**Physics for Information Science - PH3256**

**Unit-I Electrical Properties of Materials**

**PART-B**

**1. What are the basic assumptions of classical free electron theory? Based on the assumptions derive an expression for electrical and thermal conductivity of metals. What are the success and failures of this theory?**

**Classical Free Electron Theory**

**📌 Basic Assumptions of Classical Free Electron Theory:**

1. **Free Electrons:**
   * Valence electrons are treated as free particles, like gas molecules, inside the metal.
2. **Obeys Classical Laws:**
   * Electrons follow Maxwell-Boltzmann statistics.
3. **Random Motion:**
   * Electrons move in random directions with high speed and collide with positive ions.
4. **No Potential Energy Inside:**
   * Potential inside the metal is constant; electrons move freely except at the boundary.
5. **Collision Causes Resistance:**
   * Resistance in metals arises due to electron collisions with lattice ions.

**📌 Derivation of Electrical Conductivity (σ):**

Using **Drude’s model**, consider:

* **m:** mass of electron
* **e:** charge of electron
* **τ:** relaxation time (average time between collisions)
* **E:** applied electric field
* **v\_d:** drift velocity

**👉 Drift Velocity:**

vd=eEτmv\_d = \frac{eE\tau}{m}

**👉 Current Density (J):**

J=nevd=ne(eEτm)⇒J=ne2τmEJ = n e v\_d = n e \left( \frac{eE\tau}{m} \right) \Rightarrow J = \frac{n e^2 \tau}{m} E

**👉 Electrical Conductivity (σ):**

σ=JE=ne2τm\sigma = \frac{J}{E} = \frac{n e^2 \tau}{m}

**📌 Derivation of Thermal Conductivity (K):**

Using kinetic theory of gases:

K=13nvλCK = \frac{1}{3} n v \lambda C

* **n:** number density of electrons
* **v:** average speed of electrons
* **λ:** mean free path
* **C:** specific heat per electron

For free electrons:

K=13nv2τkBK = \frac{1}{3} n v^2 \tau k\_B

**📌 Wiedemann-Franz Law:**

The ratio of thermal to electrical conductivity:

Kσ=π23(kBe)2T=LT\frac{K}{\sigma} = \frac{\pi^2}{3} \left( \frac{k\_B}{e} \right)^2 T = L T

* **L** is the Lorentz number.

**Success of Classical Free Electron Theory:**

* Explains Ohm’s law.
* Describes thermal and electrical conductivities.
* Justifies Wiedemann-Franz Law.

**❌ Failures:**

* Could not explain specific heat of metals (observed values were too low).
* Cannot explain the behavior of semiconductors and insulators.
* Does not account for quantum nature of electrons.
* Fails to explain magnetic and optical properties.

**2. Derive Schrödinger equation for a particle in 3- dimensional box. Determine the Eigen values and Eigen functions for the same.**

**Schrödinger Equation for 3D Box**

**📌 Assumptions:**

* A particle is confined in a 3D box with dimensions Lx,Ly,LzL\_x, L\_y, L\_z
* Potential energy V=0V = 0 inside the box
* V=∞V = \infty outside the box

**📌 Time-independent Schrödinger Equation:**

−ℏ22m∇2ψ(x,y,z)=Eψ(x,y,z)- \frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) = E \psi(x, y, z) ⇒∂2ψ∂x2+∂2ψ∂y2+∂2ψ∂z2+2mEℏ2ψ=0\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2mE}{\hbar^2} \psi = 0

Let:

ψ(x,y,z)=X(x)Y(y)Z(z)\psi(x, y, z) = X(x)Y(y)Z(z)

Use **Separation of Variables**:

⇒1Xd2Xdx2+1Yd2Ydy2+1Zd2Zdz2=−2mEℏ2\Rightarrow \frac{1}{X} \frac{d^2X}{dx^2} + \frac{1}{Y} \frac{d^2Y}{dy^2} + \frac{1}{Z} \frac{d^2Z}{dz^2} = -\frac{2mE}{\hbar^2}

Each term is equal to a separation constant:

d2Xdx2=−kx2X,X(x)=sin⁡(nxπxLx)\frac{d^2X}{dx^2} = -k\_x^2 X, \quad X(x) = \sin\left(\frac{n\_x \pi x}{L\_x}\right)

Similarly,

Y(y)=sin⁡(nyπyLy),Z(z)=sin⁡(nzπzLz)Y(y) = \sin\left(\frac{n\_y \pi y}{L\_y}\right), \quad Z(z) = \sin\left(\frac{n\_z \pi z}{L\_z}\right)

**📌 Eigenfunctions:**

ψnxnynz(x,y,z)=Asin⁡(nxπxLx)sin⁡(nyπyLy)sin⁡(nzπzLz)\psi\_{n\_x n\_y n\_z}(x, y, z) = A \sin\left(\frac{n\_x \pi x}{L\_x}\right) \sin\left(\frac{n\_y \pi y}{L\_y}\right) \sin\left(\frac{n\_z \pi z}{L\_z}\right)

Where nx,ny,nz=1,2,3,...n\_x, n\_y, n\_z = 1, 2, 3, ...

**📌 Eigenvalues (Energy Levels):**

Enxnynz=ℏ2π22m(nx2Lx2+ny2Ly2+nz2Lz2)E\_{n\_x n\_y n\_z} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n\_x^2}{L\_x^2} + \frac{n\_y^2}{L\_y^2} + \frac{n\_z^2}{L\_z^2} \right)

If Lx=Ly=Lz=LL\_x = L\_y = L\_z = L, then:

Enxnynz=ℏ2π22mL2(nx2+ny2+nz2)E\_{n\_x n\_y n\_z} = \frac{\hbar^2 \pi^2}{2mL^2}(n\_x^2 + n\_y^2 + n\_z^2)

**✅ Conclusion:**

* Energy levels are **quantized**.
* Wavefunctions represent **stationary states**.
* The particle **cannot have zero energy** (minimum energy ≠ 0).

**Unit II Semiconductor Physics**

**1. Derive an expression for the carrier concentrations of electron and holes in an intrinsic semiconductor. And also explain the variation of carrier concentration with temperature.**

**Carrier Concentration in an Intrinsic Semiconductor**

**📌 Definition:**

An **intrinsic semiconductor** is a pure semiconductor without any doping. In such materials, the number of **electrons (n)** in the conduction band is equal to the number of **holes (p)** in the valence band:

n=p=nin = p = n\_i

Where:

* nin\_i = intrinsic carrier concentration.

**✅ Part 1: Derivation of Electron and Hole Concentrations**

**🔷 1. Electron Concentration in the Conduction Band (n):**

The number of electrons in the conduction band is given by:

n=∫Ec∞Dc(E)f(E) dEn = \int\_{E\_c}^{\infty} D\_c(E) f(E) \, dE

Where:

* Dc(E)D\_c(E) = density of states in the conduction band
* f(E)f(E) = Fermi-Dirac distribution function
* EcE\_c = energy at bottom of conduction band

Using approximations valid for intrinsic semiconductors:

n=Ncexp⁡(−(Ec−EF)kT)n = N\_c \exp\left( \frac{-(E\_c - E\_F)}{kT} \right)

Where:

* NcN\_c = effective density of states in the conduction band

Nc=2(2πme∗kTh2)3/2N\_c = 2 \left( \frac{2\pi m\_e^\* k T}{h^2} \right)^{3/2}

Thus,

n=2(2πme∗kTh2)3/2exp⁡(−(Ec−EF)kT)n = 2 \left( \frac{2\pi m\_e^\* k T}{h^2} \right)^{3/2} \exp\left( \frac{-(E\_c - E\_F)}{kT} \right)

**🔷 2. Hole Concentration in the Valence Band (p):**

p=∫−∞EvDv(E)[1−f(E)]dEp = \int\_{-\infty}^{E\_v} D\_v(E) \left[ 1 - f(E) \right] dE

Using approximation,

p=Nvexp⁡(−(EF−Ev)kT)p = N\_v \exp\left( \frac{-(E\_F - E\_v)}{kT} \right)

Where:

* NvN\_v = effective density of states in the valence band

Nv=2(2πmh∗kTh2)3/2N\_v = 2 \left( \frac{2\pi m\_h^\* k T}{h^2} \right)^{3/2}

**🔷 3. Intrinsic Carrier Concentration nin\_i:**

In intrinsic semiconductors:

ni=p=n⇒ni2=n⋅pn\_i = p = n \Rightarrow n\_i^2 = n \cdot p

Substitute:

ni2=NcNvexp⁡(−(Ec−Ev)kT)n\_i^2 = N\_c N\_v \exp\left( \frac{-(E\_c - E\_v)}{kT} \right) ⇒ni=NcNv⋅exp⁡(−Eg2kT)\Rightarrow n\_i = \sqrt{N\_c N\_v} \cdot \exp\left( \frac{-E\_g}{2kT} \right)

Where Eg=Ec−EvE\_g = E\_c - E\_v is the **bandgap energy**.

**✅ Part 2: Variation of Carrier Concentration with Temperature**

From:

ni=NcNv⋅exp⁡(−Eg2kT)n\_i = \sqrt{N\_c N\_v} \cdot \exp\left( \frac{-E\_g}{2kT} \right)

* As **temperature (T)** increases:
  + NcN\_c and NvN\_v slightly increase (∝ T3/2T^{3/2})
  + The **exponential term dominates**, so nin\_i increases rapidly.

**📈 Graphical Representation (Optional for exams):**

* Log-scale plot of log⁡ni\log n\_i vs 1/T1/T is a **straight line**.
* Slope = −Eg/2k-E\_g / 2k

**✅ Summary:**

* **Electron concentration:**

n=Ncexp⁡(−(Ec−EF)kT)n = N\_c \exp\left( \frac{-(E\_c - E\_F)}{kT} \right)

* **Hole concentration:**

p=Nvexp⁡(−(EF−Ev)kT)p = N\_v \exp\left( \frac{-(E\_F - E\_v)}{kT} \right)

* **Intrinsic concentration:**

ni=NcNv⋅exp⁡(−Eg2kT)n\_i = \sqrt{N\_c N\_v} \cdot \exp\left( \frac{-E\_g}{2kT} \right)

* **With increasing temperature, nin\_i increases exponentially.**

**Unit III Magnetic properties ofmaterials**

**1.Describe (classify) dia, para, ferro, antiferro and ferrimagnetic materials and their properties with example**

**Classification of Magnetic Materials:**

Magnetic materials are classified based on their response to external magnetic fields. The five main types are:

**🔷 1. Diamagnetic Materials**

* **Definition**: Substances that create an induced magnetic field in a direction opposite to the applied magnetic field.
* **Magnetic Susceptibility (χ)**: Negative and very small (χ < 0).
* **Relative Permeability (μᵣ)**: Slightly less than 1.
* **Behavior**: Weakly repelled by a magnetic field.
* **Temperature Effect**: Independent of temperature.
* **Examples**: Bismuth, Copper, Gold, Water.

**🔷 2. Paramagnetic Materials**

* **Definition**: Materials that are weakly attracted by magnetic fields due to unpaired electrons.
* **Magnetic Susceptibility (χ)**: Positive and small (χ > 0).
* **Relative Permeability (μᵣ)**: Slightly greater than 1.
* **Behavior**: Weak attraction towards a magnetic field.
* **Temperature Effect**: Susceptibility decreases with increasing temperature (follows Curie’s Law).
* **Examples**: Aluminium, Platinum, Chromium, Oxygen.

**🔷 3. Ferromagnetic Materials**

* **Definition**: Strongly attracted by magnetic fields; they retain magnetization even after the removal of the field.
* **Magnetic Susceptibility (χ)**: Very high and positive.
* **Relative Permeability (μᵣ)**: Much greater than 1.
* **Behavior**: Strong permanent magnetism due to domain alignment.
* **Curie Temperature**: Above which it becomes paramagnetic.
* **Examples**: Iron, Nickel, Cobalt.

**🔷 4. Antiferromagnetic Materials**

* **Definition**: Materials where adjacent atomic magnetic moments align in opposite directions and cancel each other.
* **Net Magnetization**: Zero.
* **Behavior**: Weak or no net magnetic moment.
* **Néel Temperature**: Temperature above which antiferromagnetic behavior disappears.
* **Examples**: Manganese oxide (MnO), Nickel oxide (NiO).

**🔷 5. Ferrimagnetic Materials**

* **Definition**: Magnetic moments are aligned antiparallel but unequal in magnitude, resulting in net magnetization.
* **Net Magnetization**: Non-zero.
* **Behavior**: Used in magnetic storage devices.
* **Examples**: Magnetite (Fe₃O₄), Ferrites like MnFe₂O₄.

**🔷 Tabular Summary**

| **Property** | **Dia** | **Para** | **Ferro** | **Antiferro** | **Ferri** |
| --- | --- | --- | --- | --- | --- |
| Susceptibility (χ) | < 0 | > 0 small | > 0 large | = 0 net | > 0 medium |
| Net Magnetization | None | Weak | Strong | Zero | Moderate |
| Examples | Bi, Cu | Al, O₂ | Fe, Ni | MnO, NiO | Fe₃O₄ |

**2. Explain Magnetic principle in computer data storage and GMR sensor.**

**Magnetic Principle in Data Storage & GMR Sensor**

**🔷 i. Magnetic Principle in Computer Data Storage**

* **Concept**: Uses **ferromagnetic materials** to store binary data (0s and 1s).
* **Working**:
  + A **magnetic disk** (e.g., HDD) has tiny domains.
  + **Direction of magnetization** of each domain represents binary data:
    - Upwards → 1
    - Downwards → 0
  + **Read/Write head** changes or senses magnetic orientation.
* **Process**:
  + **Writing**: A current in the write head generates a magnetic field that aligns domains.
  + **Reading**: The read head detects changes in magnetic flux.
* **Materials Used**: Cobalt alloys, Ferrites.

**🔷 ii. GMR (Giant Magnetoresistance) Sensor**

* **Principle**: Based on the change in resistance of multilayered magnetic materials when exposed to magnetic fields.
* **Structure**:
  + Layers of **ferromagnetic** and **non-magnetic** metals (e.g., Fe/Cr/Fe).
  + Two ferromagnetic layers: one fixed, one free.
  + Resistance depends on relative alignment:
    - **Parallel** → Low resistance
    - **Antiparallel** → High resistance
* **Application in Hard Drives**:
  + GMR sensors used in read heads can detect tiny magnetic fields from data bits.
  + Extremely sensitive → Higher storage density.
* **Other Applications**:
  + Automotive sensors
  + Biosensors
  + Position and speed detectors

**✅ Conclusion:**

* Magnetic materials have diverse properties based on atomic magnetic moments.
* Ferromagnetic and ferrimagnetic materials are key to data storage.
* **GMR effect** revolutionized magnetic data reading and miniaturized devices.

**Unit IV Optical properties ofmaterials**

**1. How optical materials are classified depending on the interactions of the materials with visible light.**

**Classification of Optical Materials Based on Light Interaction**

Optical materials are classified depending on how they interact with **visible light** (wavelength ~400–700 nm). The interactions include **transmission**, **reflection**, **absorption**, **refraction**, and **scattering**.

**🔷 Types of Optical Materials:**

| **Type** | **Behavior with Light** | **Example Materials** |
| --- | --- | --- |
| **Transparent** | Light passes through with minimal absorption | Glass, Quartz, Plastic |
| **Translucent** | Light passes through partially; scattered | Frosted glass, Wax paper |
| **Opaque** | Does not allow light to pass; reflects/absorbs | Metals, Wood, Stone |
| **Reflective** | Light is mostly reflected | Mirrors (Aluminum-coated) |
| **Absorptive** | Absorbs most of the incident light | Black Paint, Carbon Black |

**🔷 Classification Based on Material:**

1. **Dielectrics (Insulators)**:
   * High transparency in visible region.
   * No free electrons.
   * Used in lenses and optical fibers.
2. **Semiconductors**:
   * Light can excite electrons across the band gap.
   * Show selective absorption and emission.
   * Used in photodiodes, LEDs, solar cells.
3. **Metals**:
   * Highly reflective due to free electrons.
   * Opaque; absorb and reflect light.
   * Used in mirrors, coatings.

**2.** **Explain the three types of carrier generations and recombination in semiconductors.**

**Carrier Generation and Recombination in Semiconductors**

In semiconductors, **electron-hole pairs** are generated and annihilated. There are **three main types** of **carrier generation and recombination**:

**🔷 Carrier Generation:**

1. **Thermal Generation**:
   * Due to temperature, electrons gain enough energy to jump from valence band to conduction band.
   * Creates **electron-hole pair**.
2. **Optical Generation**:
   * When a photon with energy ≥ bandgap strikes the material, it excites an electron to conduction band.
   * Used in photodiodes, solar cells.
3. **Electrical Generation**:
   * Applying voltage across a p-n junction can cause minority carrier injection and increase in carrier density.

**🔷 Carrier Recombination:**

1. **Radiative Recombination (Band-to-Band)**:
   * Electron recombines with a hole and releases energy as light (photon).
   * Occurs in direct bandgap semiconductors like GaAs (used in LEDs).
2. **Non-Radiative Recombination**:
   * Energy is released as **heat** instead of light.
   * Occurs via defect levels or trap states inside the bandgap.
3. **Auger Recombination**:
   * Energy released during recombination is given to a third carrier (electron or hole), which is excited.

**3. Explain absorption and emission of light in metals, insulators and semiconductors.**

**Absorption and Emission of Light in Metals, Insulators, and Semiconductors**

**🔷 Metals**

* **Absorption**: Very strong due to large number of free electrons. Photons excite electrons, but do not lead to band transitions.
* **Emission**: Typically do not emit visible light efficiently. Heat energy may be radiated (e.g., in incandescent filaments).
* **Behavior**: Opaque and reflective.

**🔷 Insulators**

* **Absorption**: Only high-energy photons (UV) can excite electrons due to large bandgap (> 5 eV).
* **Emission**: Poor emitters in visible range.
* **Behavior**: Transparent to visible light (e.g., glass), as visible photons don't have enough energy to excite electrons.

**🔷 Semiconductors**

* **Absorption**: Moderate. If photon energy ≥ bandgap, electrons are excited to conduction band (optical generation).
* **Emission**:
  + **Direct bandgap semiconductors** (e.g., GaAs) emit light → used in LEDs, lasers.
  + **Indirect bandgap semiconductors** (e.g., Si) emit heat → used in electronics.
* **Behavior**: Partially transparent and selectively absorptive.

**🔷 Summary Table**

| **Material** | **Absorption** | **Emission** | **Behavior** |
| --- | --- | --- | --- |
| **Metal** | Strong | Weak (thermal) | Opaque, reflective |
| **Insulator** | Weak (visible) | Negligible | Transparent |
| **Semiconductor** | Medium | Light or heat | Selective |

**Unit V NANO DEVICES**

**1. Explain Quantum confinement and quantum structures in nano materials.**

**Quantum Confinement and Quantum Structures in Nanomaterials**

**🔷 Quantum Confinement:**

Quantum confinement occurs when the size of the material becomes comparable to the **de Broglie wavelength** of electrons (~1–10 nm). In such cases, the motion of charge carriers (electrons/holes) is restricted in one or more dimensions, leading to **discrete energy levels** rather than continuous bands.

**✅ Key Features:**

* Significant change in **optical, electrical, and magnetic properties**.
* Bandgap increases as the size of the nanoparticle decreases.
* More prominent in **quantum dots** and **nanowires**.

**🔷 Quantum Structures:**

Based on the degree of confinement, nanostructures are classified into:

| **Structure Type** | **Confinement Dim.** | **Free Dim.** | **Example** |
| --- | --- | --- | --- |
| **Quantum Well** | 1D confinement | 2D | Thin films |
| **Quantum Wire** | 2D confinement | 1D | Nanowires |
| **Quantum Dot** | 3D confinement | 0D | Nanoparticles |

**✅ Applications:**

* Quantum dots in LEDs, bio-labeling.
* Quantum wells in laser diodes.
* Nanowires in transistors and sensors.

**2. Notes on:**

**(i) Band Gap of Nanomaterials:**

* In nanomaterials, the **band gap increases** as particle size decreases.
* This is due to quantum confinement which forces electrons and holes to occupy higher energy levels.
* Example: CdSe nanoparticles change color with size (blue for small particles, red for large).

**(ii) Quantum Confinement (Recap):**

* Occurs when a material’s dimension is smaller than the **exciton Bohr radius**.
* Causes the continuous energy bands to split into discrete levels.
* Enhanced **tunability of optical properties** by varying particle size.

**(iii) Coulomb Blockade:**

* In nanoscale conductors (like quantum dots), **adding a single electron requires energy** due to electrostatic repulsion.
* This phenomenon is **Coulomb blockade**.
* Seen when the capacitance is very low, and temperature is also low.
* Important in **single-electron devices**.

**3. Describe single electron phenomena and single electron transistor.**

**Single Electron Phenomena and Single Electron Transistor (SET)**

**🔷 Single Electron Phenomena:**

* Based on the idea that the **movement of individual electrons** can be controlled.
* Due to the **Coulomb blockade**, only one electron can tunnel through a nano-island at a time.
* Happens at **low temperatures** and in **nanometer-scale structures**.

**✅ Conditions Required:**

* Small capacitance (C), such that charging energy EC=e22CE\_C = \frac{e^2}{2C} is significant.
* Temperature kT<ECkT < E\_C, to prevent thermal agitation.
* Tunneling junctions with resistance R>h/e2≈25.8 kΩR > h/e^2 \approx 25.8 \, k\Omega.

**🔷 Single Electron Transistor (SET):**

**🔹 Construction:**

* Consists of:
  + **Source and Drain** electrodes.
  + **Tunnel Junctions**.
  + **Island (Quantum Dot)**.
  + **Gate Electrode** (controls potential of island).

**🔹 Working:**

* Gate voltage modulates the energy of the island.
* At certain gate voltages, electrons can tunnel one by one through the island.
* Acts like a transistor but with **ultra-low current** control using **single electrons**.

**🔹 Applications:**

* Ultra-low-power digital circuits.
* High-sensitivity charge detectors.
* Quantum computing devices.

**✅ Summary Table:**

| **Concept** | **Description** |
| --- | --- |
| **Quantum Confinement** | Discrete energy levels due to size restriction |
| **Bandgap in Nanomaterials** | Increases as particle size decreases |
| **Coulomb Blockade** | Prevents electron flow unless energy condition is met |
| **Single Electron Transistor** | Device controlling electron flow at quantum level |