



ADDIS ABABA UNIVERSITY

COLLEGE OF NATURAL AND COMPUTATIONAL SCIENCE

DEPARTMENT OF PHYSICS

**Boltzmann Transport Equation for Degenerate Electron Gas in
semiconductor in the Presence of Electric Field**

By

Desalegn Mulugeta

**A PROJECT SUBMITTED TO DEPARTMENT OF PHYSICS IN PARTIAL
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ADDIS ABABA UNIVERSITY
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DEPARTMENT OF PHYSICS

The undersigned hereby certify that they have read and recommend to the College of Natural Sciences for acceptance a project entitled "Boltzmann Transport Equation for Degenerate Electron Gas in semiconductor in the Presence of Electric Field" by Desalegn Mulugeta in partial fulfillment of the requirements for the degree of Master of Science in Physics(Statistical Physics).

Advisor:

Dr.Yitagesu Elfagd

Examiners:

1. Dr.Lemi Demeyu
2. Dr.Kenate Nemera

ADDIS ABABA UNIVERSITY

Date: February 6, 2022

Author: Desalegn Mulugeta

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ABSTRACT

The effect created by the applied electric field and temperature gradient on the electrons in a semiconductor is to change the distribution function of electrons from its equilibrium condition. In the absence of external fields, the distribution of electrons in a semiconductor under equilibrium conditions may be described by the Fermi-Dirac distribution function. Thus, the effects created by applied electric field as well as the temperature gradient on electron transport in a n-type Silicon were discussed in this project. The Boltzmann transport equation was solved by applying the relaxation time approximation method in the presence of electric field to obtain a general expression for Fermi-Dirac distribution function for the degenerate electron gas in doped semiconductor material. Employing the results of solved Boltzmann transport equation, the expression was derived for electron mobility and electron conductivity. The results of the study were described numerically, graphically and qualitatively. In the integral equation of electron concentration n , it is difficult to evaluate because the normalized Fermi energy E_F is unknown. Thus, by using iteration method for a given arbitrary value, the integral equation was evaluated mathematically using a Mathematica 5.1 software program and the results we got were in agreement with those in the literature. From the numerical computation we observed that; the Fermi energy increases exponentially with increasing electron concentration, conductivity increases linearly with increasing electron density and mobility decreases with the dopant density.

1 Introduction

1.1 Background of the study

There is no doubt that semiconductors changed the world beyond anything that could have been imagined before them. The modern information technology and the electronic product depends on tremendous progress in the technology of semiconductor device in the past half century, and marvelously changed our daily lives and the whole world itself. The use of these devices has advantages relative to the carrier transport, mainly due to the reduction of surface roughness scattering and the lower vertical electric field. Moreover, the introduction of new materials, intrinsic materials to reduce phonon scattering, Coulomb scattering and to enhance the mobility, as the strained silicon, the intrinsic silicon channel, can result in electronic transport approaching the ballistic regime [1]. By adding the right kind of dopants it is possible to make semiconductor materials, n-type materials and p-type materials. If such impurities contribute a significant fraction of the conduction band electrons and /or valance band holes, one speaks of an extrinsic semiconductors.

Measurements of conductivity in silicon have been reported by different journals. The transport properties in bulk silicon have been studied in great detail. Precise knowledge of the transport properties is important, as in applications with large drift distances, e.g. radiation sensors, even small uncertainties in the drift velocities can have noticeable effects [2]. Hence over the last three decades, there has been considerable focus on an understanding on the physics of transport parameters of which charge-carrier mobility (μ) has been the most studied. To improve the electronic properties of doped semiconductor requires knowledge concerning the mechanism by which carriers are generated and transported. So there have been many attempts to deduce the shape of the density of state and to develop a theoretical frame-work to understand their properties. Using some particular assumptions on the charge carrier transport in semiconductor materials are characterized by such transport coefficients [3].

The carrier mobility in Silicon has been deeply investigated since 1950 [4] and charge transport models are able to simulate the dependence of the carrier mobility on temperature and impurity concentration up to a carrier concentration of above 10^{19} at./cm^3 . At high doping level, a dependence of the carrier mobility on the chemical dopant species becomes evident. In particular,

the electron mobility is lower for As than P doped Si and the hole mobility is lower for Ga than B doped Si . Several authors attempted to explain the different mobility in P and as doped Si introducing impurity-core effect in the calculations but the modification is too weak to account for the experimental results [5].

The number of semiconductor materials that are today studied and employed by the electronic industry is very large and continuously increasing, in particular after the introduction of semiconductor heterostructures. These are semiconductors in which the pure state of the semiconductor material is deliberately diluted by adding very minute quantities of impurities. To be more specific, the impurities are known as dopants or doping agents. This implies that, if suitable impurities are added to the semiconductors, controlled conductivity can be provided. Some examples of semiconductors are silicon, germanium, carbon etc. [6] Semiconductors materials are materials at the heart of many electronic devices, such as transistors, switches, diodes, photovoltaic cells, etc. Silicon is widely used now a day with several applications in light emitting diodes, semiconductor lasers, microwaves lasers, and others specialized areas.

The conductivity of electrons is the most important parameter for characterizing the transport characteristics in the semiconductor devices. A great deal of attention has been paid to this parameter and many considerable efforts have also been focused on theoretical models of carrier mobility in semiconductor. The success of this models largely depends on the proper formulation of different types of scattering mechanisms and one must know which type of scattering mechanisms are predominant in a particular material under the prevalent condition of temperature and carrier concentration [7].

The electron conductivity strongly depends on the values of electron drift mobility as a function of temperature and electron (carrier) concentration. In this paper, we will limit ourselves to the most popular materials called silicon. Because, Silicon may be considered as the information carrier of our times. In the history of information there were two revolutions (approximately 500 years apart). The first was that of Johan Gutenberg who made information available to many, the other is the invention of the transistor [8]. Currently the global amount of information doubles every year. Many things we are taking for granted (such as, e.g., computers, Internet and mobile phones) would not be possible without silicon microelectronics.

In this work, the relationship between Fermi energy, electrical conductivity and the electron concentration were shown. We shall deal with the processes taking place under the influence of applied electric fields. we present the main building block of our work which is the general overview of the electron transport properties in doped n-type semiconductor devices. Silicon is by far the most used material in semiconductor industry, both because of its large availability and because of the existence of a natural oxide, very suitable for the realization of electronic devices. Hopefully, the analysis of some transport coefficients will enable the reader to understand the main electronic transport properties of n-type semiconductor materials (silicon).

1.2 Organization

The rest of this work is organized in five Chapters. In Chapter two, we present the general overview of the electron transport properties in doped semiconductor devices, which was the main building block of our work. We briefly discussed some transport coefficients that are the key parameters governing the transport properties associated with the effects in a doped n-type Silicon semiconductor are derived from the current solution of Boltzmann transport equation (BTE) using the relaxation time approximation in the presence of electric field. The methodology is presented in Chapter three. The results of numerical calculation are analyzed and discussion of the results was presented in Chapter 4. The effects created by the applied electric electric as well as the temperature gradient in a semiconductor are discussed. In the final part (Chapter 5), conclusion for this work are presented in brief and understandable way.

2 Transport Properties of Electron in Semiconductors Materials

There are several possible theoretical approaches to transport phenomena. The equations for electron transport coefficients in n-type Silicon semiconductor under the influence of applied external fields are presented in this chapter. The most widely used were the method of Boltzmann's transport equation, which can be employed to calculate the carrier mobility, the electrical conductivity, and other transport coefficients representing the behavior of a semiconductor when it is subjected to external forces. The key parameters governing the transport properties of a semiconductor (silicon) was discussed here in this section. From the standpoint of device applications, the carrier density and the carrier mobility are the parameters of greatest importance.

To the extent that electrons can be considered as particles, the electrical conductivity, the electronic contribution to the thermal conductivity and the magnetoresistance are all found by solving the Boltzmann equation. Thus, a solution of the modified Boltzmann transport equations applying the relaxation time approximation in the presence of electric field is found, which describes features of the charge transport in semiconductor to obtain the distribution function of the degenerate free electron gas in heavily doped n-type silicon [9]. Some transport coefficients in a semiconductor are therefore derived from the Boltzmann transport equation using the relaxation time approximation. The isotropic part of the distribution function was assumed to be the Fermi-Dirac distribution Function and the constant energy surface in K-space are assumed to be ellipsoidal. The effect of an applied electric field or temperature gradient on the electrons in a semiconductor is to change the distribution function of electrons from its equilibrium condition [10].

2.1 Electron Density of States

In doped semiconductor devices, the description of carriers depends on a large number of parameters such as effective mass m^* , impurity concentrations, dielectric constants, and energy band gap E_g . Ionization energy, impurity concentration, as well as some other parameters are determined by semiconductor statistic interdependences of the free minority carrier concentrations. Semiconductor statistics describes the probabilities of carrier states either at vacant or populated states [11]. Impurity states have single states with no degeneracy in the simplest case. However, it may need to be considered that an impurity may have a degenerate ground state as well as excited levels.

The density of state (DOS) describes the states of carriers in the bands and their dependence on energy. The free motion of carriers is confined to three, two, or one spatial dimensions in semiconductor devices [12]. DOS in above spatial dimensions must be known before applying semiconductor statistics to such systems of reduced dimensions. In bulk semiconductor carriers occupy either localized impurity states or delocalized continuum states in conduction or valence bands. The density of impurity states equals to the concentration of impurities, when impurity forms a single, non-degenerate state. When the impurities are sufficiently far apart, where coupling can be neglected, the energy of the impurity states is the same for all impurities. On the other hand, the density of continuum states is more complicated.

2.2 Effective Mass

A simple analytic band approximation can be described by the relationship between the K-space and m^* . The effective mass m^* plays a fundamental role in several physical problems of different nature: the electron group velocity, in a crystal subject to an external force, the electron density of states in energy space, the ratio of non-parabolicity parameter. The role of effective mass m^* in the different situations may not be the same when the band is not described by the simple parabolic band. For this reason, different types of effective mass m^* have been defined in different journals. In reality, an electron in a crystal experiences complex forces from the ionized atoms. We imagine that the atoms in the linear chain form the electrical periodic potential. If the free electron mass m is replaced by the effective mass m^* , we can treat the motion of electrons in the conduction band as free electrons [13].

2.3 Density of State Effective Mass in Degenerate Semiconductor

We shall define first the density of state in a given semiconductor material (silicon) to find the general expression of electron concentration n farther to calculate the conductivity and mobility for the discussion of the electrical properties of semiconductor. The system under consideration is n-type silicon. There are six equivalent constant energy ellipsoids for electron in silicon. The wave vector variation dK which is determined associated with energy variation dE is integrated over the entire constant energy surface to obtain the volume of K-space enclosed between two constant energy surfaces with energies between E and dE . Most actual band structures for semiconductors have ellipsoidal energy surfaces which require longitudinal and transverse effective masses in place of the three principal effective masses. Thus, the constant energy surfaces are rotational ellipsoids and two of the main axis of the ellipsoid are identical (i.e. $m_x \neq m_y = m_z$) [14].

If the mass are denoted as m_l and m_t for the longitudinal and transversal, respectively, the density of state per unit energy can be expressed as

$$N(E)dE = \frac{(2m_l m_t^2)^{1/2}}{\pi^2 \hbar^3} \left(E - E_c \right)^{1/2} dE \quad (1)$$

as carriers require a volume of $4\pi^3$ in phase space.

Now the density of states $g(E)$ can be calculated from the volume between E and dE in k-space divided by the volume of a single state in k-space.

$$g(E) = \frac{1}{2\pi^2} \left(\frac{2m_d^*}{\hbar} \right)^{3/2} (E - E_c)^{1/2} \quad (2)$$

where

$$m_d^* = (m_x m_y m_z)^{1/3}$$

which is called the density of states effective mass, and m_x , m_y , and m_z are the principal effective masses in the x, y and z directions.

2.4 Electron Concentration

If the probability that a state with energy E will be occupied states, the electron concentration in thermal nonequilibrium is expressed as:

$$n(E) = \int_0^\infty f(E)g(E)dE \quad (3)$$

where the function $f(E)$ is the temperature-dependent occupation probability in thermal nonequilibrium. In thermal equilibrium, this function will be the Fermi-Dirac distribution $f_o(E)$ and it becomes unity at absolute zero when energy E is less than Fermi-energy E_F , and zero when E is greater than E_F .

For electron occupation of the conduction band, Fermi-faction $f(E)$ can be expressed as:

$$f(E) = \frac{1}{\exp\left(\frac{E-E_F}{K_B T}\right) + 1} \quad (4)$$

where E_F is the Fermi energy:

Since the conduction band of silicon contains six equivalent ellipsoids of resolution, the total density of state (equation 2) in the bottom of conduction band (at $E_c = 0$) can be expressed as

$$g(E) = \frac{8\sqrt{2}}{\hbar^3} \pi m_n^{*3/2} (E)^{1/2} \quad (5)$$

The density of state function given by equation (5) doesn't incorporate the effects of band tails. Since the impurity distribution in an extrinsic semiconductor is not uniform, the statistical average over the entire lattice of the density of the states function shows tailing into the energy gap. Thus, the bands are no longer parabolic.

For density of states having band tails, Kane [5] has shown that if the variation in local electrostatic potential is sufficiently slow, the average density of states function for conduction band is expressed as

$$g(Z) = \frac{m_n^{*3/2} 2^{3/4} \delta^{1/2}}{\pi^2 \hbar^3} y(z) \quad (6)$$

where we have replaced a new variable $y(z)$ as forwarded by Kane [5] is given by

$$y(z) = \frac{1}{\pi^{1/2}} \int_{-\infty}^z (z - \xi)^{1/2} \exp(-\xi) d\xi \quad (7)$$

In this expression, the variable z implies the dimensionless energy expressed as

$$z = \frac{E}{\sqrt{2}\delta} \quad (8)$$

δ is the standard deviation of a Gaussian distribution function for impurity potential energy which is expressed as [15]

$$\delta = \left(\frac{2\pi N_d \lambda e^4}{16\pi^2 \epsilon_0 \kappa^2} \right)^{1/2} \quad (9)$$

where λ is the Thomas-Fermi screening length and κ is the dielectric constant of the specimen.

The equation for number of electron concentration for the density of state function that doesn't incorporate the effects of band tails is obtained by substituting equations (4) and (5) in to (3), we get

$$n(E) = \int_0^\infty \frac{1}{\exp\left(\frac{E-E_F}{K_B T}\right) + 1} \left(\frac{8\sqrt{2}}{\hbar^3} \pi m_n^{*3/2} E^{1/2} \right) dE \quad (10)$$

To make it easy to normalize, equation 4 can be written as

$$n = \left[\frac{8\sqrt{2}}{\hbar^3} \pi m_n^{*3/2} \right] \int_0^\infty \frac{E^{1/2}}{\exp\left(\frac{E-E_F}{K_B T}\right) + 1} dE \quad (11)$$

The density of states function given by equation (6) is so complicated that one can not use it to make any useful calculations. Thus, to avoid these complications, I used the the normalized equation for equation (11) suggested by Slotboom [14] in the numerical calculation given by

$$n_n = \frac{n}{10^{24}/m^3} \quad (12)$$

We assume in the numerical calculation (in section 3) that the total mobile electron concentration in the conduction band is equal to donor concentration N_d .

2.5 Fermi Energy in Degenerate Semiconductors

In semiconductors, we usually have $\frac{E-E_F}{K_B T} \gg 1$, and then $\exp\left(\frac{E-E_F}{K_B T}\right)$ becomes much greater than 1.

Therefore, equation (4) will become

$$f(E) = \frac{1}{\exp\left(\frac{E-E_F}{K_B T}\right) + 1} = \exp\left(-\frac{E-E_F}{K_B T}\right) \quad (13)$$

The electron concentration n in equilibrium from Equation (11) is

$$n = \frac{1}{2\pi^2} \left(\frac{2m_n^*}{\hbar^2}\right)^{3/2} \int_0^\infty E^{1/2} \exp\left(\frac{E_F - E}{K_B T}\right) dE \quad (14)$$

In single band, the electron concentration n is reduced to (this is known as the Boltzmann approximation)

$$n = N_v 2 \left(\frac{m_n^* K_B T}{2\pi \hbar^2}\right)^{3/2} \exp\left(\frac{E_F}{K_B T}\right) \quad (15)$$

where N_v is the degeneracy (number of bands or valleys having the same band edge energy and the same wave vector).

Solving for E_F , we have

$$E_F = K_B T \ln \left(\frac{n}{2N_v} \left(\frac{m_n^* K_B T}{2\pi \hbar^2} \right)^{-3/2} \right) \quad (16)$$

Assuming that every atom contributes one free electron to the conduction band and neglecting thermally excited electrons from the valence band, we used this equation to determine the Fermi energy of an n-type Si semiconductor doped with phosphorus with a given electron concentration n at temperature T farther to find some transport coefficients. Si has six identical conduction bands with an effective mass equal to $0.33 m_0$, where m is the free electron mass.

2.6 Boltzmann Transport Equation

The Boltzmann Transport Equation (BTE) is carrier-based because it is derived by careful consideration of carrier inflow and outflow. The carrier motion is described as a series of free flights that are decided by scattering rates. We solve the Boltzmann's transport equation (BTE) in presence of electric to obtain the isotropic part of the electron distribution function. Because, the calculation of isotropic part of electron distribution function which determines the magnitude of

the macroscopic current density is the central problem of any transport theory.

The Boltzmann transport equation is a statement that in the steady state, there is no net change in the distribution function $f(\vec{r}, \vec{k}, t)$ which determines the probability of finding an electron at position $\vec{r}$, crystal momentum $\vec{k}$ and time t . Considering the deformation due to the time dependence of $\vec{r}$ and $\vec{k}$ and using only the first term of a Taylor expansion we get [16]:

$$\frac{\partial f}{\partial t} + \frac{\partial \vec{r}}{\partial t} \cdot \vec{\Delta}_r f + \frac{\partial \vec{k}}{\partial t} \cdot \vec{\Delta}_k f = \left(\frac{\partial f}{\partial t} \right) \Big|_c \quad (17)$$

In steady state (state in which $\frac{\partial f}{\partial t} = 0$), the Boltzmann equation becomes

$$\left(\frac{\partial f}{\partial t} \right) \Big|_c = \frac{\partial \vec{r}}{\partial t} \cdot \vec{\Delta}_r f + \frac{\partial \vec{k}}{\partial t} \cdot \vec{\Delta}_k f \quad (18)$$

where

$$\frac{\partial \vec{k}}{\partial t} = \frac{d\vec{F}}{\hbar} = \frac{q}{\hbar} \left[\vec{E} + \frac{1}{c} (\vec{v} \times \vec{B}) \right] \quad (19)$$

Here $\vec{E}$ and $\vec{B}$ are the external dc electric and magnetic field, respectively and $\vec{v} = \frac{d\vec{r}}{dt} = \frac{1}{\hbar} \vec{\Delta}_k \varepsilon$ is group velocity of the electron wave packet (ε is the kinetic energy of electrons).

The first term in equation (17) gives the explicit time dependence of the distribution function and is needed for the solution of ac driving forces or for impulse perturbations. It consists in a powerful way to describe systems which is out of thermodynamic equilibrium. Generally, it involves the diffusion or transport of mass, energy or charge that makes the system evolve towards its equilibrium configuration, providing a suitable formalism to calculate a number of properties of a given physical system, such as thermal and electrical conductivities, diffusion coefficients, etc. That makes it a major tool for statistical physics, whose applicability ranges from the microscopic scale up to cosmological domains. The relaxation time approximation plays an important role in a number of methods to solve the Boltzmann equation [17].

2.6.1 Solution of Boltzmann Transport Equation in Relaxation Time Approximation

A great simplification of the BE is obtained by the assumption that the collision integral can be put in the form in this relaxation time approximation. When high electric field is applied to semiconductors, the energy of carriers will be far from the minimum energy with parabolic

band so that effective mass approximation is not suitable. However, the $E_k - K$ relation can be used with non-parabolic band correction by applying non-parabolicity parameter α . Boltzmann's equation is usually solved using two approximations [18]:

1. The perturbation due to external fields and forces is assumed to be small so that the distribution function can be linearized and written as

$$f(\vec{r}, \vec{k}) = f_0(E) + f_1(\vec{r}, \vec{k}) \quad (20)$$

where $f_0(E)$ is the equilibrium distribution function (the Fermi function) which depends only on the energy E , while $f_1(\vec{r}, \vec{k})$ is the perturbation term giving the departure from equilibrium.

2. The collision term in the Boltzmann equation is written in the **relaxation time approximation** so that the system returns to equilibrium uniformly [19]

$$\left. \frac{\partial f}{\partial t} \right|_c = -\frac{f - f_0}{\tau} \quad (21)$$

where τ denotes the relaxation time which depends only on collision process and not on the external field, f is the total deformation distribution function and f_0 is unperturbed distribution function.

Up on performing the differentiations we have

$$\frac{\partial f_0}{\partial \varepsilon} + \vec{v} \cdot \vec{\nabla}_r f_1(\vec{k}, \vec{r}) + \frac{q}{\hbar} \vec{E} \cdot \vec{\nabla}_k f_1(\vec{k}, \vec{r}) + \frac{q}{\hbar c} (\vec{v} \times \vec{B}) \cdot \vec{\nabla}_k f_1(\vec{k}, \vec{r}) = \frac{-f_1(\vec{k}, \vec{r})}{\tau} \quad (22)$$

The relaxation time follows a Poisson distribution indicating that collisions relax the distribution function exponentially to f_0 with a time constant τ . With these approximations, the Boltzmann equation is solved to find the distribution function which in turn determines the number density and current density.

Substituting equation (21) in to the steady state BTE which describes the transport of electrons under the influence of external fields takes the form:

$$\frac{\partial \vec{r}}{\partial t} \cdot \vec{\Delta}_r f + \frac{\partial \vec{k}}{\partial t} \cdot \vec{\Delta}_k f = -\frac{f - f_0}{\tau} \quad (23)$$

2.7 The electrical current density in Degenerate Semiconductor

Current is defined as the time rate at which charge is transported across a given surface in a direction normal to it, the current will depend on both number of charges free to move and the speeds at which they move. To begin with we shall calculate the current density associated with a single ellipsoid, which we shall assume to be symmetric about the x-axis. The electrical current density is given by [20]

$$J = -q \int_{Cb}^{\infty} v(k)g(k)f(k)d^3k \quad (24)$$

where $g(k)$ is the total density of states in k-space, $f(k)$ is the distribution function given by

$$f(k) = f_0 + q\tau E_x v \frac{\partial f_0}{\partial E} \quad (25)$$

$v(k)$ is the group velocity in k-space, d^3k is the volume element in k-space and C_b indicates that the integration is over the whole conduction band.

Equation (24) can be written as

$$J = -\frac{2q}{(2\pi)^3} \int v f(k) d^3k \quad (26)$$

Since no current flows in equilibrium, f_0 does not contribute to the electric field current. Therefore, substituting equation 20 in to equation (26), we obtain

$$J = \frac{-2q^2}{(2\pi)^3} E \int \tau v_k^2 \frac{df_0}{d\varepsilon} d^3k \quad (27)$$

Since we have applied the electric field along the x-direction, only the x-component of electric current density is finite and is

$$J_x = \frac{-2q^2}{(2\pi)^3} E_x \int \tau v_x^2 \frac{df_0}{d\varepsilon} d^3k \quad (28)$$

Using the relation

$$n = \frac{2}{(2\pi)^3} \int f_0 d^3k \quad (29)$$

For electron moving under applied electric field, we can write the electrical conductivity in terms of the conductivity tensor as

$$\vec{j}_x = \sigma_x \cdot \vec{E}_x \quad (30)$$

Equation (28) is written as

$$J_x = -q^2 n E_x \frac{\int \tau v_x^2 \frac{df_0}{d\varepsilon} d^3k}{\int f_0 d^3k} \quad (31)$$

From the relation $f_0(\varepsilon) = \frac{1}{e^{\varepsilon - \varepsilon_F / K_B T} + 1}$, we have

$$\frac{\partial f_0(\varepsilon)}{\partial \varepsilon} = \frac{-1}{K_B T} f_0(1 - f_0) \quad (32)$$

Therefore, equation (31) becomes

$$J_x = \frac{q^2 n E_x}{K_B T} \frac{\int \tau v_x^2 f_0(1 - f_0) d^3k}{\int f_0 d^3k} \quad (33)$$

Since the term $\tau(1 - f_0)$ in the integral of (33) is a function of the energy ε , we express it as $\phi(\varepsilon)$

and it is true that $\int v_x^2 \phi(\varepsilon) d^3k = \int v_y^2 \phi(\varepsilon) d^3k = \int v_z^2 \phi(\varepsilon) d^3k = \frac{1}{3} \int v^2 \phi(\varepsilon) d^3k$

We have

$$J_x = \frac{q^2 n E_x}{3 K_B T} \frac{\int \tau v^2 f_0(1 - f_0) d^3k}{\int f_0 d^3k} \quad (34)$$

The integral with respect to d^3k is changed in to an integral with respect to ε by using the relation

$\varepsilon = \frac{\hbar^2 k^2}{2m^*}$, we obtain

$$d^3k = 4\pi k^2 dk = \frac{8\pi m^{*3/2}}{\sqrt{2}\hbar^3} \varepsilon^{1/2} d\varepsilon \quad (35)$$

Therefore equation (34) will be

$$J_x = \frac{q^2 n E_x}{3 K_B T} \frac{\int_0^\infty \tau v^2 \varepsilon^{1/2} f_0(1 - f_0) d\varepsilon}{\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon} \quad (36)$$

Using $v = \frac{\hbar k}{m^*}$ and $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$, we get

$$J_x = \frac{2q^2 n E_x}{3 K_B T m^*} \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0(1 - f_0) d\varepsilon}{\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon} \quad (37)$$

Although the upper limit of the integral should be the upper edge of the band, it is replaced by infinity, taking account of the exponential decay of the distribution function in the higher energy region.

In case of **Degenerate Semiconductor**, the Fermi energy ε_F is located in the conduction band, and the term $-df_0/d\varepsilon = f_0(1 - f_0)/K_B T$ has a large value near the Fermi energy only.

Therefore, the term $-df_o/d\varepsilon$ may be approximated by the Dirac δ -function.

In addition, the following relations,

$$f_o \cong 1 \quad \varepsilon \leq \varepsilon_F,$$

$$f_o \cong 0 \quad \varepsilon > \varepsilon_F$$

hold for the Fermi distribution function, and therefore we obtain

$$\frac{1}{K_B T} \int_0^\infty \tau(\varepsilon) \varepsilon^{3/2} f_o(1 - f_o) d\varepsilon = - \int_0^\infty \tau(\varepsilon) \varepsilon^{3/2} \frac{df_o}{d\varepsilon} d\varepsilon \cong \tau(\varepsilon_F) \varepsilon_F^{3/2} \quad (38)$$

$$\int_0^\infty \varepsilon^{1/2} f_o d\varepsilon = \int_0^{\varepsilon_F} \varepsilon^{1/2} d\varepsilon = \frac{2}{3} \varepsilon_F^{3/2} \quad (39)$$

Inserting these relations into equation (37), we obtain

$$J_x = \frac{ne^2 \tau(\varepsilon_F)}{m^*} E_x \quad (40)$$

where $\tau(\varepsilon_F)$ is the relaxation time of an electron at $\varepsilon = \varepsilon_F$ (or at the Fermi surface).

The relation between the Fermi energy ε_F and the electron density n will becomes

$$\varepsilon_F = \frac{\hbar^2}{2m^*} (3\pi^2 n)^{2/3} \quad (41)$$

2.8 Electrical conductivity in Heavily Doped n-type Semiconductor

Electrical conduction is transport processes resulting from the motion of charge carriers under the action of internal or external field. Conduction of electron in an n-type silicon is the one in which the conductivity is due to the excess electrons. Current is defined as the time rate at which charge is transported across a given surface in a direction normal to it, the current will depend on both number of charges free to move and the speeds at which they move. Electrical conduction takes place as a result of the motion of the free electrons under the action of an applied electric field.

The current density is defined as flow of charges per area per unit time. The electrical conductivity σ is a material constant which connects the component of electrical current density J

with the electrical field strength E . Actually, the conductivity s is not strictly constant but it rather depends on different parameters like temperature and the impurity concentrations.

For the second term in the Boltzmann equation (18), $\vec{v}(\vec{k}) \cdot f(\vec{r}, \vec{k}, t) / \partial \vec{r}$, we note that

$$\frac{\partial f}{\partial \vec{r}} \simeq \frac{\partial f_0}{\partial \vec{r}} = \frac{\partial f_0}{\partial T} \frac{\partial T}{\partial \vec{r}} \quad (42)$$

For the third term in equation (18), which we write as

$$\dot{\vec{k}} \cdot \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial \vec{k}} = \sum_{\alpha} \dot{k}_{\alpha} \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial k_{\alpha}} \quad (43)$$

where the right hand side shows the summation over the vector components, we do get a contribution, since the equations of motion ($F = ma$) gives

$$\hbar \dot{\vec{k}} = e \vec{E} \quad (44)$$

and

$$\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial \vec{k}} = \frac{\partial f_0 + f}{\partial \vec{k}} = \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial \vec{k}} + \frac{\partial f_1}{\partial \vec{k}} \quad (45)$$

In considering the linearized Boltzmann equation, we retain only the leading terms in the perturbing electric field, so that $\partial f_1 / \partial \vec{k}$ can be neglected and only the term $(\partial f_0 / \partial E) \hbar \vec{v}(\vec{k})$ need be retained. We thus obtain the linearized Boltzmann equation for the case on an applied electric field and no thermal gradients:

$$\dot{\vec{k}} \cdot \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial \vec{k}} = \frac{\phi \partial f_0}{\tau \partial E} = \frac{-f_1}{\tau} \quad (46)$$

In order to show the $\partial f_0 / \partial E$ dependence explicitly, it is convenient to write:

$$f_1 = -\phi \frac{\partial f_0}{\partial E} \quad (47)$$

Substituting equations (23) and (46) into equation 46 yields

$$f_1 = \left[\frac{e \vec{E}}{\hbar} \frac{\partial f_0}{\partial E} \right] \cdot \left[\hbar \vec{v}(\vec{k}) \right] = \frac{\phi(\vec{k})}{\tau} \left(\frac{\partial f_0}{\partial E} \right) \quad (48)$$

so that

$$\phi(\vec{k}) = e\tau \vec{E} \cdot \vec{v}(\vec{k}) \quad (49)$$

Thus we can relate $\phi(\vec{k})$ to $f_1(\vec{k})$ by

$$f_1(\vec{k}) = -\phi(\vec{k}) \frac{\partial f_0(E)}{\partial E} = -e\tau \vec{E} \cdot \vec{v}(\vec{k}) \frac{\partial f_0(E)}{\partial E} \quad (50)$$

The current density is then found from the distribution function $f(\vec{k})$ by calculation of the average value of $\langle ne\vec{v} \rangle$ over all k-space

$$\vec{j} = \frac{1}{4\pi^3} \int e \vec{v}(\vec{k}) f(\vec{k}) d^3k = \frac{1}{4\pi^3} \int e \vec{v}(\vec{k}) f_1(\vec{k}) d^3k \quad (51)$$

since

$$\frac{1}{4\pi^3} \int e \vec{v}(\vec{k}) f_0(\vec{k}) d^3k = 0 \quad (52)$$

Equation (51) states that no net current flows in the absence of an applied electric field, another statement of the equilibrium condition.

Substitution for $f_1(\vec{k})$ given by equation (50) into (51) for $\vec{j}$ yields

$$\vec{j} = \frac{-e^2 \vec{E}}{4\pi^3} \cdot \int \tau \vec{v} \vec{v} \frac{\partial f_0}{\partial E} d^3k \quad (53)$$

where in general $\tau = \tau(\vec{k})$ and $\vec{v} = \frac{\hbar \vec{k}}{m^*}$.

A comparison of equations (41) and (53) thus yields the desired result for the conductivity tensor σ

$$\sigma = \frac{-e^2}{4\pi^3} \cdot \int \tau \vec{v} \vec{v} \frac{\partial f_0}{\partial E} d^3k \quad (54)$$

where σ is a symmetric second rank tensor $\sigma_{ij} = \sigma_{ji}$.

The evaluation of the integral in equation (54) over all k-space depends on the $E(\vec{k})$ relations through the $\vec{v} \vec{v}$ terms and the temperature dependence comes through the $\partial f_0 / \partial E$ term.

To get the general expression for electrical conductivity in the presence of electric field strength, equation (53) can be written as

$$J_x = \left[\frac{16\sqrt{2}\pi e^2 m_n^{*1/2} E_x \tau^3 (K_B T)^{3/2}}{\hbar^3} \right] \int_0^\infty \frac{\epsilon^2 d\epsilon}{1 + \exp(\epsilon - \epsilon_f)} \quad (55)$$

From the general relation of $J_x = \sigma_x E_x$, we have

$$\sigma_x = \frac{J_x}{E_x} \quad (56)$$

Using equations (50) and (55), we get

$$\sigma_x = \left[\frac{2ne^2\tau_0}{\int_0^\infty \frac{(E)^{1/2}}{1+\exp(\epsilon-\epsilon_f)} d\epsilon} \right] (m_n^{*1/2}) \int_0^\infty \frac{\epsilon^2 d\epsilon}{1+\exp(\epsilon-\epsilon_f)} \quad (57)$$

The dimensionless electrical conductivity is given by

$$\sigma_x^d = \left[\frac{2ne^2\tau_0}{m_n^*} \right] \frac{\int_0^\infty \frac{\epsilon^2 d\epsilon}{1+\exp(\epsilon-\epsilon_f)}}{\int_0^\infty \frac{(\epsilon)^{1/2}}{1+\exp(\epsilon-\epsilon_f)} d\epsilon} \quad (58)$$

2.8.1 Electrical Conductivity in Isotropic Parabolic Density of State

By writing the electrical conductivity as a product of the carrier density with the mobility, it is easy to contrast the temperature dependence of conductivity for semiconductors. We shown in this section that, the simple Drude model ($\sigma = ne^2\tau/m^*$) can also be recovered for a semiconductor from the general relation given by equation (56), using a simple parabolic band model and a constant relaxation time. When a more complete theory is used, departures from the simple Drude model will result.

In deriving the Drude model for a semiconductor we make three approximations:

(i). **Approximation #1**

In the case of electron states in intrinsic semiconductors having no donor or acceptor impurities, we have the condition $(E - E_F) \gg k_B T$ since E_F is in the band gap and E is the energy of an electron in the conduction band.

Thus, the first approximation is equivalent to writing

$$f_0(E) = \frac{1}{1 + \exp\left((E - E_F)/k_B T\right)} \simeq \exp\left(-(E - E_F)/k_B T\right) \quad (59)$$

which is equivalent to using the Maxwell-Boltzmann distribution in place of the full Fermi-Dirac

distribution. Since E is usually measured with respect to the bottom of the conduction band, E_F is a negative energy and it is therefore convenient to write $f_0(E)$ as

$$f_0(E) \simeq e^{-|E_F|/K_B T} e^{-E_F/K_B T} \quad (60)$$

so that the derivative of the Fermi function becomes

$$\frac{\partial f_0(E)}{\partial E} = -\frac{e^{-|E_F|/K_B T}}{K_B T} e^{-E_F/K_B T} \quad (61)$$

(ii). **Approximation #2**

For simplicity we assume a constant relaxation time τ independent of $\vec{k}$ and E . This approximation is made for simplicity and is not valid for specific cases. Some common scattering mechanisms yield an energy dependent relaxation time such as acoustic deformation potential scattering or ionized impurity scattering where $r = -1/2$ and $r = +3/2$ respectively in the relation $\tau = \tau_0(E/K_B T)^r$.

(iii). **Approximation #3**

To illustrate the explicit evaluation of the integral in equation (58), we consider the simplest case, assuming an isotropic, parabolic band $E = \hbar^2 k^2 / 2m^*$ for the evaluation of $v = \hbar k / m^*$ about the conduction band extrema. Using this approximation we can write

$$\begin{aligned} k^2 &= 2m^* E / \hbar^2 \\ 2k dk &= 2m^* dE / \hbar^2 \\ v^2 &= 2E / m^* \end{aligned}$$

We next convert equation (58) to an integration over energy and write

$$d^3 k = 4\pi k^2 dk = 4\pi \sqrt{2} (m^* / \hbar^2)^{3/2} \sqrt{E} dE \quad (62)$$

so that equation (58) becomes

$$\sigma = \frac{e^2 \tau}{4\pi^3} \left(\frac{8\sqrt{2\pi\sqrt{m^*}}}{3\hbar^3 k_B T} \right) e^{-|E_F|/k_B T} \int_0^\infty E^{3/2} dE e^{-E/k_B T} \quad (63)$$

in which the integral over energy E is extended to ∞ because there is negligible contribution for

large E and because the definite integral

$$\int_0^\infty x^p dx e^{-x} = \Gamma(p+1) \quad (64)$$

can be evaluated exactly, $\Gamma(p)$ being the Γ function which has the property

$$\Gamma(p+1) = p\Gamma(p) \quad (65)$$

Substitution into equation (63), yields

$$\sigma = \frac{2e^2\tau}{m^*} \left(\frac{\sqrt{m^*}k_B T}{2\pi\hbar^2} \right)^{3/2} e^{-|E_F|/k_B T} \quad (66)$$

which gives the temperature dependence of σ .

Now the carrier density calculated using the same approximations becomes

$$\begin{aligned} n &= \frac{1}{4\pi^3} \int f_0(E) d^3k = \frac{1}{4\pi^3} e^{-|E_F|/k_B T} \int e^{-E/k_B T} 4\pi k^2 dk \\ &= (\sqrt{2}/\pi^2) (m^*/\hbar^2)^{3/2} e^{-|E_F|/k_B T} \int_0^\infty \sqrt{E} dE e^{-E/k_B T} \end{aligned} \quad (67)$$

where $\int_0^\infty \sqrt{E} dE e^{-E/k_B T} = \frac{\sqrt{\pi}}{2} (k_B T)^{3/2}$ which gives the final result for the temperature dependence of the carrier density

$$n = \left(\frac{m^* K_B T}{2\pi\hbar^2} \right)^{3/2} e^{-|E_F|/k_B T} \quad (68)$$

so, by substitution into equation (66), the Drude formula is recovered

$$\sigma = \frac{ne^2\tau}{m^*} \quad (69)$$

for a semiconductor with constant τ and isotropic, parabolic dispersion relations.

This implies that in the absence of magnetic field, conductivity, mobility, and concentration are related by $\sigma = nq\mu$.

To find conductivity for a semiconductor with more than one spherical carrier pocket, the conductivities per carrier pocket are added

$$\sigma = \sum_i \sigma_i \quad (70)$$

where i is the carrier pocket index. We use these simple formulae to make rough estimates for the carrier density and conductivity of semiconductors. For more quantitative analysis, the details of the $E(\vec{k})$ relation must be considered, as well as an energy dependent τ and use of the complete Fermi function. The electrical conductivity and carrier density of a semiconductor with one carrier type exhibits an exponential temperature dependence so that the slope of $\ln \sigma$ vs $1/T$ yields an activation energy.

2.9 Electron Scattering Mechanism in n-type semiconductor

There are different scattering mechanisms like acoustic phonon scattering, ionized impurity scattering, carrier-carrier scattering among others responsible for the resistivity of the material. Conwell and Weisskopf [9] have calculated the rate of change of distribution function due to ionized impurity scattering by using the following assumptions:

- (a). In the electron ionized impurity scattering only the direction of electrons changes
- (b). An electron gets scattered by a single ion at a time i. e. by the one which is closest to it at that particular instant of time.

Therefore, the number of electrons per unit volume per second into a solid angle $d\Omega'$ at polar angle θ' , and ϕ' can be expressed as:

$$N f(u, \theta, \Omega) \sigma(\theta, \theta') u d\Omega \quad (71)$$

where N is the number of electron per unit volume, $N f(u, \theta, \Omega) d\Omega$ is the number of electrons per unit volume with solid angle $d\Omega$ and $\sigma(\theta, \theta')$ is the Rutherford scattering cross-section given by.

$$\sigma(\theta, \theta') = \left(\frac{ze^2}{8\pi\epsilon_0\epsilon_d} \right)^2 \frac{1}{\sin^4(\theta - \theta')/2} \quad (72)$$

The Conwell and Weisskopf [9] formula for ionized impurity relaxation time is:

$$\tau = \tau_0 \left(\frac{E}{K_B T} \right)^{3/2} = \tau_0 \epsilon^{3/2} \quad (73)$$

Where ϵ is the dimensionless kinetic energy. Among various scattering mechanisms responsible for resistivity in the temperature range $100 - 800^\circ K$ and for electron concentration $n \geq 10^{16}/m^3$ the ionized impurity scattering is the dominant scattering mechanism. We shall use the above

expression of relaxation time for ionized impurity scattering in subsequent sections to obtain the explicit expression for thermal conductivity.

2.9.1 Electron mobility in Doped n-type Silicon

Although carrier mobility (μ) in Si is a fundamental property deeply investigated since 40 years, a complete understanding of its characteristics over a large range of carrier concentration is still lacking. The mobility of electrons in silicon depends on many parameters. Some of them are the electric and magnetic field, temperature, carrier density etc. Among the transport properties of a semiconductor, a chief role is played by the carrier mobility. It indicates, in fact, the potentiality of the charge to move in the material and to respond to field changes. At higher mobilities, transit times and switching times are shorter, and frequency cutoffs are higher [22].

In describing the electrical conductivity of semiconductors, it is customary to write the conductivity from equation (69) as

$$J_x = \sigma_x E_x = \frac{ne^2 \langle \tau \rangle}{m^*} E_x \quad (74)$$

where σ_x is the electron conductivity of the semiconductor material (silicon) defined as

$$\sigma_x = \frac{J_x}{E_x} = \frac{ne^2 \langle \tau \rangle}{m^*} = nq\mu \quad (75)$$

where μ is mobility of electron and $\langle \tau \rangle$ is the average time between the scattering events (collisions) or the scattering rate (collision rate) given by

$$\langle \tau \rangle = \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0 d\varepsilon}{\int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon} \quad (76)$$

Among various scattering mechanisms responsible for resistivity in the temperature range 100 – 800⁰K and for electron concentration $n \geq 10^{16}/m^3$ the ionized impurity scattering is the dominant scattering mechanism. Using Boltzmann transport equation in relaxation time approximation, ionized impurity scattering mobility μ_I (the dominant impurity scattering mechanism in these ranges) is expressed as [9]

$$\mu_I = \frac{128\sqrt{2}\pi\epsilon^2(K_B T)^{3/2}}{ne^3\sqrt{m^*}} \quad (77)$$

This implies that the temperature dependence of mobility due to impurity scattering is $T^{+3/2}$.

2.9.2 Motion of electrons in Presence Electric Field

We begin with a discussion of the transport properties associated with free electron gas, since the model serves as a basis for understanding the electron transport behavior of normal semiconductors. Transport is the phenomenon of currents flowing in response to applied fields. The electric field E is interfered with two processes which are the electric current density j and the temperature gradient ∇T . The currents and fields are linearly related and it will be our goal to calculate the coefficients (known as transport coefficients) of these linear relations. Implicit in our discussion is the assumption that we are always dealing with systems near equilibrium.

Whenever the semiconductor is subjected to an external electric field, temperature and concentration gradient a non vanishing macroscopic current density arises. But, when a semiconductor is in uniform thermal equilibrium in the absence of external fields, the distribution of electrons over the eigenstates available to them in each region of the semiconductor is in accordance with the Fermi Dirac distribution function and the electric current density vanishes everywhere in semiconductor. Under the influence of these fields and gradients the equilibrium distributions of electrons in each region of semiconductor is then deformed and becomes isotropic because electron move from field states to adjacent empty states.

3 METHODOLOGY

For the purposes of this work, the symbolic mathematical computation program (Mathematica 5.1 software program) were used. It is sometimes called a computer algebra program used in many scientific, engineering, mathematical, and computing fields. It was conceived by Stephen Wolfram and is developed by Wolfram Research of Champaign, Illinois [23]. Mathematica is good at handling numerical work, widely used computational tool in data science and it is a perfect programming system. The most widely used was the method of Boltzmann's transport equation in relaxation time approximation to calculate some transport coefficients representing the behavior of a semiconductor when it is subjected to external forces.

This software was to compute the numerical values for some transport coefficients in n-type Silicon semiconductor under the influence of applied external fields in the method of Boltzmann transport equation, which can be employed to calculate the carrier mobility and the electrical conductivity as a function of electron concentration and temperature. The equations derived in part two for some transport coefficients were used. By inserting some known constant parameters, the transport properties of electron in a doped semiconductor at the variable electron concentration and temperature were discussed.

In general, Mathematica is a great tool for solving problems, because it integrates all functionalities you can imagine: symbolic calculations, sophisticated manipulation with equations, very good numerics, pretty graphical output. Although the classical free electron theory gave good results for electrical and thermal conductivities. These failure was eliminated by having the free electron obeys the Fermi-Dirac distribution. The ground state is state of the N electron system at absolute zero. What happens as the temperature is increased? The solution is given by the Fermi-Dirac distribution and all the result obtained by using this software were presented in next chapter.

4 RESULTS AND DISCUSSION

The effects created by the applied electric fields as well as the temperature gradient in a semiconductor are discussed in this chapter. The electric field E is interfered with two processes which are the electric current density j and the temperature gradient ΔT . We use the equations for transport coefficients in a semiconductor derived from the Boltzmann transport equation using the relaxation time approximation in part two.

The effect of an applied electric field or temperature gradient on the electrons in a semiconductor is to change the distribution function of electrons from its equilibrium condition. In the absence of external fields, the distribution of electrons in a semiconductor under equilibrium conditions may be described by the Fermi-Dirac distribution function equation (59). This equation shows that in thermal equilibrium the electron distribution function $f_0(E)$ depends not only on the electron energy but also on the Fermi energy E_F , a many-body parameter, and the temperature T .

4.1 Numerical Calculations and Discussion of Results

We shall first discuss the procedure to compute the dimensionless electrical conductivity and electron drift mobility as a function of electron concentration n which is in this work equal to the dopant density N_d in an n-type Si in the impurity concentration range approximately from 1×10^{16} to $1 \times 10^{21} \text{ cm}^{-3}$. I have used the Fermi level distribution function for electrons at the lower edge of the conduction band (when the dopant density N_d exceeds the effect level density N_c). Since this requires the knowledge of the Fermi energy E_F as a function of electron concentration n ($n = N_d$), the position of Fermi Energy were calculated first.

We use Equation (68), the normalized formula for electron concentration n_n for density of state having band tails.

Thus, Equation (68) can also be written as

$$n_n = \frac{m_n^{3/2} 2^{5/4} \delta^{3/2}}{10^{24} \pi^2 \hbar^3} \Psi_0 \cong N_d \quad (78)$$

where,

$$\Psi_0 = \frac{1}{2\pi^{1/2}} \int_{-\infty}^{0.601} \exp(-z^2) \left[\frac{0.319 + 0.906 \exp(2z)}{(1 + \exp(\frac{\sqrt{2}\delta}{K_B T} z - \eta))} \right] dz + \int_{0.601}^{+\infty} z^{1/2} \frac{(1 - \frac{1}{16z^2})}{1 + \exp(\frac{\sqrt{2}\delta}{K_B T} z - \eta)} dz$$

and η is dimensionless Fermi Energy $\frac{E_f}{K_B T}$.

The dimensionless electrical conductivity (σ_x^d) can be normalized as

$$\sigma_x^d = \frac{\sigma_x}{\frac{ne^2 \tau_0}{m_n^*}} \quad (79)$$

The integral of equation (78) for electron concentration n is difficult to evaluate because the normalized Fermi energy E_F is unknown. Therefore, by using iteration method in such a way that for a given arbitrary value of the left side of the integral in this equation can be evaluated by using a Mathematica 5.1 software program. In the calculation, we have used the constant values of various parameters including; $T = 300^0 K$ (to calculate the numerical value of conductivity as a function of number of electron concentration), $k_B = 1.38 \times 10^{-23} J/Kg$, $m_n^* = 1.18m_0$ where $m_0 = 9.11 \times 10^{-31} Kg$ and $\varepsilon = \frac{E}{K_B T}$.

The value of the normalized electron concentration obtained by this numerical calculation will be compared with the known initial value $n_n = 0.04628$. I continue my calculation until I get the precise value of the normalized Fermi energy E_F corresponding to the given normalized electron concentration $n_n = 0.04628$ at $300^0 K$.

This iteration method is used again to get the other values of the normalized Fermi energy (E_F) corresponding to the given electron concentration (n_n) in the table. These values are used to calculate dimensionless electrical conductivity (σ_x^d) corresponding to the given value of the normalized electron concentration as shown in the below table. We can see from the table (1) and from figure (1) below that, the normalized Fermi energy increases with increasing normalized dop-

Table 1: The dimensionless Fermi energy (E_F^d) and dimensionless electrical conductivity (σ_x^d) using the given value of normalized electron concentration (n_n).

n_n	E_F^d	σ_x^d
0.0462845	-4.23354	4.528399
0.12039	-3.26945	4.5527
0.1605	-2.97748	4.565182
0.240398	-2.56469	4.590962
0.5095	-1.80185	4.675266
0.750925	-1.36966	4.756477
1.0009	-1.05497	4.837995
1.50085	-0.59533	5.002002
2.008	-0.25354	5.167141
2.50075	0.0223557	5.33409
3.007	0.259635	5.50086
3.50065	0.46734	5.669359
4.0006	0.65422	5.838826
4.50055	0.825143	6.009266
5.0005	0.983438	6.180707
5.50045	1.131475	6.352981
6.0004	1.27101	6.526144
6.50035	1.403375	6.700136
7.0003	1.529607	6.874981
7.50025	1.65025	7.050141
8.0002	1.766795	7.226896
8.50015	1.878955	7.407064
9.0001	1.987462	7.581702
9.50005	2.092687	7.760182
10	2.19496	7.939213

ing concentration. The numerical values are used to draw the graph of normalized Fermi energy (E_F^d) vs normalized electron concentration (n_n) and to draw the graph of dimensionless electrical conductivity (σ_x^d) vs normalized electron concentration (n_n).

Figure (1) shown that the normalized Fermi energy increases exponentially as the doping concentration or the normalized electron concentration (n_n) increases. The negative sign means that the Fermi energy is below the conduction band edge. The silicon bandgap at room temperature is 1.12 eV. Thus, the Fermi energy is within the band gap. In fact, only in this case, the Boltzmann approximation we used in Equation (58) is applicable because the electron energy inside the conduction band, minus the Fermi energy, is much greater than $k_B T$ ($(E - E_F)/k_B T \gg 1$). If the Fermi energy is close to the band edge or falls inside the conduction band, which is the case when the semiconductors are heavily doped.

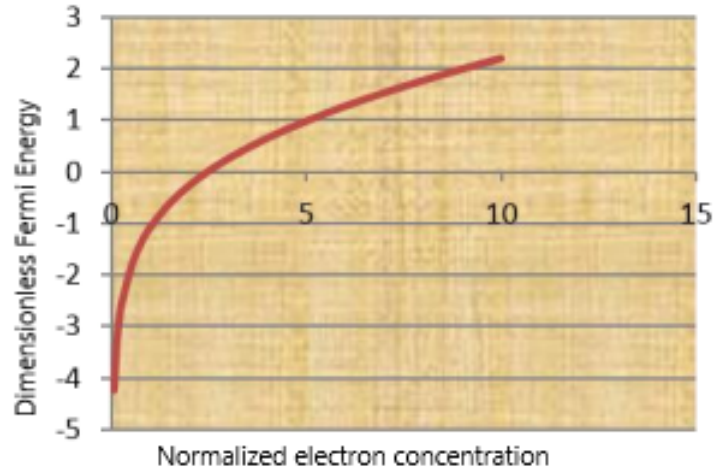


Figure 1: Dimensionless Fermi energy vs normalized electron concentration.

Generally, when we increase the normalized electron concentration by doping it from time to time, the Fermi energy level increases with it. We get negative Fermi energy when the location of the Fermi level is below the bottom of the conduction band and a positive Fermi energy when the location of the Fermi level is above the bottom of the conduction band.

Figure (2) shown us that the electrical conductivity of the semiconductor increases by increasing the electron concentration in the conduction band as a result of doping. Under the influence

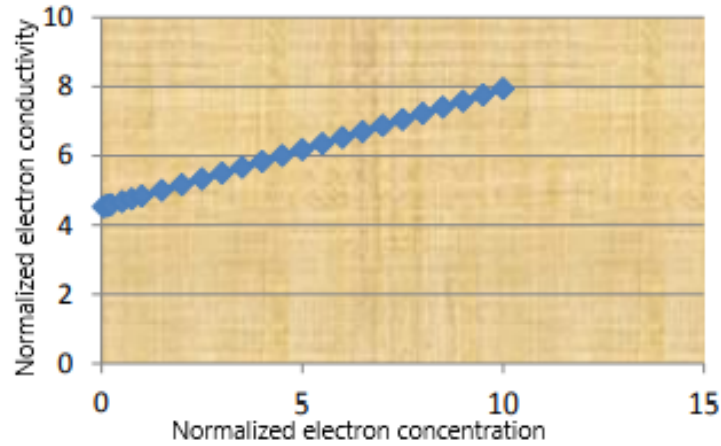


Figure 2: Normalized electrical conductivity vs. normalized electron concentration.

of external fields, $f_0(E)$ may change from its equilibrium distribution function in a semiconductor. This was explained by considering the case in which an electric field is applied to the semiconductor specimen.

When an electric field is applied to the semiconductor, the Lorentz force will tend to change the wave vector of electrons along the direction of the applied fields. As a result, the distribution function is modified by the changing wave vector of electrons under the influence of Lorentz force.

Furthermore, since f_0 depends on both the energy and temperature as well as the electron concentration, one expects that the non-equilibrium distribution function of electrons will also be a function of the position in space when a temperature gradient or a concentration gradient is presented across the semiconductor specimen.

4.1.1 Temperature Dependence of Electron mobility in Doped n-type Silicon

Temperature affects the properties of electronic systems in a number of fundamental ways. Assuming for the moment that each donor contributes one electron to the conduction band, then the donors can contribute an excess carrier concentration up to N_d , where N_d is the donor impurity concentration. The concentration of electrons thermally ionized into the conduction band is given by

$$N_d - n_d = \frac{N_d}{1 + 2e^{(E_d - E_F^e)/k_B T}} = n_e - n_h \quad (80)$$

where n_e and n_h are the mobile electron and hole concentrations. At low temperatures, where $E_d \sim k_B T$, almost all of the carriers in the conduction band will be generated by the ionized donors, so that $n_h \ll n_e$ and $(N_d - n_d) \simeq n_e$. The Fermi level will then adjust itself so that the following equation determines E_F^e

$$n = 2 \left(\frac{m_e K_B T}{2\pi \hbar^2} \right)^{3/2} e^{-E_F^e/k_B T} \simeq \frac{N_d}{12e^{(E_d - E_F^e)/k_B T}} \quad (81)$$

Solution of this equation shows that the presence of the ionized donor carriers (electron) moves the Fermi level up above the middle of the band gap and close to the bottom of the conduction band. For the donor impurity problem, the Fermi level will be close to the position of the donor level E_d . The position of the Fermi level also varies with temperature. Almost all the donor electrons are ionized and are in the conduction band, which is typical of temperatures where the n-type silicon would be used.

We have

$$E_F = E_c - k_B T \ln(N_c/N_d) \quad (82)$$

where $N_c = 2m_e k_B T / (2\pi \hbar^2)$.

The conductivity of a substance is determined by the concentration and mobility of charge carriers and it takes place as a result of the motion of the free electrons under the action of an applied electric field. Conductivity of n-type silicon is the one in which the conductivity is due to the excess electrons.

Figure (3) shows the variation of electron mobility as a function of dopant density at temperature range $100 \leq T \leq 800$ where ionized impurity scattering is the dominant scattering mechanism.

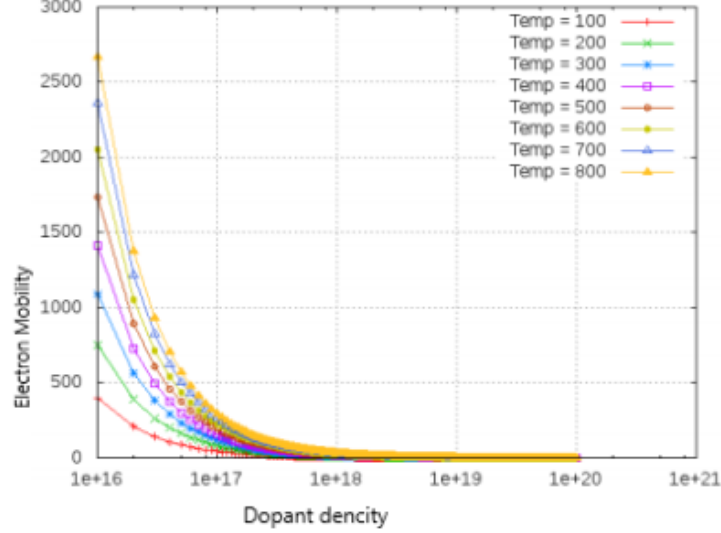


Figure 3: Impurity scattering mobility μ_I (in $cm^2/V.s$) as a function of doping density N_D (in cm^{-3}).

This figure shown that electron drift mobility depends on both dopant density (carrier concentration) and temperature. One can see from the figure that, when the impurity scattering mobility as a function of electron concentration in the presences of electric field increases at high temperature the doping density will decreases because of scattering from straight line path. This can be understood qualitatively by considering that with increasing temperature, electrons can travel faster and this makes it easier to escape the ionized impurities.

So there are a variety of possible temperature dependencies for conductivity or mobility. For instance, at fairly low temperature (less than 200 K), the dominant scattering mechanism might be impurity scattering ($\mu \propto T^{3/2}$) while the carrier concentration is determined by extrinsic doping ($n = N_D^+$). Therefore, conductivity would be seen to increase with temperature ($\sigma \propto T^{3/2}$). One particularly interesting case occurs at high temperatures (above 400 k or higher) when carrier concentration is intrinsic and mobility is dominated by lattice scattering ($\mu_{lattice} \propto T^{-3/2}$).

We understand the property that the transport of carrier is substantially disturbed by scattering due to ionized impurities, distributed randomly in heavily doped regions. This can be evidenced from two facts, the impurity scattering is especially pronounced for low-energy carriers, and the carriers do not acquire high energy levels from low electric fields in heavily doped regions.

5 Conclusion

In this thesis, the most important transport coefficients including electron conductivity and electron drift mobility as a function of both number of electron concentration and temperature gradients has been studied. The Boltzmann transport equation were solved by applying the relaxation time approximation method in the presence of electric field to obtain a general expression for Fermi-Dirac distribution function for the degenerate electron gas in doped n-type silicon. Employing the results of solved Boltzmann transport equation, the expression were derived for electron mobility and electron conductivity. The investigation of the effects created by applied electric field as well as the temperature gradient on transport of electron gas in degenerate doped semiconductor material (Silicon) was discussed.

With the help of Mathematica 5.1 software, we carried out a numerical computation for electron conductivity coefficient using iteration method. Based on our numerical values, we have plotted the variation of Fermi energy and electron conductivity with electron concentration n . One can see from the result that the electrical conductivity of n-type silicon increases as the electron concentration increases, and the Fermi energy increases from the result of the Fermi level increases. We have also computed the variation of electron drift mobility μ_I with dopant density N_d that ranges from 1×10^{16} to $1 \times 10^{21} \text{ cm}^{-3}$ at temperature between $100 \leq T \leq 800 \text{ K}$. We observed that, when the impurity scattering mobility as a function of electron concentration in the presences of field strength increases at high temperature the doping density will decreases because of scattering from straight line path. So with increasing temperature, electrons can travel faster and this makes it easier to escape the ionized impurities. At low temperatures carriers move more slowly, so there is more time for them to interact with charged impurities.

In general, based on the results we can conclude that;

- (i). the Fermi energy increases exponentially with increasing electron concentration (n_n).
- (ii). conductivity increases linearly with increasing density of electron.
- (iii). mobility decreases with dopant density.

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