



Sudan University of Science and Technology

College of Graduate Studies



**Effect of Temperature on Density of State Function and the
Valence Band in Semiconductors**

أثر الحرارة على كثافة دالة الحالة و نطاق التكافؤ في اشباه الموصلات

***A thesis submitted for partial fulfillments of the requirement
of the degree of science master in physics***

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DEDICATION

This research to the great **prophet Mohammed** "Peace & prayers be upon him" Whom we love for their Encouragement and Support... To those who are the reasons for my presence in life ... **My parents...**
To the road friends.

Greetings

Acknowledgement

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Abstract

In this thesis the characteristic of semiconductor made of silicon diode was investigated.

The energy gap was calculated and density of state function was studied as function of temperature variation and it was found that it was proportional to $T^{\frac{3}{2}}$ as prescribed in theoretical consideration.

The relation of semiconductor resistivity with temperature variation also investigated which reveals exponential relations.

المستخلص

يهدف البحث لتوضيح أثر درجة الحرارة علي شبه الموصل وفيه تمت دراسة خصائص الجهد والتيار لثنائي مصنوع من السيلكون. و حساب فجوة الطاقة وكثافة دالة الحالة كدالة في درجة الحرارة ووجد انها تتناسب مع $T^{\frac{3}{2}}$ كما تمت دراسة العلاقة بين القدرة المستهلكة مع ارتفاع درجة الحرارة التي اظهرت علاقة خطية. ايضا درست العلاقة بين المقاومة مع درجة الحرارة ووجد انها تتناسب معها عكسيا.

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Chapter One

Introduction

1.1 Preface

So far, we have been considering a general crystal and applying to it the concepts of quantum mechanics in order to determine a few of the characteristics of electrons in a single-crystal lattice. In this chapter, we will apply these concepts specifically to a semiconductor material. In particular, we will use the density of quantum states in the conduction band and the density of quantum states in the valence band along with the Fermi-Dirac probability function to determine the concentration of electrons and holes in the conduction and valence bands, respectively.

We will also apply the concept of the Fermi energy to the semiconductor material. This chapter deals with the semiconductor in equilibrium. Equilibrium, or thermal equilibrium, implies that no external forces such as voltages, electric fields, magnetic fields, or temperature gradients are acting on the semiconductor. All properties of the semiconductor will be independent of time in this case. Equilibrium is our starting point for developing the physics of the semiconductor. We will then be able to determine the characteristics that result when deviations from equilibrium occur, such as when a voltage is applied to a semiconductor device. We will initially consider the properties of an intrinsic semiconductor, that is, a pure crystal with no impurity atoms or defects. We will see that the electrical properties of a semiconductor can be altered in desirable ways by adding controlled amounts of specific impurity atoms. Called dopant atoms, to the crystal. Depending upon the type of dopant atom added, the dominant charge carrier in the semiconductor will be either electrons in the conduction band or holes in the valence band. Adding dopant atoms changes the distribution of electrons among the

available energy states, so the Fermi energy becomes a function of the type and concentration of impurity atoms. Finally, as part of this discussion, we will attempt to add more insight into the significance of the Fermi energy.

1.2 Charge Carriers in Semiconductors

Current is the rate at which charge flows. In a semiconductor. Two types of charge carrier, the electron and the hole, can contribute to a current. Since the current in a semiconductor is determined largely by the number of electrons in the conduction band and the number of holes in the valence band, an important characteristic of a semiconductor is the density of these charge carriers. The density of electrons and holes is related to the density of states function and the Fermi distribution function, both of which we have considered. A qualitative discussion of these relationships will be followed by a more rigorous mathematical derivation of the thermal-equilibrium concentration of electrons and holes.

1.3 The Problem:

Temperature has great influences in the I-V characteristic for semiconductor devices as a semiconductor plays an important role in today's technology so it is important to fix the important characteristics in practice.

1.4 The Objective:

The objective of this thesis is

1. To find the effective density of state as a function in the valence band.
2. To study the effect of temperature on the resistivity of a semiconductor diode
3. To find the energy gap
4. The obtained results compared with theoretical considerations

1.5 Thesis Layout:

This thesis consist of four chapters, chapter one Introduction, chapter two Basic Principles of Semiconductors its properties, chapter three discussion of the band theory and Fermi level, chapter four the material and methods

1.6 Previous studies:

In 1979 Ansgar Liebsch (Liebsch 1979) study effect of Self-Energy Corrections on the Valence-Band Photoemission Spectra of Ni, his study shown that the experimentally observed band narrowing, the large quasiparticle damping, the small exchange splitting, and the existence of satellites can be reproduced semi quantitatively with use of the low-density approximation to describe correlations between Ni 3d electrons. The exchange splitting of t_{2g} states (~0.37 eV) is found to be considerably larger than that between e.g. states (~0.21 eV). A new satellite is predicted about 2 eV below the main "6-eV" satellite. {1}

In 1984 L. E. Brus (Brus 1984) study the Electron–electron and electron-hole interactions in small semiconductor crystallites: The size dependence of the lowest excited electronic state in an elementary way, the excited electronic states of semiconductor crystallites sufficiently small (~50 Å diam) that the electronic properties differ from those of bulk materials. In this limit the excited states and ionization processes assume a molecular-like character. However, diffraction of bonding electrons by the periodic lattice potential remains of paramount importance in the crystallite electronic structure. Schrödinger's equation is solved at the same level of approximation as used in the analysis of bulk crystalline electron–hole states (Wannier excitons). Kinetic energy is treated by the effective mass approximation, and the potential energy is due to high frequency dielectric solvation by atomic core electrons. An approximate formula is

given for the lowest excited electronic state energy. This expression is dependent upon bulk electronic properties, and contains no adjustable parameters. The optical f -number for absorption and emission is also considered. The same model is applied to the problem of two conduction band electrons in a small crystallite, in order to understand how the redox potential of excess electrons depends upon crystallite size. {2}

Chapter Two

Basic Principles of Semiconductors

2.1 The diode:

The Diode is one of the simplest semiconductor devices around, and which has the characteristic of passing current in only one direction only. However, unlike a resistor, a diode does not behave linearly with respect to the applied voltage as the diode has an exponential current-voltage (I-V) relationship and therefore we cannot described its operation by simply using an equation such as Ohm's law.

If a suitable positive voltage (forward bias) as show figure is applied between the two ends of the PN junction, it can supply free electrons and holes with the extra energy they require to cross the junction as the width of the depletion layer around the PN junction is decreased.

By applying a negative voltage (reverse bias) results in the free charges being pulled away from the junction resulting in the depletion layer width being increased. This has the effect of increasing or decreasing the effective resistance of the junction itself allowing or blocking current flow through the diode.

2.2 The Depletion Region

The depletion region, also called depletion layer, depletion zone, junction region, space charge region or space charge layer, is an insulating region within a conductive, doped semiconductor material where the mobile charge carriers have been diffused away, or have been forced away by an electric field. The only elements left in the depletion region are ionized donor or acceptor impurities.

Then the depletion layer widens with an increase in the application of a reverse voltage and narrows with an increase in the application of a forward voltage. This

is due to the differences in the electrical properties on the two sides of the PN junction resulting in physical changes taking place. One of the results produces rectification as seen in the PN junction diodes static I-V (current-voltage) characteristics. Rectification is shown by an asymmetrical current flow when the polarity of bias voltage is altered as shown below.

But before we can use the PN junction as a practical device or as a rectifying device we need to firstly bias the junction, ie connect a voltage potential across it. On the voltage axis above, “Reverse Bias” refers to an external voltage potential which increases the potential barrier. An external voltage which decreases the potential barrier is said to act in the “Forward Bias” direction.

There are two operating regions and three possible “biasing” conditions for the standard Junction Diode and these are:

1. Zero Bias – No external voltage potential is applied to the PN junction diode.
2. Reverse Bias – The voltage potential is connected negative, (-ve) to the P-type material and positive, (+ve) to the N-type material across the diode which has the effect of Increasing the PN junction diode’s width.
3. Forward Bias – The voltage potential is connected positive, (+ve) to the P-type material and negative, (-ve) to the N-type material across the diode which has the effect of Decreasing the PN junction diodes width.

2.3 Reduction in the Depletion Layer due to Forward Bias

This condition represents the low resistance path through the PN junction allowing very large currents to flow through the diode with only a small increase in bias voltage. The actual potential difference across the junction or diode is kept

constant by the action of the depletion layer at approximately 0.3v for germanium and approximately 0.7v for silicon junction diodes.

Since the diode can conduct “infinite” current above this knee point as it effectively becomes a short circuit, therefore resistors are used in series with the diode to limit its current flow. Exceeding its maximum forward current specification causes the device to dissipate more power in the form of heat than it was designed for resulting in a very quick failure of the device.

2.4 Zero Biased Junction Diode

When a diode is connected in a Zero Bias condition, no external potential energy is applied to the PN junction. However if the diodes terminals are shorted together, a few holes (majority carriers) in the P-type material with enough energy to overcome the potential barrier will move across the junction against this barrier potential. This is known as the “Forward Current” and is referenced as I_F

Likewise, holes generated in the N-type material (minority carriers), find this situation favourable and move across the junction in the opposite direction. This is known as the “Reverse Current” and is referenced as I_R . This transfer of electrons and holes back and forth across the PN junction is known as diffusion, as shown below.

The potential barrier that now exists discourages the diffusion of any more majority carriers across the junction. However, the potential barrier helps minority carriers (few free electrons in the P-region and few holes in the N-region) to drift across the junction.

Then an “Equilibrium” or balance will be established when the majority carriers are equal and both moving in opposite directions, so that the net result is zero

current flowing in the circuit. When this occurs the junction is said to be in a state of “Dynamic Equilibrium“.

The minority carriers are constantly generated due to thermal energy so this state of equilibrium can be broken by raising the temperature of the PN junction causing an increase in the generation of minority carriers, thereby resulting in an increase in leakage current but an electric current cannot flow since no circuit has been connected to the PN junction.

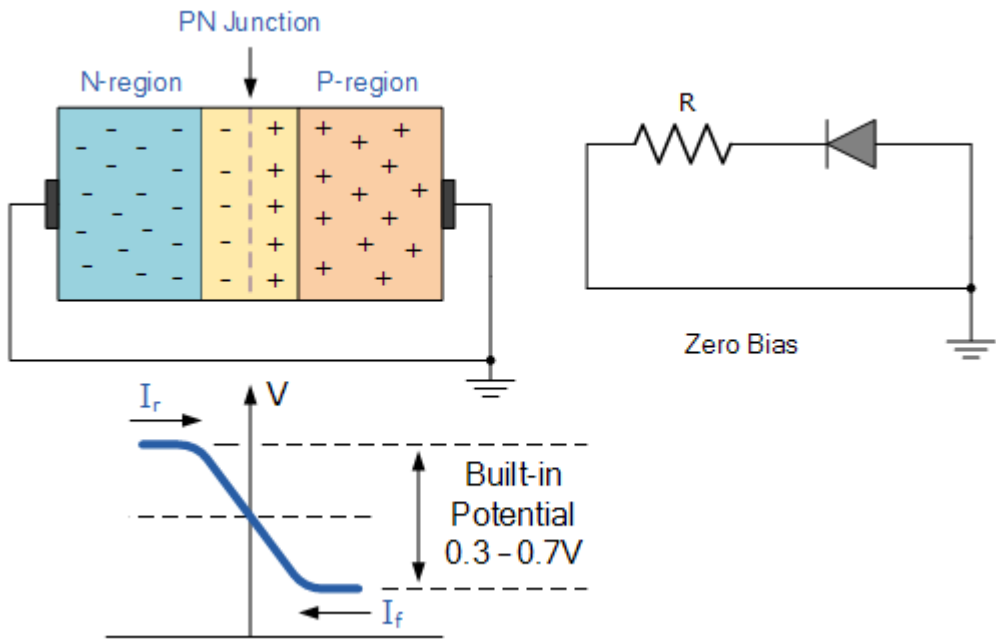


Figure 2.1 Zero Biased Junction Diode

2.5 Reverse Biased PN Junction Diode

When a diode is connected in a Reverse Bias condition, a positive voltage is applied to the N-type material and a negative voltage is applied to the P-type material.

The positive voltage applied to the N-type material attracts electrons towards the positive electrode and away from the junction, while the holes in the P-type end are also attracted away from the junction towards the negative electrode.

The net result is that the depletion layer grows wider due to a lack of electrons and holes and presents a high impedance path, almost an insulator. The result is that a high potential barrier is created thus preventing current from flowing through the semiconductor material.

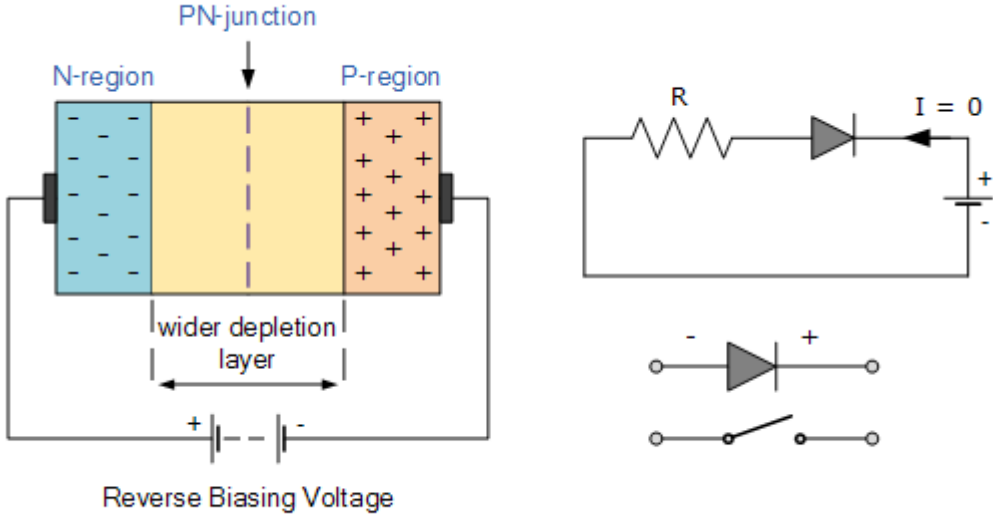


Figure 2.2 Reverse Biased PN Junction Diode

This condition represents a high resistance value to the PN junction and practically zero current flows through the junction diode with an increase in bias voltage. However, a very small leakage current does flow through the junction which can be measured in micro-amperes, (μA).{3}

One final point, if the reverse bias voltage V_r applied to the diode is increased to a sufficiently high enough value, it will cause the diode’s PN junction to overheat and fail due to the avalanche effect around the junction. This may cause the diode

to become shorted and will result in the flow of maximum circuit current, and this shown as a step downward slope in the reverse static characteristics curve below. {4}

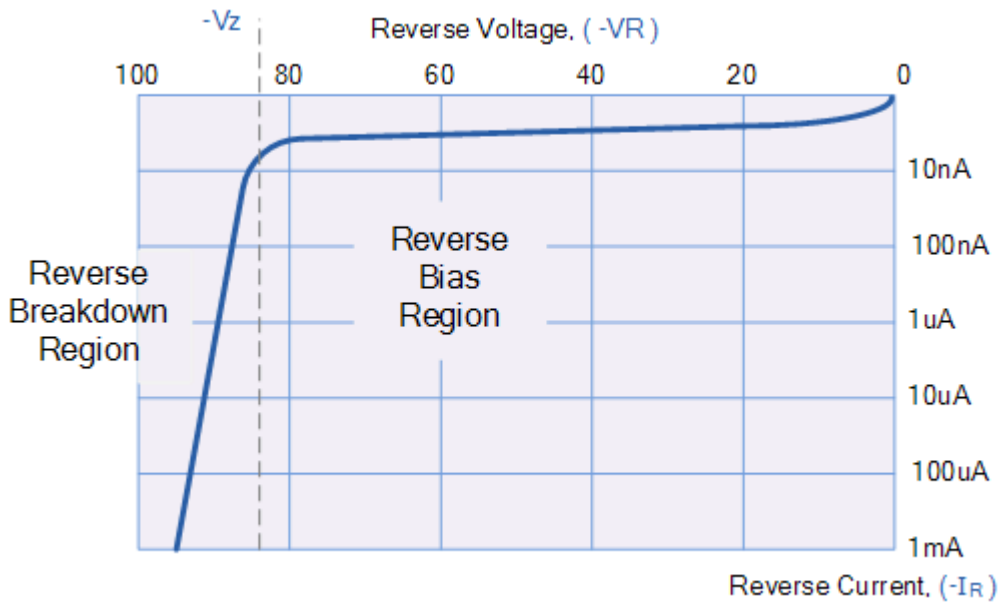


Figure 2.3 Forward Biased PN Junction Diode

2.6 Forward Biased PN Junction Diode

When a diode is connected in a Forward Bias condition, a negative voltage is applied to the N-type material and a positive voltage is applied to the P-type material. If this external voltage becomes greater than the value of the potential barrier, approx. 0.7 volts for silicon and 0.3 volts for germanium, the potential barriers opposition will be overcome and current will start to flow.

This is because the negative voltage pushes or repels electrons towards the junction giving them the energy to cross over and combine with the holes being pushed in

the opposite direction towards the junction by the positive voltage. This results in a characteristics curve of zero current flowing up to this voltage point, called the “knee” on the static curves and then a high current flow through the diode with little increase in the external voltage as shown below.

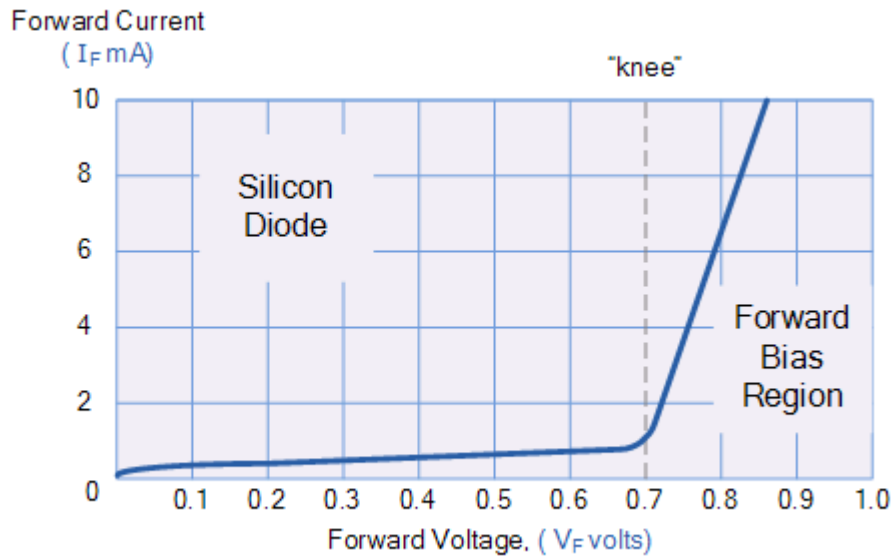


Figure 2.4 Forward Voltage

2.7 Exceed Breakdown Voltage

Now here the applied voltage is greater than the breakdown voltage. We don't know what the breakdown voltage of this diode is, but it is greater than that. What's going to happen at this point is, even though it is reverse bias, current will be forced to flow through this device. The device is effectively breaking down and was going to have the current through here will be the applied voltage minus whatever drop there is across this device. This usually damages the diode.

2.8 The unit cell concept:

A unit cell is the most basic and least volume consuming repeating structure of any solid. It is used to visually simplify the crystalline patterns solids arrange themselves in. When the unit cell repeats itself, the network is called a lattice. {5}

The unit cell has a number of shapes, depending on the angles between the cell edges and the relative lengths of the edges. It is the basic building block of a crystal with a special arrangement of atoms. The unit cell of a crystal can be completely specified by three vectors, a , b , c that form the edges of a parallelepiped. A crystal structure and symmetry is also considered very important because it takes a role in finding a cleavage, an electronic band structure, and an optical property. There are seven crystal systems that atoms can pack together to produce 3D space lattice. {6}

The unit cell is generally chosen so as to contain only complete complement of the asymmetric units. In a geometrical arrangement, the crystal systems are made of three set of (a) , (b) , (c) , which are coincident with unit cell edges and lengths. The lengths of a , b , c are called the unit cell dimensions, and their directions define the major crystallographic axes. A unit cell can be defined by specifying a , b , c , or alternately by specifying the lengths $|a|$, $|b|$, $|c|$ and the angles between the vectors, (α) , (β) , and (γ) as shown in Fig. 1.1. Unit

cell cannot have lower or higher symmetry than the aggregate of asymmetric units. There are seven crystal systems and particular kind of unit cell chosen will be determined by the type of symmetry elements relating the asymmetric units in the cell.

The unit cell is chosen to contain only one complete complement of the asymmetric units, which is called primitive (P). Unit cells that contain an asymmetric unit greater than one set are called centered or nonprimitive unit cells. The additional asymmetric unit sets are related to the first simple fractions of unit cells edges. For example, $(1/2, 1/2, 1/2)$ for the body centered cell (I) and $(1/2, 1/2, 0)$ for the single-face-centered cell (C). The units can be completely specified by three vectors (a, b, c) and the lengths of vectors in angstroms are called the unit cell dimensions. Vectors directions are defined the major crystallographic axes. Unit cell can also be defined by specifying the lengths ($|a|$, $|b|$, $|c|$) and the angles between the vectors (α), (β), and (γ)

2.9 Charge Carrier

Charge carrier is a particle free to move, carrying an electric charge, especially the particles that carry electric charges in electrical conductors. Examples are electrons, ions and holes. In a conducting medium, an electric field can exert force on these free particles, causing a net motion of the particles through the medium; this is what constitutes

an electric current. In different conducting media, different particles serve to carry charge:

2.9.5 Metals

In metals the charge carriers are electrons. One or two of the valence electrons from each atom is able to move about freely within the crystal structure of the metal. The free electrons are referred to as conduction electrons, and the cloud of free electrons is called a Fermi gas.

2.9.6 Electrolytes

In electrolytes, such as salt water, the charge carriers are ions, which are atoms or molecules that have gained or lost electrons so they are electrically charged. Atoms that have gained electrons so they are negatively charged are called anions, atoms that have lost electrons so they are positively charged are called cations. Cations and anions of the dissociated liquid also serve as charge carriers in melted ionic solids (see e.g. the Hall–Héroult process for an example of electrolysis of a melted ionic solid). Conductors are electrolytic conductors employing positive hydrogen ions as carriers.

2.9.7 Plasma

In a plasma, an electrically charged gas which is found in electric arcs through air, neon signs, and the sun and stars, the electrons and cations of ionized gas act as charge carriers.

2.9.8 Vacuum

In a vacuum, free electrons can act as charge carriers. In the electronic component known as the vacuum tube (also called *valve*), the mobile electron cloud is generated by a heated metal cathode, by a process called thermionic emission. When an electric field is applied strong enough to draw the electrons into a beam, this may be referred to as a cathode ray, and is the basis of the cathode ray tube display widely used in televisions and computer monitors until the 2000s.

2.9.9 Semiconductors

In semiconductors (the material used to make electronic components like transistors and integrated circuits), in addition to electrons, the travelling vacancies in the valence-band electron population (called "holes"), act as mobile positive charges and are treated as charge carriers. Electrons and holes are the charge carriers in semiconductors.

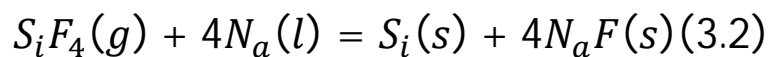
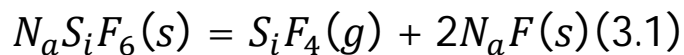
It can be seen that in some conductors, such as ionic solutions and plasmas, there are both positive and negative charge carriers, so an electric current in them consists of the two polarities of carrier moving in opposite directions. In other conductors, such as metals, there are only charge carriers of one polarity, so an electric current in them just consists of charge carriers moving in one direction.

2.10 Obtaining ultra-pure Silicon

In 1823, Berzelius obtained iron-free silicon by reducing SiF_4 gas, which came from the heat decomposition of K_2SiF_6 , with red-hot potassium metal above 520°C . From then on, the processes of producing silicon with precursor silicon tetra fluoride or trichlorosilane have been extensively studied.

Current industrial manufacturing of high purity silicon adopts the Siemens method using purified trichlorosilane, SiHCl_3 . With hydrogen gas, SiHCl_3 , obtained by converting crude silicon with hydrogen chloride, decomposes and deposits silicon onto high-purity silicon rods and enlarges the rods at 1150°C .

The well-known Stanford Research Institute International (SRI) reduction process involves that purified silicon tetrafluoride (SiF_4) gas through fractional distillation is reduced to silicon by metal sodium above 500°C . SiF_4 is from the heat decomposition of sodium hex fluorosilicate (Na_2SiF_6) at 647°C :



An alternative method to transform SiF_4 gas into elemental silicon with NaAlH_4 , in which silane (SiH_4) gas is decomposed at 727°C to generate elemental silicon, was used by Ethyl Corporation. In 2006, Renewable

Energy Corporation announced construction of a plant based on the fluidized bed method using SiH_4 gas, which was obtained by conversion of metallurgical grade silicon into SiHCl_3 and redistribution/distillation to SiH_4 . The continuous flow process recycles all hydrogen and chloride materials back to the initial reactors, while continuous distillation steps purify the SiH_4 gas.

However, there are many drawbacks with these methods, including high deposition temperature, high cost for constructing durable reactors, high energy consumption, operation with explosive raw materials, and post-treatment of hazardous exhausted gas and amorphous silicon dust waste. Much of the recent research effort to produce solar cell grade silicon has thus focused on electrochemical reduction of silica in molten salts –at 850°C , or metallo-thermic reduction of silicon compounds. Among them, the magnesio-thermic reduction method above 650°C was well-known.

The preparation of crystalline silicon using other silicon precursors has also been reported. Among them, the synthesis of nanometer-sized silicon crystals by reducing SiCl_4 with metal sodium in a nonpolar organic solvent at high temperature (385°C) and high pressure (> 100 atmospheres) was reported.

To our knowledge, no studies have been conducted on electrochemical sodium reduction to obtain crystalline silicon using one step process at

temperature less than 180°C and in nitrogen atmosphere with a pressure of less than 1 atm. Moreover, this method does not involve silicon precursor gas purification that is necessary to all above-stated industrial processes. The silicon preparation carried out at low temperature may effectively reduce amounts of impurities from side reactions and containers.

2.11 The Diode Characteristics

- When a diode is Zero Biased no external energy source is applied and a natural Potential Barrier is developed across a depletion layer which is approximately 0.5 to 0.7v for silicon diodes and approximately 0.3 of a volt for germanium diodes.
- When a junction diode is Forward Biased the thickness of the depletion region reduces and the diode acts like a short circuit allowing full current to flow.
- When a junction diode is Reverse Biased the thickness of the depletion region increases and the diode acts like an open circuit blocking any current flow, (only a very small leakage current).
- Semiconductors contain two types of mobile charge carriers, “Holes” and “Electrons”.
- The holes are positively charged while the electrons negatively charged.

- A semiconductor may be doped with donor impurities such as Antimony (N-type doping), so that it contains mobile charges which are primarily electrons.
- A semiconductor may be doped with acceptor impurities such as Boron (P-type doping), so that it contains mobile charges which are mainly holes.
- The junction region itself has no charge carriers and is known as the depletion region.
- The junction (depletion) region has a physical thickness that varies with the applied voltage.

We have also seen above that the diode is two terminal non-linear device whose I-V characteristic are polarity dependent as depending upon the polarity of the applied voltage, V_D the diode is either *Forward Biased*, $V_D > 0$ or *Reverse Biased*, $V_D < 0$. Either way we can model these current-voltage characteristics for both an ideal diode and for a real silicon diode.

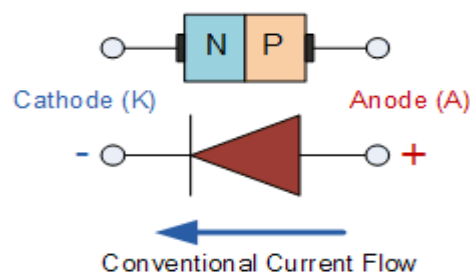


Figure 2.5 the Diode Characteristics

2.12 The Diode Resistance

Resistance is the opposition offered to the flow of current through the device. Hence, diode resistance can be defined as the effective opposition offered by the diode to the flow of current through it. Ideally speaking, a diode is expected to offer zero resistance when forward biased and infinite resistance when reverse biased. However, no device can ever be ideal. Thus, practically speaking, every diode is seen to offer a small resistance when forward biased, and a considerable resistance when reverse biased. One can characterize the given diode regarding its forward and reverse resistances.

2.13 Forward Resistance

Even after forward biasing, the diode will not conduct until it reaches a minimum threshold voltage level. After the applied voltage exceeds this threshold level, the diode starts to conduct. We refer the resistance, offered by the diode under this condition as the forward resistance of the diode. That is, the forward resistance is nothing but the resistance offered by the diode when the diode is working in its forward biased condition.

Forward resistance is classified into two type's viz., static or dynamic depending on whether the current flowing through the device is DC (Direct Current) or AC (Alternating Current), respectively.

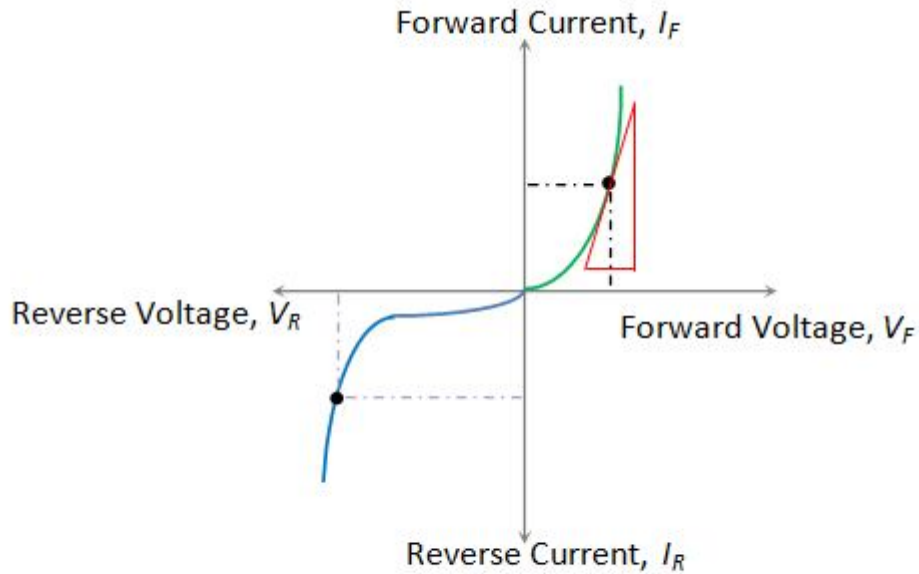


Figure 1 Diode resistance shown as a part of diode characteristics

2.14 Static or DC Resistance

It is the resistance offered by the diode to the flow of DC through it when we apply a DC voltage to it. Mathematically the static resistance is expressed as the ratio of DC voltage applied across the diode terminals to the DC flowing through it

$$R_{dc} = \frac{V_{dc}}{I_{dc}} \quad (3.3)$$

2.15 Dynamic or AC Resistance

It is the resistance offered by the diode to the flow of AC through it when we connect it in a circuit which has an AC voltage source as an active circuit element. Mathematically the dynamic resistance is given as the ratio of change in voltage applied across the diode to the resulting

change in the current flowing through it. This is shown by the slope-indicating red solid lines in Figure 1 and is expressed as

$$r_{ac} = \frac{V_{ac}}{i_{ac}}(3.4)$$

2.16 Reverse Resistance

When we connect the diode in reverse biased condition, there will be a small current flowing through it which is called the reverse leakage current. We can attribute the cause behind this to the fact that when the diode functions in its reverse mode, it will not be completely free of charge carriers. That is, even in this state, one can experience the flow of minority carriers through the device. Due to this current flow, the diode exhibits reverse resistance characteristic which is shown by the purple dotted line in Figure 1. The mathematical expression for the same is similar to that for the forward resistance and is given by

$$R_r = \frac{V_r}{I_r} \quad (3.5)$$

2.17 Electrical properties of solids in solid state chemistry:

Electrical properties of solids are measured in terms of conductivity. Conductivity may be defined as the ease with which electric current can pass through a given substance. All solids do not conduct electricity in equal amounts. Some of them have high conductivity, whereas some of them do not conduct electricity at all. On the basis of conduction of electricity, solids can be broadly divided into three categories:

2.18 Conductors:

Conductors are the solids that allow easy passage of electric current through them. Metals are generally good conductors of electricity. Electrical conductivity in metals is due to the presence of mobile electrons. The conductivity of metals is of the order of $10^7(\Omega\text{m})^{-1}$. There is no gap between the conduction band and the valence band. Thus electrons can easily flow from the valence band to the conduction band under the influence of electric field, making them good conductors of electricity.

2.19 Semiconductors:

The gap between the conduction band and the valence band is very less; therefore whenever sufficient energy is provided to the electrons in a semiconductor, electrons jump from the valence band to the conduction band. The conductivity of the semiconductors increases with an increase in temperature, for semiconductors, it lies in between 10^{-6} to $10^{-4}(\Omega\text{m})^{-1}$. There are two types of semiconductors:

2.19.1 Intrinsic semiconductor:

When heat is provided to the semiconductors, sometimes they eject electrons from their position leaving a positive hole behind them. The semiconductors can now conduct electricity because, on the application of electric field, electrons will now move in one direction and the holes in the opposite direction. These type of materials are known as undoped or intrinsic semiconductors. Example: Silicon, Germanium.

2.19.2 Extrinsic semiconductor:

Silicon and germanium generally have a low conductivity in their pure state at room temperature. To increase the conductivity of the semiconductors small

amount of impurity is added to the semiconductor (group 13 and group 15 elements). This process of adding the impurities to improve the conductivity of semiconductors is known as doping and the semiconductors are referred to as extrinsic semiconductors or doped semiconductors.

2.20 Insulators:

These materials do not conduct electricity. The band gap between the valence band and conduction band is very large. Even if a large amount of energy is provided to these solids, they do not conduct electricity. Example: Wood, plastics etc.

This was just a brief layout of electrical properties of solids and its classification on the basis of electrical conductivity. To know more about the solids and their properties please download BYJUS the learning app.

2.21 The Band Theory

Band theory derives these bands and band gaps by examining the allowed quantum mechanical wave functions for an electron in a large, periodic lattice of atoms or molecules. Band theory has been successfully used to explain many physical properties of solids, such as electrical resistivity and optical absorption, and forms the foundation of the understanding of all solid-state devices (transistors, solar cells, etc.).

According to the band theory, semiconductors will actually act as insulators at absolute zero. Above this temperature and yet still staying below the melting point of the solid, the material would act as a semiconductor. Semiconductors are classified by the fully occupied valence band and unoccupied conduction band. With the small band gap in between these two bands, it takes a certain amount of energy to excite the electrons from the valence to conduction band. Thus it follows that the higher the temperature.

2.22 Valence Band

It is defined as the band of energy where all of the valence electrons reside and are involved in the highest energy molecular orbital.

2.23 Conduction Band

It is defined as the band energy where positive or negative mobile charge carriers exist. Negative mobile charge carriers are simply electrons that had enough energy to escape the valence band and jump to the conduction band. Here, they move freely throughout the crystal lattice and are directly involved in the conductivity of semiconductors. Positive mobile charge carriers are also referred to as holes. Holes refer to the lack of an electron in the conduction band. In other words, a hole refers to the fact that within the band there is a place where an electron can exist (i.e. negative mobile charge carrier), and yet the electron ceases to exist at that particular location. Because the electron has the *potential* to be there and yet *isn't* there, it is referred to as positive mobile charge carrier.

2.24 The State Function

Function of state is a function defined for a system relating several *state* variables or state quantities that depends only on the current equilibrium state of the system. For example a gas, a liquid, a solid, crystal, or emulsion. State functions do not depend on the path by which the system arrived at its present state. A state function describes the equilibrium state of a system and thus also describes the type of system. For example, a state function could describe an atom or molecule in a gaseous, liquid, or solid form; a heterogeneous or homogeneous mixture; and the amounts of energy required to create such systems or change them into a different equilibrium state. (Callen, 1985)

For example, internal energy, enthalpy, and entropy are state quantities because they describe quantitatively an equilibrium state of a thermodynamic system, irrespective of how the system arrived in that state. In contrast, mechanical work and heat are process quantities or path functions, because their values depend on the specific *transition* (or path) between two equilibrium states. Heat in certain discrete amounts can describe a certain state function, such as enthalpy, but in general, does not truly describe the system unless it is defined as the state function of a certain system, and thus enthalpy is described by an amount heat. This can also apply to entropy when heat is compared to temperature. The mode of description breaks down for quantities exhibiting hysteresis effects. (Mandl, 1988)

2.25 The Fermi Level:

The Fermi level chemical potential for electrons (or electrochemical potential for electrons), usually denoted by μ or E_F ,^[1] of a body is a thermodynamic quantity, whose significance is the thermodynamic work required to add one electron to the body (not counting the work required to remove the electron from wherever it came from). A precise understanding of the Fermi level—how it relates to electronic band structure in determining electronic properties, how it relates to the voltage and flow of charge in an electronic circuit—is essential to an understanding of solid-state physics.

the Fermi level can be considered to be a hypothetical energy level of an electron, such that at thermodynamic equilibrium this energy level would have a 50% probability of being occupied at any given time. The position of the Fermi level with the relation to the band energy levels is a crucial factor in determining electrical properties. The Fermi level does not necessarily correspond to an actual energy level (in an insulator the Fermi level lies in the band gap), nor does it require the existence of a band structure. Nonetheless, the Fermi level is a precisely

defined thermodynamic quantity, and differences in Fermi level can be measured simply with a voltmeter. (*Kittel, Charles, 1998*)

2.26 Fermi Level Referencing and the Location of Zero Fermi Level

Much like the choice of origin in a coordinate system, the zero point of energy can be defined arbitrarily. Observable phenomena only depend on energy differences. When comparing distinct bodies, however, it is important that they all be consistent in their choice of the location of zero energy, or else nonsensical results will be obtained. It can therefore be helpful to explicitly name a common point to ensure that different components are in agreement. On the other hand, if a reference point is inherently ambiguous (such as "the vacuum", see below) it will instead cause more problems.

A practical and well-justified choice of common point is a bulky, physical conductor, such as the electrical ground or earth. Such a conductor can be considered to be in a good thermodynamic equilibrium and so its μ is well defined. It provides a reservoir of charge, so that large numbers of electrons may be added or removed without incurring charging effects. It also has the advantage of being accessible, so that the Fermi level of any other object can be measured simply with a voltmeter.

2.27 The Fermi Level and Temperature

The Fermi level, μ , and temperature, T , are well defined constants for a solid-state device in thermodynamic equilibrium situation, such as when it is sitting on the shelf doing nothing. When the device is brought out of equilibrium and put into use, then strictly speaking the Fermi level and temperature are no longer well defined. Fortunately, it is often possible to define a quasi-Fermi level and quasi-temperature for a given location, that accurately describe the occupation of states

in terms of a thermal distribution. The device is said to be in *quasi-equilibrium* when and where such a description is possible.

In some situations, such as immediately after a material experiences a high-energy laser pulse, the electron distribution cannot be described by any thermal distribution. One cannot define the quasi-Fermi level or quasi-temperature in this case; the electrons are simply said to be *non-thermalized*. In less dramatic situations, such as in a solar cell under constant illumination, a quasi-equilibrium description may be possible but requiring the assignment of distinct values of μ and T to different bands (conduction band vs. valence band). Even then, the values of μ and T may jump discontinuously across a material interface (e.g., p–n junction) when a current is being driven, and be ill-defined at the interface itself.

2.28 Bonding Models

Atoms or ions in minerals are glued together by electrical bonds that are ionic, covalent, or metallic. The types and intensities of these bonds in a mineral determine its physical and chemical properties, including hardness, cleavage, and conductivity

2.29 Ionic Bonding Model

Atoms have a tendency to achieve a completely filled valence shell like the inert gases. Metals like sodium tend to lose electrons to achieve full valence shells, and nonmetals like chlorine tend to gain electrons. The process of gaining or losing electrons creates ions, and electrostatic forces bring the ions together to form compounds. For example, sodium may lose an electron to chlorine to create Na^+ and Cl^- , and the

Coulombic attraction between the resulting ions makes NaCl, or table salt. The attraction between the oppositely charged ions constitutes the ionic bond. {7}

2.30 Covalent Bonding Model

Whereas atoms exchange electrons to achieve a full valence shell in ionic bonds, they share electrons in covalent bonds because neither atom has a strong tendency to give them up completely. For example, when an atom of chlorine bonds with another atom of chlorine, the result is an overlap of the atoms' electron clouds that simultaneously fills the valence shells of both atoms. Covalent bonds are expressed symbolically with Lewis notation, in which valence electrons appear as dots surrounding an atom.

2.31 Metallic Bonding Model

Minerals like native gold and silver have properties that cannot be explained in terms of ionic or covalent bonds. For example, the malleability and electrical conductivity of either metal cannot be readily explained by the localized sharing or complete transfer of electrons. Instead, the bonding electrons in native metals like gold and silver are modeled as highly delocalized and free to move from one atom to the next. The electrons compose a mobile electron glue that keeps the positively charged metal ions from flying apart. {8}

2.32 Dipole-dipole Bonds

When the bond between atoms is neither perfectly ionic nor perfectly covalent, shared electrons are located closer to the more electronegative atom. This asymmetric distribution of electrons makes the bond polar and the molecule has a dipole moment. In HCl, for example, the more electronegative chlorine atom has a partial negative charge (δ^-) and the hydrogen atom has a partial positive (δ^+) charge.

2.33 Vander Waals Bonds

Gases such as O_2 , N_2 , and the inert gases all have crystalline forms at very low temperatures even though their molecules are not polar. This results from van der Waals bonds. Van der Waals bonds are electrostatic bonds between atoms or molecules that result from instantaneous asymmetric charge distributions in the atoms and molecules.

2.34 Hydrogen Bonds

A hydrogen bond is a special type of dipole-dipole bond between a positive hydrogen ion and a negative ion like O_2^- . Because the hydrogen ion is an unshielded proton, it can get very close to negative ions or the negative ends of polar molecules and create strong intermolecular bonds. These bonds are considerably stronger than van der Waals bonds. The best known example of hydrogen bonds is the attraction between hydrogen and oxygen among molecules of water.

The Energy Band Model -Metal, Semiconductor, Insulator

Band formation:

The energy band model can be explained using the molecular orbital theory. Solids are regarded as aggregations of an almost infinite number of atoms. The linear combination and overlap of N atomic orbitals in a solid leads to N molecular orbitals, which are closely spaced in energy and spread over the whole crystal (energy band). An almost continuous band of energy levels is formed. The molecular orbitals are not allowed to have the same energy (Hund's rule). The 1s-band is separated (not for all solids, the band may also overlap) from the 2s-band by a band gap. In a band gap no molecular orbital occur. The width of a band gap depends on the energy-difference of the atomic orbitals and the strength of interactions between the crystal atoms. A band consists of countable number of near-continuum energy levels. There is only a narrow spread of orbital energies.

2.35 Fermi level

The highest occupied orbital at $T = 0\text{K}$ is called the Fermi level.

Densities of states

2.36 The Density of States (DOS)

is defined as the quantity of energy levels in an energy range divided by the range's width. It is not uniform across a band. The energy levels may be more closely or less closely.

2.37 Conductivity of Metals

In metals the valence band overlap with the next higher band (e.g. for alkaline earth metals) or a not fully occupied band exists (e.g. for alkaline metals). Electrons can travel in unoccupied energy levels. There is a decrease of electrical conductivity with increasing temperature. Increasing vibration of atoms with increasing temperature leads to an increasing number of collisions between electrons and atoms.

2.38 Conductivity of Semiconductors

The electrical conductivity increases with increasing temperature.

2.39 Intrinsic Semiconductors (band gap 1-3 eV)

The band gap between the empty conduction band and the full valence band is so small that electrons can populate the empty upper band by slight thermal excitation. The absence of electrons in the valence band introduces positive charges.

2.40 Extrinsic Semiconductors (impurity semiconductors):

They are intentionally doped with impurities. The doping is substitutional, the dopant atom takes the place of the host atom. n-type semiconductors: Host material doped with an element with more valence electrons than the host element. The doping material supply electrons to the conduction band. The filled donor band is commonly near the empty conduction band. (electron conduction).

p-type semiconductors: Host material doped with an element with less valence electrons than the host element. Doping atoms form an empty acceptor band lying above the full valence band of the host material. Electrons of the host material occupy this band and electron gaps in host material are formed. Conductivity because of migration of positive holes in the valence band (hole conduction).

2.41 Conductivity of Insulators:

The valence band is completely filled, while the conduction band is empty. The band gap is higher than 3 eV (e.g. NaCl: 7 eV, Diamond: 5.5 eV). A thermal excitation of electrons in the conducting band is difficult or not possible.

Chapter Three

Material and Method

3.1 Introduction

Silicon and germanium are commonly used as semiconductor materials in solid state electronic devices such as diodes, transistors, integrated circuits, these two elements distinguishes by filled valence band and empty conduction band and small energy gap between them. In case of low temperature, heating isn't enough to transfer electrons to conduction band thus these materials behave as insulators. And by increasing temperature, heating provide energy to electrons to transfer to conduction band and this materials called conductors. Semi-conductors are used in an experiment to know the density of a status function according to a valence band with an increase in temperature.

3.2 materials

Electric heater, clamps, connecting wires, sand, voltmeter for measuring the voltage, Ammeter for measuring electric current.

3.3 Method

The diode (silicon)was connected to the clamps and through connecting wires the voltmeter and Ammeter were connected with the diode and electric current, to protect the diode from damage and burn external resistor was connected as show in plant.

- putted in a container then silicone diode inserted into sand, current and voltage wasmeasured at room temperature to investigate the I-V characteristic..
- I-V characteristic also recorded with varying temperature step 10 up to 240⁰c

- Density of state function calculated according to valence band with aid of equation (4.1):

$$N_V = 2 \left(2\pi \frac{m_p kT}{h^2} \right)^{\frac{3}{2}} \quad (4.1)$$

- The relation between temperature (T_C) was explained and status function density (N_V) was explained from equation (4.1).
- And valence band value has been calculated using this formula

$$R_T = R_0 e^{-E_g/2kT} \quad (4.2)$$

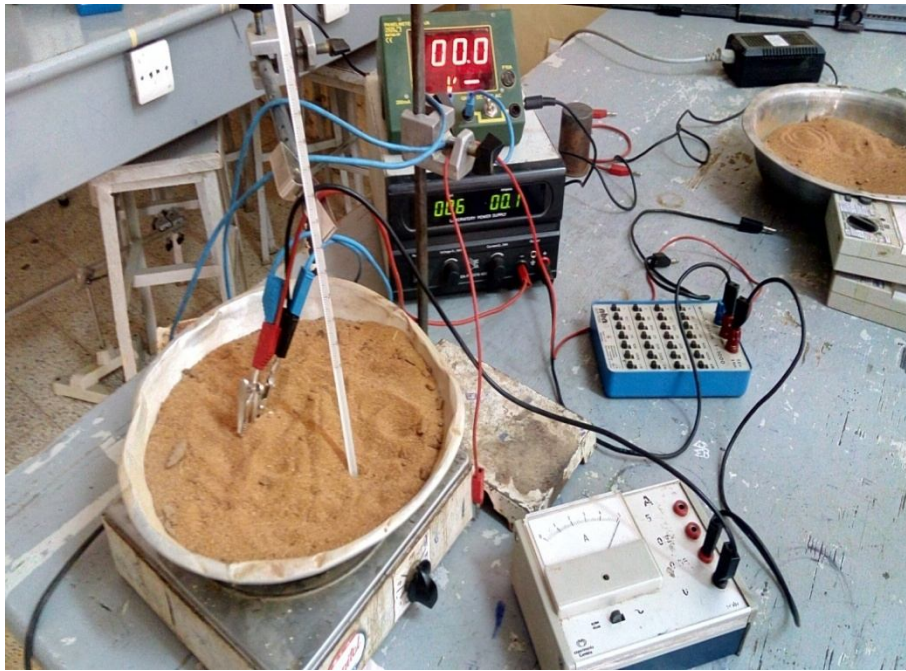


Figure (4.1) shows experimental set up

Chapter Four

The Table Result and Dissection

4.1 Result

Table (4.1) shows the result obtained I-V characteristic versus temperature

T_c	I_A	V	$P=IV$ m_w	R $=V/I$	$N_V = 2 \left(2\pi \frac{MpkT}{h^2} \right)^{\frac{3}{2}}$	$L_n(R_T)$	$\frac{1}{T}$
30	6	0.67	4.02	111	8.97×10^{31}	4.7	3.3
40	6	0.63	3.87	105	21.2×10^{31}	4.65	3.19
50	6	0.61	3.66	101	41.5×10^{31}	4.61	309
60	6	0.61	3.66	101	71.7×10^{31}	4.61	3
70	6	0.58	3.48	96	113×10^{31}	4.56	2.9
80	6	0.55	3.3	91	190×10^{31}	4.51	2.8
90	6	0.53	3.1	88	242×10^{31}	4.47	2.75
100	6	0.51	3.01	85	323×10^{31}	4.44	2.68
110	6	0.50	3	83	442×10^{31}	4.41	2.61
120	6	0.49	2.94	81	574×10^{31}	4.39	2.54
130	6	0.46	2.76	79	729×10^{31}	4.44	2.48
140	6.5	0.45	2.92	69	911×10^{31}	4.23	2.42
150	6.5	0.44	2.86	67	1120×10^{31}	4.2	2.36
160	6.5	0.43	2.79	66	1360×10^{31}	4.13	2.3
170	6.8	0.43	2.92	63	1630×10^{31}	4.14	2.25
180	6.9	0.42	2.89	60	1930×10^{31}	4.09	2.2
190	6.9	0.41	2.82	59	2270×10^{31}	4.07	2.15
200	7	0.40	2.8	57	2650×10^{31}	4.04	2.11

4.2 Discussion:

From results of table (4.1) it was obvious the I-V characteristic reveals semiconductors made of silicone which explained in figure (4.1).

Figure (4.2) shows the I-V characteristic at different temperature ranged from (30 up to 200)C⁰. It was found that the current maintains constant value for a period time at 6mA during temperature change from (30-130), and then increases (6.5-7) when the temperature increased (from 140 to 200) while the voltage's increases as shown in the previous.

The relation between the power ($p=IV$) and temperature, shown in figure (4.3) realized decreasing in regular rates for power with the increasing of temperature which means that the dissipated power decreases (from 4.02 to 2.8) mW due to increases in temperature.

Figure (4.5) shows the change of the diode resistance R versus temperature TC⁰ it was clear that reduction of resistance value with increase of temperature in a full agreement with theoretical consideration.

Figure (4.5) shows the probability density of states the versus temperature TC⁰ from which one can conclude that $N_v \sim T^{\frac{3}{2}}$

Finally energy gap has been calculated from figure (4.6) by fitting the curve and was found to be $E_g = 0.89175 \text{ eV}$.

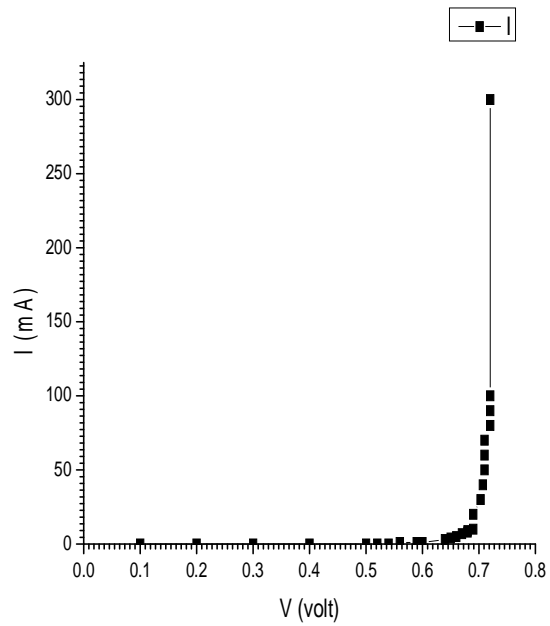


Figure (4.1) shows the I-V characteristic at room temperature 26°C

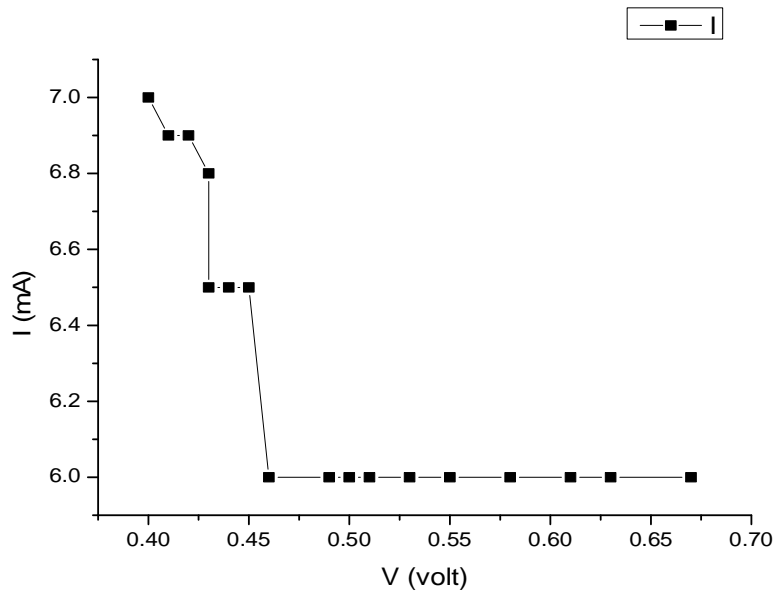


Figure (4.2) shows the I-V characteristic at different temperature ranged from (30 up to 200) $^{\circ}\text{C}$

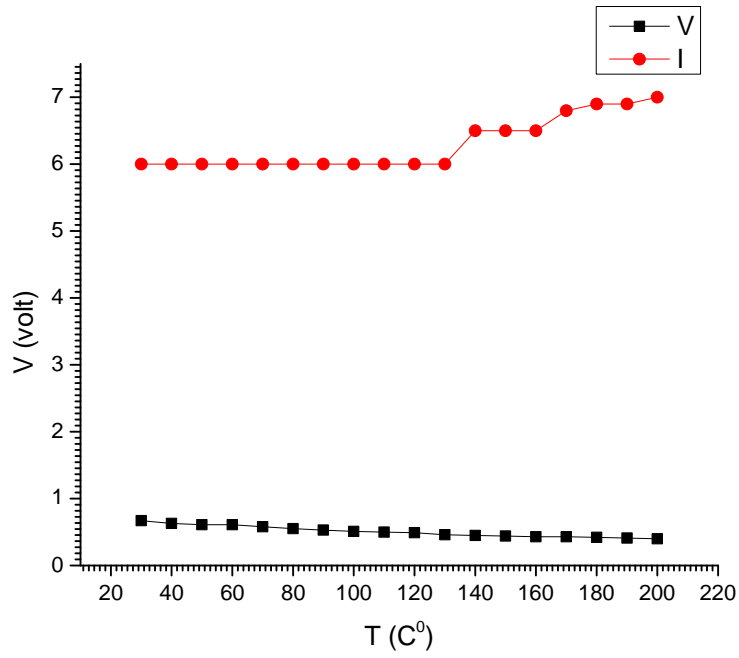


Figure (4.3) shows the I-V characteristic versus temperature TC⁰

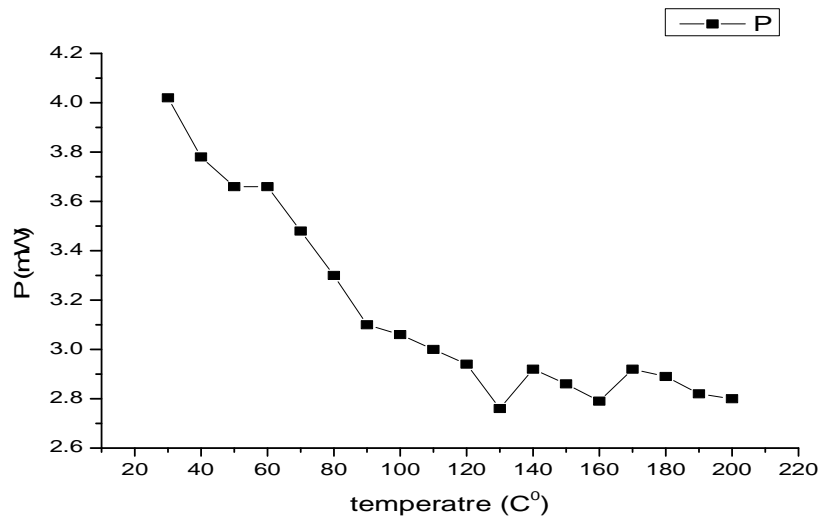


Figure (4.4) shows the power dissipated by diode versus temperature TC⁰

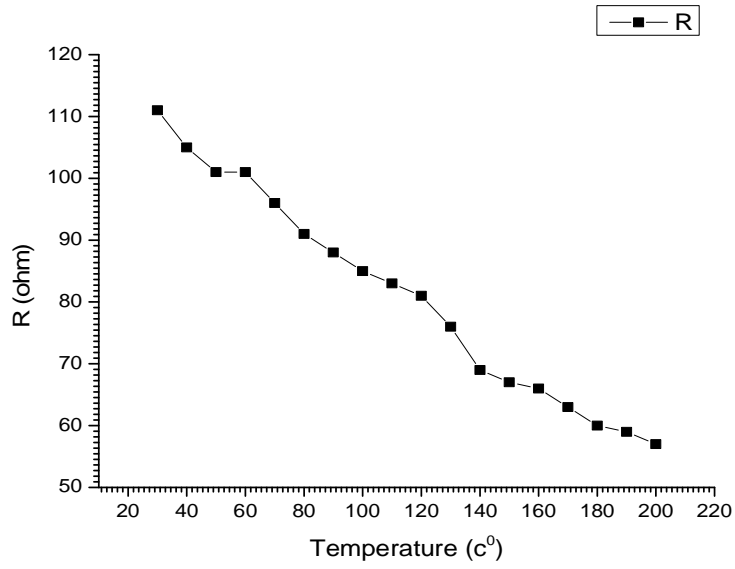


Figure (4.5) shows the change of the diode resistance R versus temperature TC^0

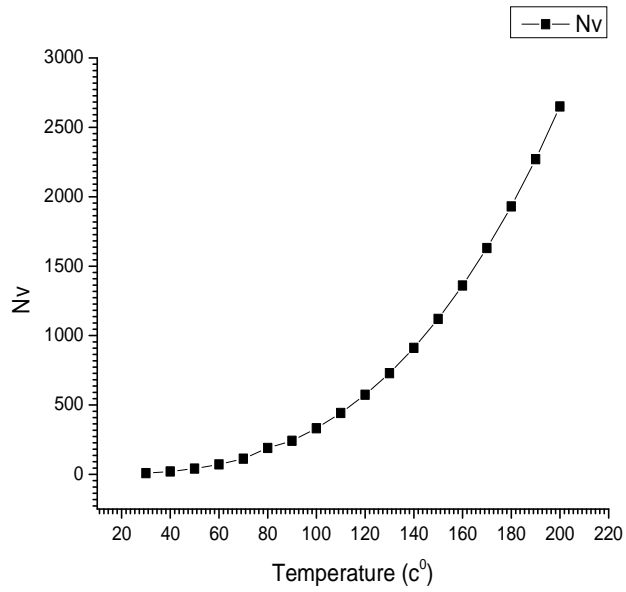


Figure (4.5) shows the probability density of states the versus temperature TC^0

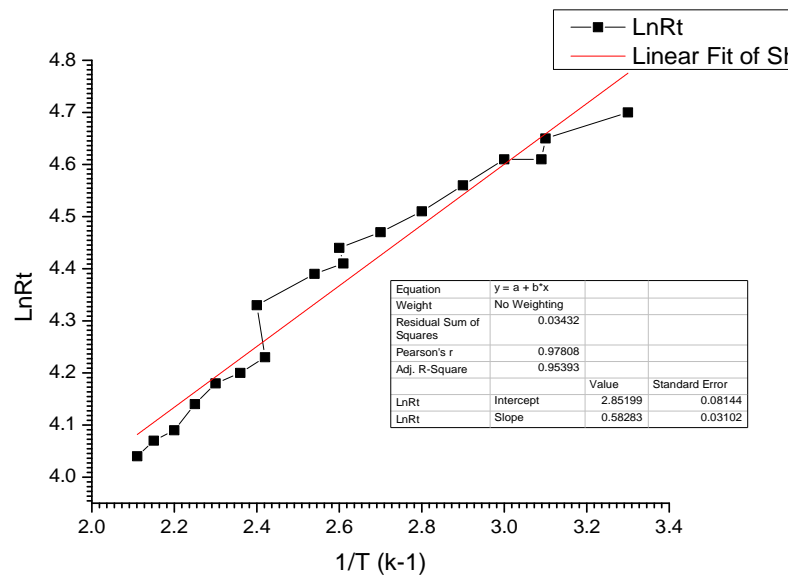


Figure (4.6) shows $\text{Ln}R_T$ versus temperature $1/T$ (K^{-1})

4.3 Conclusion:

It was concluded that through the graphs which illustrated the relationship between the intensity of the status function and temperature $N_v \sim T^{\frac{3}{2}}$ as prescribed in theoretical consideration.

Also energy gab obtained is considerably $E_g = 0.89175 \text{ eV}$ while the theoretical value is 0.7 eV.

4.4 Recommendation:

1. Semiconductors must be available because they are used in all electrical circuits that provide us with everything new in this field.
2. Accurate devices such as voltmeter and Ampermeter must be available.
3. Diodes(germanium)are cheap so must be available in the laboratory.
4. The accuracy of the connection must be observed to get good results.
5. The study of status function density according to valence band give us opportunity to create new electrons devices suit with a various bodies temperature depending on the type of using to contribute in society development in all industrial,economical,technical fields.

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