Band Structure and Electrical Conductivity in Semiconductors *

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Semiconductors are one of the technologically most important class of materials. According to the band theory of solids, which is an outcome of quantum mechanics, semiconductors possess a band gap, i.e., there is a range of forbidden energy values for the electrons and holes. In this experiment, we will calculate the energy band gap in the intrinsic region and the temperature dependence of the majority carrier mobility in the extrinsic region.

KEYWORDS

Semiconductor · intrinsic conduction · extrinsic conduction · energy band gap · conduction band · valence band · conductivity · resistivity · mobility · unijunction transistor · temperature control · low temperature physics

Approximate Performance Time 2 weeks.

Contents

1 Objectives

In this experiment, we will,

1. understand how conductivity in semiconductors depends on carrier concentration and mobility, and how these depend on temperature,
2. distinguish between intrinsic and extrinsic temperature regimes and identify the applicable temperature range from an examination of measured data,
3. calculate the energy band gap for doped Si,
4. understand how temperature-dependent measurements are a major experimental technique,
5. calculate the temperature dependent coefficient α of the majority carriers and
6. through experimental realizations, appreciate a physical understanding of the band gap structure of semiconductors.

References

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2 Theoretical introduction

2.1 Semiconductors

The available energies for electrons help us to differentiate between insulators, conductors and semiconductors. In free atoms, discrete energy levels are present, but in solid materials (such as insulators, semiconductors and conductors) the available energy states are so close to one another that they form bands. The band gap is an energy range where no electronic states are present. In insulators, the valence band is separated from the conduction band

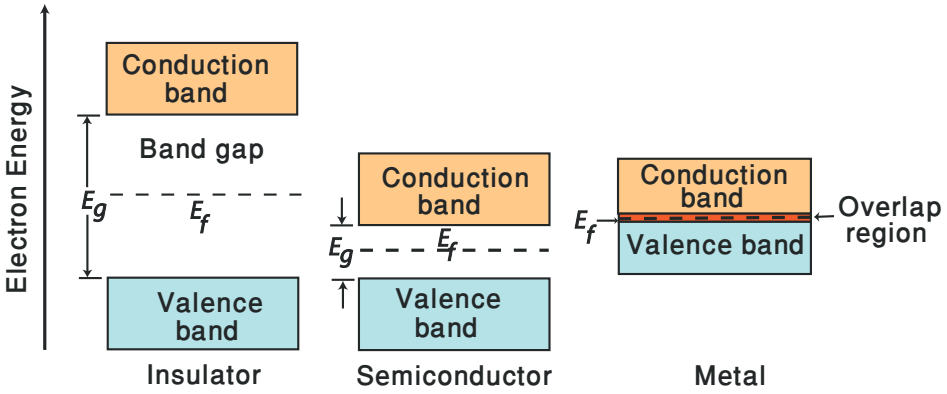

Figure 1: Simplified diagram of the electronic band structure of insulators, semiconductors and metals. The position of the Fermi level is when the sample is at absolute zero temperature (0 K).

by a large gap, in good conductors such as metals the valence band overlaps the conduction band, whereas in semiconductors there is a small gap between the valence and conduction bands, small enough allowing thermal excitation of electrons from the valence to conduction band. The overall picture is shown in Figure (1).

The Fermi level is an important consequence of band theory, the highest occupied quantum state of electrons at absolute zero temperature. The position of the Fermi level relative to the conduction band is an important parameter that contributes to determine the electrical properties of a particular material. The position of the Fermi level position is also indicated in Figure (1).

For a semiconductor, the electrical resistivity lies between a conductor and an insulator, i.e., in the range of 10^3 Siemens/cm to 10^{-8} S/cm. An externally applied electrical field may change the semiconductor's resistivity. In conductors, current is carried by electrons, whereas in semiconductors, current is carried by the flow of electrons or positively charged holes.

Q 1. Explain (or sketch) the temperature dependence of resistance for metals and semiconductors. Why does the resistance of a semiconductor decrease with increasing temperature?

2.2 Intrinsic and extrinsic semiconductors

An intrinsic semiconductor is a pure semiconductor having no impurities. In an intrinsic semiconductor, the numbers of excited electrons and holes are equal, i.e., $n = p$ as shown

in Figure (2a). A semiconductor in which doping has been introduced, thus changing the relative number and type of free charge carriers, is called an extrinsic semiconductor.

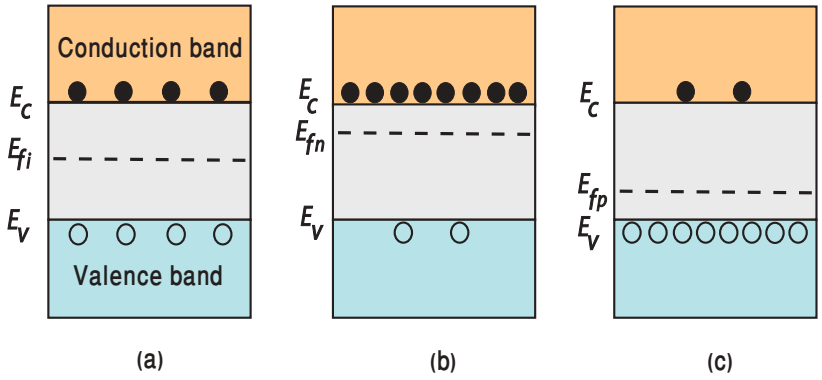

Figure 2: Energy band diagrams for (a) intrinsic, (b) n-type, and (c) p-type semiconductors. E_f is the Fermi energy level, and the letters i, n, p indicate intrinsic, n and p-type materials. E_c and E_v are the edges of the conduction and valence bands.

An extrinsic semiconductor, in which conduction electrons are the majority carriers is an n-type semiconductor and its band diagram is illustrated in Figure (2b), one in which the holes are the majority charge carriers is a p-type semiconductor and is indicated in Figure (2c). In extrinsic semiconductors, when they are *really* behaving in extrinsic region, the dopant concentration N_d is much larger than the thermally generated electron-hole pairs n_i and is temperature independent at room temperature.

Q 2. Why is doping introduced in semiconductors? How does it effect the conductivity of a semiconductor?

2.3 The ubiquitous role of semiconductor devices

Semiconductor devices are the foundation of the electronic industry. Most of these devices can be constructed from a set of building blocks. The first building block is the metal-semiconductor interface as shown in Figure (3a). This interface can be used as a rectifying contact, i.e., the device allows current in one direction as in ohmic contact. By using the rectifying contact as a gate, we can form a MESFET (metal-semiconductor field-effect transistor), an important microwave device.

The second building block is the p-n junction, a junction of p-type and n-type materials indicated in Figure (3b). The p-n junction is the key compound for numerous semiconductor devices. By combining two p-n junctions, we can form the p-n-p bipolar transistor, and combining three p-n junctions to form a p-n-p-n structure, a switching device called a thyristor can be formed.

The third important building block is the heterojunction interface depicted in Figure (3c). It is formed between two dissimilar semiconductors, for example gallium arsenide (GaAs) and aluminium arsenide (AlAs) and is used in band gap engineering. Band gap engineering is a useful technique to design new semiconductor devices and materials. Heterojunctions and molecular beam epitaxy (MBE) are the most important techniques in which required

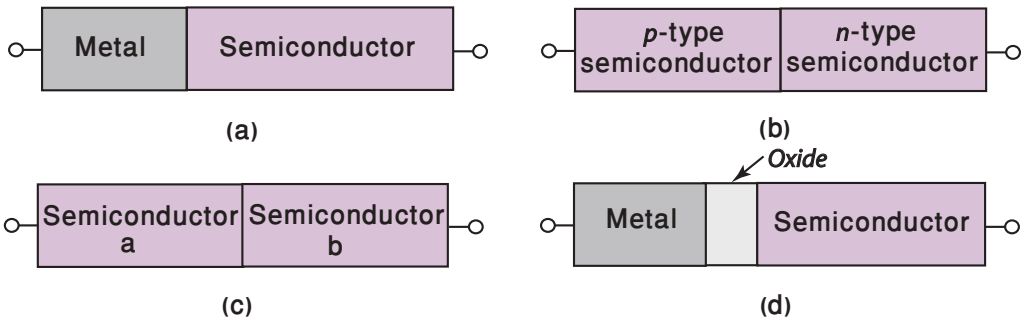

Figure 3: Basic device building blocks of (a) metal-semiconductor interface, (b) p-n junction, (c) heterojunction interface, (d) metal-oxide-semiconductor structure.

band diagrams are devised by continuous band-gap variations. A new generation of devices, ranging from solid-state photomultipliers to resonant tunneling transistors and spin polarized electron sources, is the result of this technique.

The fourth building block is the metal-oxide-semiconductor (MOS) structure. It is a combination of a metal-oxide and an oxide-semiconductor interface indicated as in Figure (3d). The MOS structure used as a gate and the two semiconductor-metal oxide junctions are the source and drain; the result is the MOSFET (MOS field-effect transistor). The MOSFET is the most important component of modern integrated circuits, enabling the integration of millions of devices per chip.

2.4 Conduction in intrinsic semiconductors

The process in which thermally or optically excited electrons contribute to the conduction is called intrinsic semiconduction. In the absence of photonic excitation, intrinsic semiconduction takes place at temperatures above 0 K as sufficient thermal agitation is required to transfer electrons from the valence band to the conduction band [**?**].

The total electrical conductivity is the sum of the conductivities of the valence and conduction band carriers, which are holes and electrons, respectively. It can be expressed as

$$\sigma = n_e q_e \mu_e + n_h q_h \mu_h, \tag{1}$$

where n_e, q_e, and μ_e are the electron's concentration, charge and mobility, and n_h, q_h, and μ_h are the hole's concentration, charge and mobility, respectively.

The mobility is a quantity that directly relates the drift velocity υ_d of electrons to the applied electric field E across the material, i.e.,

$$\upsilon_d = \mu E. \tag{2}$$

In the intrinsic region the number of electrons is equal to the number of holes, so Equation (1) implies that,

$$\sigma = n_e q_e (\mu_e + \mu_h). \tag{3}$$

The electron density (electrons/volume) in the conduction band is obtained by integrating $g(E)f(E)dE$ (density of states×probability of occupancy of states) from the bottom to top

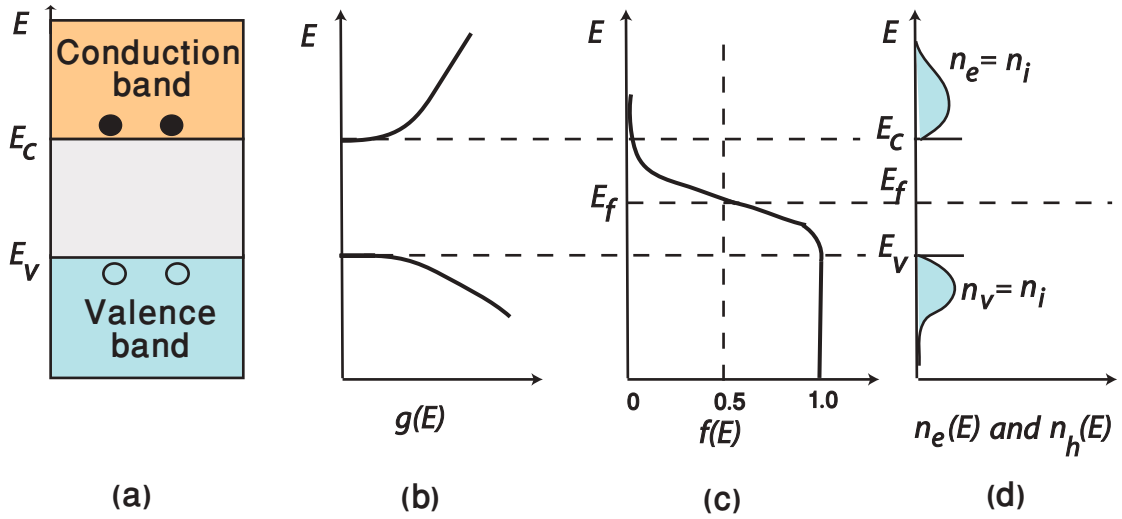

Figure 4: Band gap structure of an intrinsic semiconductor. (a) Schematic band diagram, (b) density of states $g(E)$, (c) Fermi distribution function $f(E)$, (d) carrier concentration $n_e(E)$ and $n_h(E)$. E_c, E_v and E_f represent the conduction band energy, valence band energy and Fermi energy level, respectively.

of the conduction band,

$$n_e = \int_{E_c}^{\infty} g(E)f(E)dE. \tag{4}$$

There are two important quantities introduced in the above expression: $g(E)$ is the number of states per unit energy per unit volume known as the density of sates. The density of states in the conduction band can be derived from first principle and is given by,

$$g(E) = \frac{(\sqrt{2})m_e^{*3/2}}{\pi^2\hbar^3}\Big(E - E_c\Big)^{1/2}. \tag{5}$$

The function $f(E)$ is the probability of an electronic state of energy E being occupied by an electron, and is given by the Fermi-Dirac distribution function,

$$f(E) = \frac{1}{1 + \exp\left(\frac{(E-E_f)}{k_BT}\right)}. \tag{6}$$

The profiles of $g(E)$ and $f(E)$ are depicted in Figure (4). If we suppose that $E - E_f \gg k_BT$, then Equation (6) can be approximated as,

$$f(E) \approx \exp\left(-\frac{E - E_f}{k_BT}\right). \tag{7}$$

Thus, we can replace the Fermi-Dirac distribution by the Boltzmann distribution under the assumption that the number of electrons in the conduction band is far less than the number of available states in this band ($E - E_f$ is large as compared to k_BT).

The number of mobile charge carriers (i.e., n_e in the conduction band and n_h in the valence band) can be obtained by performing the integration in Equation (4), and is given by,

$$n_e = N_c \exp\left(\frac{-(E_c - E_f)}{k_B T}\right), \tag{8}$$

and

$$n_h = N_v \exp\left(\frac{-(E_f - E_v)}{k_B T}\right), \tag{9}$$

where

$$N_c = 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2}, \tag{10}$$

$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2}. \tag{11}$$

N_c and N_v are the effective density of states for the edges of conduction and valence bands, respectively [1].

Q 3. Derive the expressions (10) and (11) for the effective density of states for the conduction band, N_c, and for the valence band, N_v.

The terms m_e^* and m_h^* are the effective masses of electrons and holes respectively, k_B is Boltzmann's constant, T is the absolute temperature, and h is Planck's constant.

Q 4. What do you understand by the term 'effective mass' of an electron? How is it different from the conventional electron mass?

In an intrinsic semiconductor, the number of electrons is equal to the number of holes, so the charge carrier concentration is given by,

$$n_i = \sqrt{n_e n_h} = \left(N_c N_v\right)^{1/2} \exp\left(\frac{-E_g}{2k_B T}\right), \tag{12}$$

where, $E_g = E_c - E_v$ is the energy band gap. The term $(N_c N_v)^{1/2}$ in Equation (12) depends on the band structure of the semiconductor. It will be shown later that for intrinsic behavior, n_i varies as some power of T, so Equation (12) can be written as,

$$n_i = C T^{3/2} \exp\left(\frac{-E_g}{2k_B T}\right), \tag{13}$$

where, C is some constant. Substituting the expression (13) into (3) yield the following expression for the intrinsic conductivity,

$$\boxed{\sigma = C T^{3/2} q_e \left(\mu_e + \mu_h\right) \exp\left(\frac{-E_g}{2k_B T}\right)}. \tag{14}$$

Equation (14) shows that the electrical conductivity of intrinsic semiconductors or extrinsic semiconductors in the intrinsic regime, decreases with increasing temperature. This relationship is extremely important and will be used to measure the band gap. So make sure you take a breath of fresh air here, and understand what this relationship means.

Q 5. Derive Equation (12).

Q 6. Using Equation (14), explain how the conductivity of a semiconductor changes at high temperatures. You will find two competing factors here, $T^{3/2}$ and $\exp(\frac{-E_g}{2k_BT})$. Which of these factors dominates and why?

Q 7. What is the difference between Fermi-Dirac and Boltzmann distributions? Which distribution is being followed by the majority carriers in semiconductors?

Q 8. Given that the effective masses of electrons and holes in Si are approximately 1.08 m_e and 0.60 m_e, respectively, the electron and hole drift mobilities at room temperature are 1350 and 450 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, respectively, and the energy band gap value is 1.10 eV, calculate the intrinsic concentration and intrinsic resistivity of Si [2].

2.5 Conduction in extrinsic semiconductors

In doped semiconductors, the dopant concentrations ($n_e \simeq N_d$ for n-type and $n_h \simeq N_a$ for p-type doping) at room temperatures are greater than the the thermally generated intrinsic carrier concentrations n_i. The conductivity depends on the carrier concentrations and the mobility. So in order to determine the temperature dependent conductivities, one has to consider, separately, how temperature affects both the carrier concentration and the mobility [2].

2.5.1 Temperature dependence of charge carrier concentration

Consider an n-type semiconductor with dopant carrier concentration (N_d) of arsenic atom (As). The As atoms introduce a donor energy level E_d, that is located at a gap ΔE below E_c. The ionization of As atoms leads to electrons jumping across ΔE into the conduction band. The scenario is depicted in Figure (5).

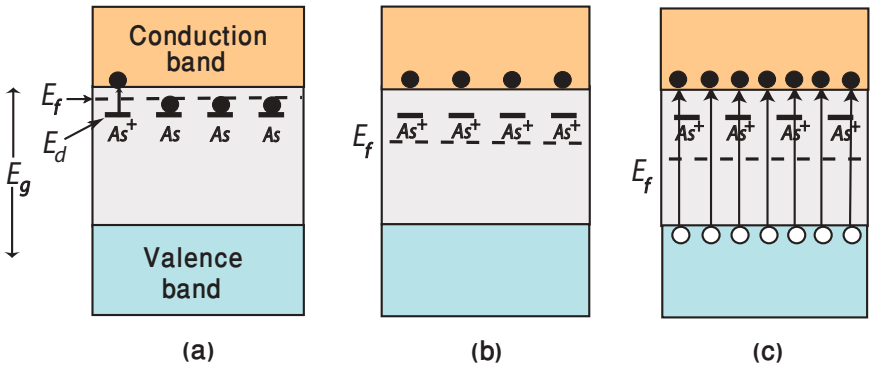

Figure 5: Electron concentration of an n-type semiconductor in (a) low temperature regime, (b) medium temperature regime, (c) high temperature regime. E_f and E_d are the Fermi and donor atom energy levels, respectively.

1. **Low temperature regime** At very low temperatures, conductivity is almost zero because donor atoms are not ionized due to the small thermal vibrational energy. As

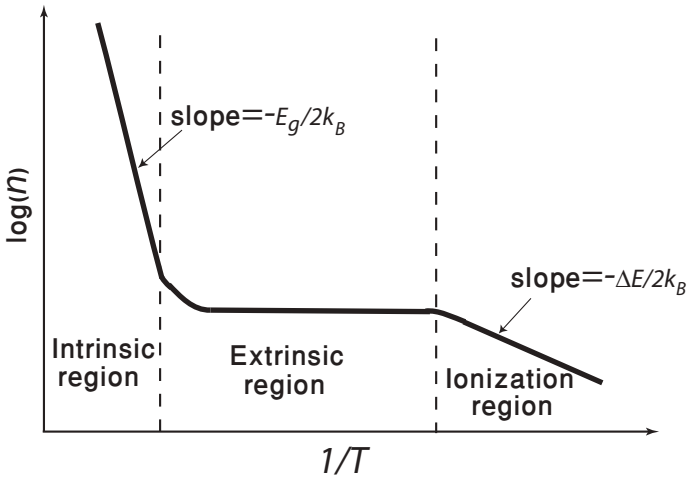

Figure 6: The temperature dependence of the electron concentration in an n-type semiconductor, showing the ionization, extrinsic and intrinsic regimes. Note that the horizontal axis is $1/T$ instead of T.

temperature slightly increases, the donor atoms get ionized and move to the conduction band as shown in Figure (5a). The electron concentration at such low temperature is given by,

$$n_e = \left(\frac{1}{2}N_c N_d\right)^{1/2} \exp\left(-\frac{\Delta E}{2k_B T}\right), \tag{15}$$

where, $\Delta E = E_c - E_d$ is the energy difference from donor energy level to bottom of conduction band. The low temperature regime is also called the ionization regime.

Q 9. What are the similarities and differences between Equations (12) and (15)?

Q 10. Explore the origin of the extra factor of one half in Equation (15).

2. **Medium temperature regime** In this temperature range, the process of ionization has continued to the extreme that all donor atoms have been ionized as shown in Figure (5b). This temperature range is often called the extrinsic range and is also indicated in Figure (6). Since the electrical conductivity depends on carrier concentration n and mobility μ,

$$\sigma = qn\mu, \tag{16}$$

and $n = N_d \simeq$constant in the extrinsic region, the conductivity is solely determined by the temperature variation of the mobility. The mobility is proportional to some power α of the temperature,

$$\boxed{\sigma = T^{\alpha}} \tag{17}$$

In the medium temperature regime, a plot of $\log(\frac{1}{\sigma})$ versus $\log(\frac{1}{T})$ will give the value of temperature dependent coefficient α. Extrinsic semiconductors are almost always operated in this region.

3. **High temperature regime** As temperature increases, the electron concentration n_i due to thermal agitations across the band gap is much larger than the dopant concentrations N_d. In this regime, excitations from valence band to conduction band are also

possible due to which hole concentration becomes equal to the electron concentration $n_h = n_e$ depicted in Figure (5c). This range is referred as the intrinsic range and is shown in Figure (6). This is the regime where the purpose of doping is defeated and the material behaves as an intrinsic semiconductor. In this temperature range, the slope of $\log(n)$ versus $1/T$ yields $(-E_g/2k_B)$. Also compare this with Eq. (14).

Q 11. An n-type Si sample has been doped with 10^{15} phosphorus atoms cm^{-3}. The donor level for P in Si is 0.045 eV below the conduction band edge energy [2]. (a) What would be the temperature above which the sample behaves as intrinsic? (b) What is the lowest temperature above which most of the donors are ionized?

2.5.2 Temperature and impurity dependence of drift mobility

Now that we have established how temperature affects carrier concentration, we turn attention to the mobility. Drift mobility μ determines the average velocity v_d in the presence of an applied external field. The variation with temperature follows two distinct regions.

1. **High temperature region** Let suppose an electron in the conduction (C_B) or valence band (V_B) suffers collisions from a scattering ion (As^+). These scattering events depend on how strongly the ions vibrate, the amplitude depends on the temperature T. The mean free time τ between scattering events, is given by,

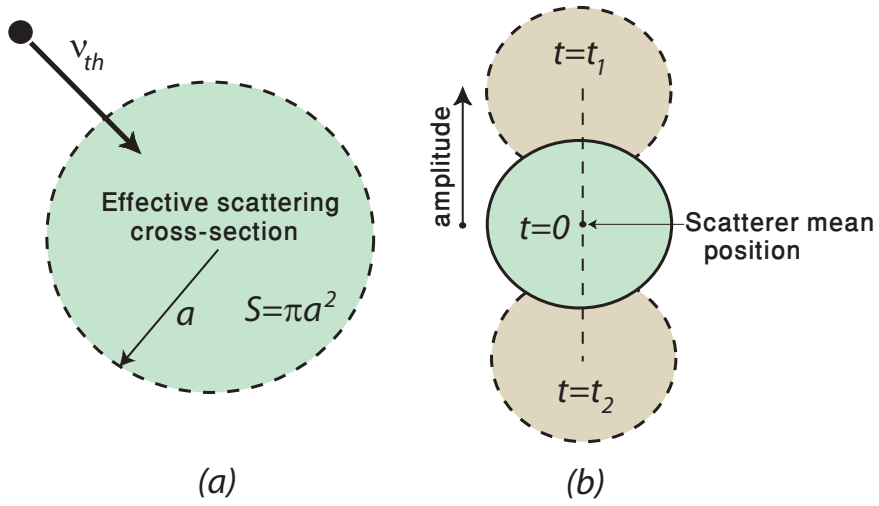

Figure 7: (a) Scattering cross-section, (b) scatterer position at three different times $t = 0, t = t1, t = t2$.

$$\tau = \frac{1}{S v_{th} N_s}. \tag{18}$$

According to the Drude model [2], the drift mobility is,

$$\mu = \frac{e\tau}{m_e^*}. \tag{19}$$

In Equation (18), S is the cross-sectional area of the scatterer shown in Figure (7a), v_{th} is the mean speed of the electrons, called the thermal velocity and N_s is the number of scatterers per unit volume. Now both the scatterer amplitude a and the thermal velocity of the electron v_{th} is temperature dependent. We unveil these dependences, one by one. The scatterer amplitude increases with temperature as $a^2 \propto T$. Now an electron in the conduction band has only kinetic energy and the mean kinetic energy per electron in the conduction band is $\frac{3}{2}k_BT$. Applying kinetic molecular theory to the gas of electrons in the conduction band, we obtain,

$$\frac{1}{2}m_e^* v_{th}^2 = \frac{3}{2}k_BT, \tag{20}$$

implying $v_{th} \propto T^{1/2}$. Using the above derived temperature dependences of v_{th}, the scatterer mean time τ_L due to lattice vibrations will become,

$$\tau_L = \frac{1}{Sv_{th}} \propto \frac{1}{T^{3/2}} = T^{-3/2}, \tag{21}$$

resulting in lattice vibration scattering limited mobility, μ_L,

$$\mu_L \propto T^{-3/2}. \tag{22}$$

Clearly as the temperature goes up, μ_L decreases.

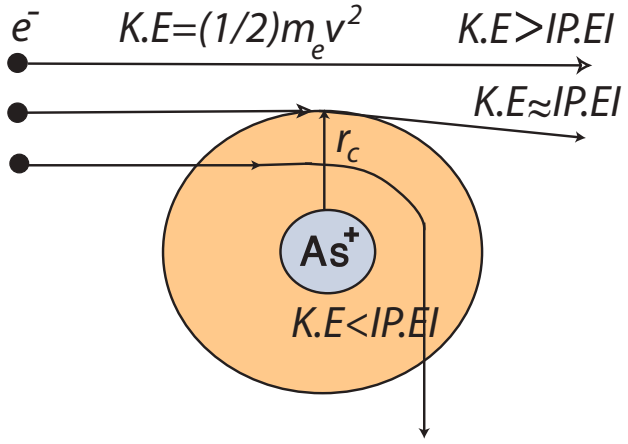

Figure 8: Electron scattering by an ionized impurity (As^+) that is fixed in position.

2. **Low temperature region** At low temperatures, the scattering of electrons by thermal lattice vibrations is not strong enough. The electron scattering is performed by the electrostatic interaction with the ionized donor impurities. Let we consider a case in which an electron passes by an ionized donor As^+. The deflection from the rectilinear path depends on the following factors,

   - If the $K.E$ of the electron is larger than the $P.E$ of the ionized donor impurity (As^+) at a distance r ($K.E > |P.E|$), then the electron will not feel the $P.E$ and will continue its course unhindered, unswayed.
   - If the $K.E < |P.E|$, then the columbic interaction energy is strong enough to deflect the electron. The two cases are depicted in Figure (8).

- $K.E \approx |P.E|$ at $r = r_c$, the critical radius at which the electron is just scattered, leading to,

$$\frac{3}{2}k_BT = \frac{e^2}{4\pi\varepsilon_o\varepsilon_r r_c^2}, \tag{23}$$

from which one can deuce the critical radius,

$$r_c = \frac{e^2}{6\pi\varepsilon_o\varepsilon_r kT}. \tag{24}$$

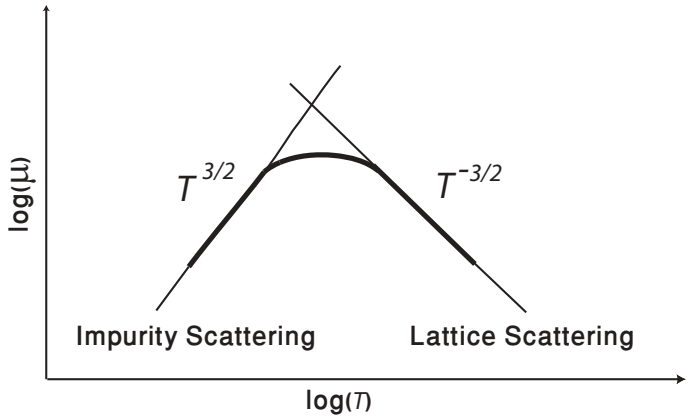

Figure 9: Temperature dependence of mobility including effects of both lattice and impurity scattering in the two temperature regimes.

Thus, the critical scattering radius r_c also possesses the inverse temperature dependence and decreases as temperature increases. By adding the value of r_c into scattering cross section, $S = \pi r_c^2$, one may infer that $S \propto T^{-2}$. Therefore, the ionized impurity scattering limited mobility, μ_I comes out as replacing the same argument given before Equation (22)

$$\mu_I \propto \frac{T^{3/2}}{N_I}, \tag{25}$$

where N_I is the ionized impurity concentration. Thus in the low temperature regime, μ_I decreases with increasing ionized impurity concentration.

The lattice limited and impurity limited regimes of the mobility are shown in Figure (9). It is observed from Equations (22), (25) and Figure (9) that the mobility has a divergent behavior with respect to temperature. At low temperature, mobility increases with increasing temperature, and starts decreasing as temperature increases in the high temperature regime.

Q 12. Calculate the temperature dependence of the mean free time τ between impurities and derive Equation (25).

2.6 Temperature dependence of conductivity

We have determined the temperature dependence of the carrier concentration and mobility for a doped semiconductor. Hence, the electrical conductivity in extrinsic semiconductors

can be determined by combining the results of Figures (6) and (9), and is shown in Figure (??).

3 The experiment

3.1 Overview of the experiment

In this experiment we will investigate the conductivity temperature variation of an n-doped semiconductor sample (the base region of a unijunction transistor (UJT)). A UJT is a semiconductor device, having three leads but only one junction. Figure (10) shows the schematic of a unijunction transistor with an N-type base and P-type emitter. Conductivity measurement between pins B_1 and B_2 of the UJT is equivalent to that of a doped semiconductor.

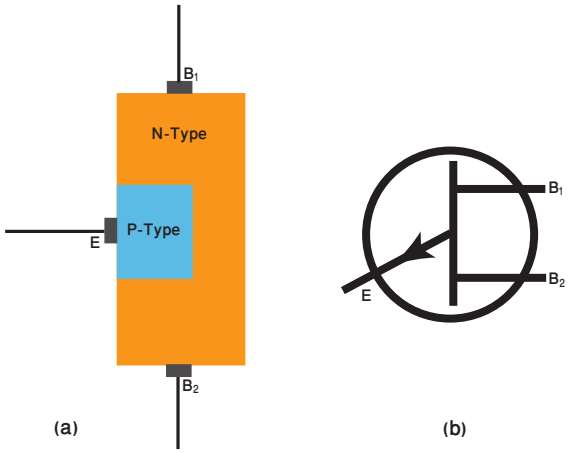

Figure 10: Schematic diagram (a) and symbol (b) of a unijunction transistor.

The semiconductor sample is placed inside a sample cell and the resistance of the sample is measured while its temperature is monitored. The sample cell is placed inside a flow cryostat which can be filled by liquid nitrogen. The cell is cooled by the cool vapor of N_2. Alternatively, the cell can be heated to elevated temperatures by passing current through a heater wire wound around it. The flow cryostat is sketched in Figure (11a) highlighting the various components.

Resistance of the UJT sample is measured using an ohmmeter. The measured resistance at different temperatures yields the conductivity versus temperature behavior of the semiconductor sample, from which the energy band gap E_g and the temperature dependent coefficient of mobility α can be calculated.

3.2 Apparatus

The experiment involves the following major components.

1. Cryostat: it is a copper cylinder with one end sealed, so that liquid N_2 can be poured into it for low temperature measurements.The sample cell is situated inside the cryostat

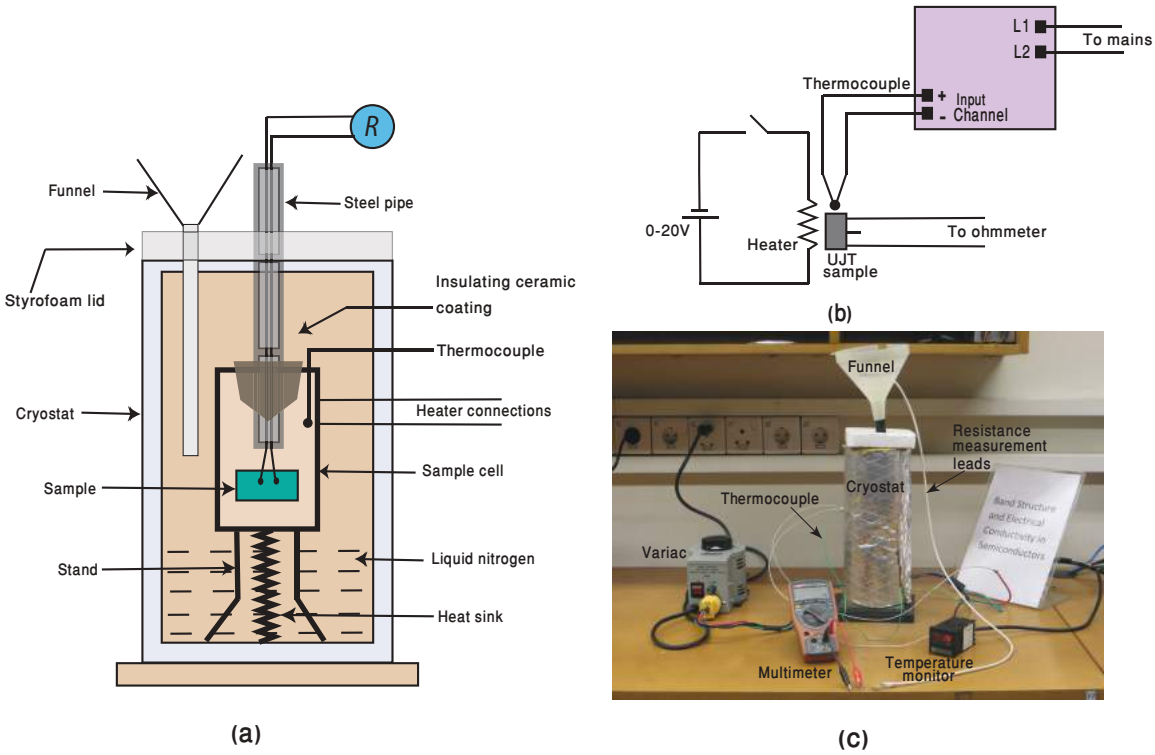

Figure 11: Experimental setup: (a) A schematic of the cryostat and sample cell assembly, (b) electrical diagram of the apparatus, and (c) a view of the experimental setup.

and is cooled by the N_2 vapor as it boils. An insulating sheet is wrapped around the cylinder to reduce thermal losses.

2. Battery or power supply used to energize the heater wrapped around the sample cell.
3. Sample cell wound with heater wire and containing the sample.
4. Thermocouple to sense the temperature of the sample.
5. Temperature monitor: receives input from the thermocouple and displays the temperature ^oC.
6. Digital multimeter to measure the resistance of the sample.
7. supply of liquid nitrogen N_2 to achieve low temperature.

3.3 Experimental procedure

1. You are provided with a unijunction transistor (UJT) to which leads are already connected for resistance measurement, as shown in Figure (12).
2. The insulated wires, enshrouded in a ceramic rod, have to be passed through a steel pipe coated with ceramic on one end.
3. Connect the multimeter to the resistance measurement leads of sample and set the dial to the appropriate resistance scale.

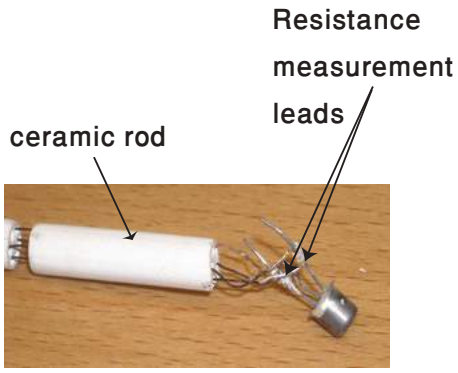

Figure 12: Unijunction transistor (UJT) with connected wires.

4. After passing through the opening on one side of the cryostat, place the thermocouple inside the sample cell.

5. Turn on the controller. It should show room temperature.

6. Place the ceramic coated end of the steel pipe on the sample cell in such a way that the UJT is completely inside the cell. The top of the cryostat needs to be covered with the styrofoam lid and the nozzle of the funnel passed through the space provided in it.

   We will start with low temperature measurements.

7. Now slowly pour liquid nitrogen into the cryostat and wait for the controller to show a temperature of around $-150°$C.

8. Note down the resistance of the sample with every $5°$ change in temperature until the sample reaches room temperature.

   We now move on to high temperature measurements.

9. Connect the heater to the battery or power supply as shown in Figure (11b).

10. Now set the battery voltage to about 20 V. The controller should indicate a rise in temperature.

11. When the temperature of the sample reaches $\sim 250°$C, switch OFF the supply and make a table of the resistance readings for every $5°$C fall in temperature.

Q 13. Plot a graph of the resistance, R, versus T in Kelvins, and distinguish the intrinsic and extrinsic regions for the UJT.

Q 14. Calculate the energy band gap from the intrinsic region data. As conductivity depends on both the charge carrier concentration and mobility, so in calculating band gap take both of these factors into account. The published energy band gap values for pure silicon (Si) is 1.12 eV, while the base of a UJT is an n-doped material. See Eq. (14) and the discussion in Q6.

Q 15. Calculate the temperature coefficient α of the carriers mobility from the extrinsic region data of the UJT. The published value of the mobility of the charge carriers, α is 2.3.

Q 16. What is the uncertainty in the energy band gap measurement?

Q 17. Find the uncertainty in the mobility measurement.