0 or 1), quantum computers use qubits, which can exist in superposition (both 0 and 1 simultaneously) and entanglement (interconnected states).
- Quantum computers use particles such as electrons or photons to represent qubits. The charge or polarization of these particles is used to encode quantum information as 0, 1, or a superposition of both.
- A classical computer has processing speed of few gigahertz (GHz). Thus about 10^9 operations are possible per second.
- In quantum computing the processing speed is measured in teraflops. Thus about 10^{12} operations can be performed per second.
- In 2015, Google and NASA reported that then developed 1097-qubit D-Wave quantum computers would be almost 100 million times faster than a regular computer chip.
- It is estimated that quantum computer would process the information within few seconds that classical computer would take 10,000 years to solve.
- **Potential Applications of Quantum Computing**
- Currently, quantum computers are in the stage of development. Based on estimation, it is predicted that quantum computers has tremendous potential to deal with many challenges that are almost impossible to handle by the existing classical computers.
- **Artificial intelligence**
- Artificial intelligence requires analysis of data from images, videos and text. This data is available in vast quantity. For analyzing and processing this huge data, traditional computers would require thousands years. Quantum computers would be able to process this data in few seconds.
- **Drug Design**
- For many of the drugs, it requires trial and error methods to understand how they will react. These methods are very expensive, complex and require much processing time. Using quantum computers the process can be simulated more effectively.
- **Financial Optimization**
- Currently classical computers are analyzing many financial tasks such as market analysis, estimated returns, risk assessment, financial transactions, etc. It requires complex algorithms and tremendous computational time. By utilizing quantum technology great improvements could be achieved in terms of time saving and more accuracy.
- **Development of new materials**
- In materials science to develop new materials or to increase efficiency of existing materials, it requires lot of simulating. Although classical computers deal with these simulations, they have limitations in terms of speed, accuracy and time. Quantum computers would be able to deal with these challenges more effectively.
- **Logistics and scheduling**
- In industry optimizations are used in logistics and scheduling. Few examples, to optimize route based on real time traffic analysis. At present classical computing is heavily used to optimize these tasks. Some of the processes are very complicated for classical computers to handle. Quantum computing would be able to perform these tasks provide a solution in terms of less time and more accuracy.



- **Cyber Security**

- Cyber security is one of the biggest challenges of today. Malware and viruses spread through internet within fraction of seconds. It is very difficult for classical computing to handle these threats. Various techniques can be developed to deal with cyber security threats using quantum machine learning approaches.

- **Dealing with encryption**

- Security encryption methods are heavily used in defense, financial sectors, banks, user data security, etc. Despite of heavy deployment of security measures using classical computing, these organizations are under constantly under threat of cyber attack. The complex encryptions such as 2048 bit RSA encryptions are extremely difficult to deal with existing computing technologies. It would take around 10^{15} years for classical computers to decode these algorithms. It has been demonstrated that quantum computing would deal with these tasks very easily.

- **Software testing, Fault Simulation**

- Very large software programs have billions of lines of codes. Using classical computers, it becomes difficult and expensive to verify the correctness of the codes. Quantum computers can deal with these tasks very efficiently.



Que. No.	Questions
1	Explain Physical vapour deposition method for synthesis of nanoparticles.
2	What is Qubit? Summarize the applications of quantum computing.
3	Explain why the properties of materials changes when particle size is reduced below the critical size.
4	Classify nanomaterials on the basis of their dimensions.
5	Assuming spherical shape of a nanoparticle, show that surface area to volume ratio is very large for nanoparticles compared to bulk materials.
6	What is top down and bottom-up approach for nanomaterial synthesis.
7	Summarize the applications of nanomaterials in automobiles.
8	Elaborate high energy ball milling synthesis method to prepare nanomaterials.
9	Discuss the electrical properties of nanomaterials.
10	Elucidate the importance of nanomaterials in automobile applications.
11	Summarize the applications of aerogels.
12	Compare top down and bottom-up approach of preparation of nanomaterials.
13	Explain with the help of experimental arrangement and Lamer diagram, synthesis of nanoparticles by colloidal route.
14	Explain why surface area to volume ratio is large in nanoparticles as compared to bulk materials? Explain it for spherical nanoparticle.
15	Explain in brief, the principle of quantum computing on the basis of superposition and entanglement.
16	Explain optical properties of metal nanoparticles with the help of G. Mie theory.
17	Explain quantum computing on the basis of superposition and entanglement.
18	Illustrate the basic principle of quantum computing.
19	Justify the need of nanomaterials in energy applications.
20	Draw and explain Lamer diagram to relate with nucleation and growth of nanoparticles.
21	Explain the concept of quantum confinement effect in nanomaterials.
22	Discuss the applications of nanomaterials in medicine.
23	Explain the use of nanomaterials in energy.
24	Draw and explain Lamer diagram to understand nucleation and growth of nanomaterials.
25	List any four applications of nanomaterials in automobile.
26	Show that surface area to volume ratio is decreasing with increasing the dimensions in the case of sphere.
27	What are nanomaterials? Discuss the electrical properties of nanomaterials.
28	Discuss in detail the method of chemical route for preparation of nanomaterials.
29	List the factors responsible for change of properties of nano scale material from that of the bulk material.
30	Summarize the role of nanomaterials in medical field.



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Sample Question Paper for Summative Assessment (SA) Examination

F. Y. Year B. Tech.

Engineering Physics [BSH21BS03]

(Regulation: 2023)

Odd / Even Semester (2024-25)

Total No. of Questions-04

[Time: 1 Hr.]

Total No. of Printed Pages-XX

[Max. Marks: 30]

Instructions:

IMP: Verify that you have received a question paper with correct course, code, branch etc.

- i) Assume suitable data wherever necessary.
- ii) Neat labelled diagrams must be drawn wherever necessary.
- iii) Figure to right indicates full marks.
- iv) Use of a non-programmable calculator is allowed.

		Marks
Q.1	Attempt any Two of the following	
	a) In Hall effect, deduce the expression for Hall voltage V_H and Hall coefficient R_H	4
	b) Write the equation of electrical conductivity in semiconductor. Calculate the number of donor atoms which must be added to an intrinsic semiconductor to obtain conductivity as 10^4 mho/cm. Given $\mu_e = 1000 \text{ cm}^2/\text{V.s}$	4
	c) Write Fermi-Dirac distribution function with the terms involved in it. Show that at all temperatures ($T > 0K$) probability of occupancy of Fermi level by an electron is 50%.	4
Q.2	Attempt the following	
A	What is quantum tunnelling effect? The lowest energy of an electron trapped in a rigid box is 4.19 eV. Find the width of the box in Å.	4
B	Attempt any one of the following	
	a) State De-Broglie hypothesis of matter waves. Show that de-Broglie wavelength of the particle is inversely proportional to the square root of accelerated potential.	3
	b) What is wave wavefunction? Write Schrodinger time independent wave equation with terms involved in it.	3
Q.3	Attempt the following	
A	Describe adiabatic demagnetization method with experimental set up to achieve low temperature.	4
B	Attempt any one of the following	
	a) Explain AC Josephson effect.	3
	b) The critical field of niobium is $1 \times 10^5 \text{ A/m}$ at 8 K and $2 \times 10^5 \text{ A/m}$ at 0 K. Calculate the critical temperature of the element.	3
Q.4	Solve any Two of the following	
	a) Discuss optical properties of metal nanoparticles.	4
	b) Elucidate Physical vapour deposition (PVD) for preparation of nanoparticles	4
	c) Summarize applications of nanoparticles in automobile field.	4



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