TEMPERATURE AND DOPANT DENSITY DEPENDENCE OF ELECTRON CONDUCTIVITY IN N-TYPE SILICON

By

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Abstract

The electrical conductivity of n-type silicon depends on the doping concentration and temperature where ionized impurity scattering and acoustical phonon scattering are the dominant scattering mechanisms. In this work, it is seen that the electrical conductivity of n-type silicon increases as the electron concentration increases e.i., when there are more ionized impurity there are more scattering from straight line path, so this reduces mobility. The expressions for computing conductivity as a function of dopant density and temperature has been formulated for n-type silicon. The electrical conductivity of n-type silicon was calculated numerically by appropriately combining ionized impurity and acoustical phonon scattering and the result we got are in agreement with those in the literature. The calculation cover at various ranges of dopant densities and temperatures. As the data of numerical computation show, as temperature increases both mobility and conductivity increase where as relaxation time decreases. Moreover, as the dopant density increases, both relaxation time and conductivity increase where as mobility decreases.

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Chapter 1

Introduction

Semiconductors are materials at the heart of many electronic devices, such as transistors, switches, diodes, photovoltaic cells, etc. Its a material that has a conductance value between that of an insulators and conductors. In addition, their resistance between them. They are only different from insulators because of conduction brought about by thermally generated charge carries (extrinsic conduction) called dopants in semiconductor devices only extrinsic conduction is desirable, the charge carries are electrons and holes. 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. Silicon is widely used now a day with several applications in light emitting diodes, semiconductor lasers, microwaves lasers, and others specialized areas [1-2].

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 type 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. In n-type Silicon, the important scattering mechanisms for electrons are mainly due to acoustical phonon and ionized impurity scattering.

The electron conductivity strongly depends on the value electron drift mobility as a function of temperature and electron concentration. At high temperature, the deformation potential acoustic phonon scattering is the dominant scattering source for n-type semiconductor (silicon), while ionized impurity scattering becomes important when dopant density exceeds 10^{18} cm^{-3} [1-2,3].

Measurements of conductivity in n-type silicon have been reported by previous investigators. Irvin [4] first showed complete conductivity versus dopant density curves for both n- and p-type silicon at 300 K, using mostly previously published data. Recently, Mousty et al.[5] reported the conductivity versus phosphorus density in n-type silicon. The electrical properties of heavily-doped silicon were also reported by Chapman et al.[6]. Most of these efforts focused on conductivity measurements near room temperature. A theoretical analysis of the conductivity as a function of dopant density for n-type silicon has been reported by Norton et al.[7] and Rode[8]; their calculations of conductivity were also confined to room temperature.

In this work, we have extended the theoretical calculations to illustrate the variation of conductivity with electron concentration and temperature in n-type silicon for various ranges of doping density N_D and temperature T. In the derivation of ionized impurity scattering mobility in n-type Si, I have used Brooks-Herring model which is based on the quantum mechanical treatment and is fundamentally much more accurate than Conwell-Weisskopf model and also, the screened Coulomb potential is used in the Hamiltonian. It can be shown that for dopant density exceeds $N_D \leq 10^{18} m^{-3}$ it is important to include electron scattering by acoustic phonon impurities. Therefore, I have used the deformation potential theory proposed by Bardeen and Shockley which is based on the energy change of an electron due to lattice deformation to drive an expression for acoustical phonon scattering mobility. The relaxation time approximation approach is used in this thesis, to investigate conductivity characteristics of electrons taking in to account elastic mechanism types. We carried out simulation of total electron conductivity calculating numerically as a function of temperature and electron concentration.

This dissertation is organized as the following five chapters: In Chapter 2, the constant energy surfaces of conduction energy band structure and the quantum density of states on n-type silicon is predicted briefly. In addition to this, the Boltzmann transport equation is solved using the relaxation time approximation in quantum mechanical treatment. At the end of this chapter, the general expression for mobility of scattering mechanisms that holds true for arbitrary degeneracy (i.e., at arbitrary temperature and carrier concentration) of electron and the expression for electrical conductivity in terms of total scattering mobilities are presented. In third chapter, the expression for both scattering mechanisms that we use in chapter for simulations are discussed briefly . The fourth chapter is result and discussion. Under this chapter the main findings of the study are discussed. We use the expressions of total electron conductivity discussed in chapter 3 to compute the electrical conductivity in n-type silicon as a function of electron concentration and temperatures. The fifth chapter is conclusion. In this part the main findings of the study are explained briefly.

Chapter 2

Carrier Scattering Phenomena

In this chapter, we will derive the expressions for relaxation time τ and differential scattering cross-section σ in terms of scattering rate further be used to obtain electron mobility expression in a given scattering mechanisms. Using quantum mechanical treatment and relaxation time approximation, the Boltzmann transport equation (BTE) discussed in the first section. Using the solution of BTE in the presence of applied electric field, relaxation time is expressed in terms of the angle between scattering states.

2.1 Density of State in Doped N-Type Semiconductor

In doped semiconductor devices the description of carriers depends on a large number of parameters such as m^*, impurity concentrations, dielectric constants and E_g. The density of states (DOS) describes the states of carriers in the bands and their dependence on energy [8]. Thus, we shall define first the DOS in n-type silicon to find the general expression of electron concentration n for both degenerate and non-degenerate semiconductor.

2.1.1 Constant Energy Surfaces And Density of States in N-Type Silicon

The system under consideration is n-type silicon. There are six equivalent constant energy ellipsoids for electron in silicon. These are six equivalents energy minimum along the six 100 directions [9-10]. 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.

The constant energy surfaces are rotational ellipsoids and two of the main axis of the ellipsoid are identical(i.e. $m_x \neq m_y = m_z$). The short and long axis are then denoted as the transversal and the longitudinal axes, respectively. A relatively heavy mass is associated with the longitudinal and transversal axis. If the mass are denoted as m_l and m_t for the longitudinal and transversal, respectively, the DOS per unit energy can be expressed as

$$N(E)dE = \frac{(2m_l m_t^2)^{1/2}}{\pi^2\hbar^3}E^{1/2}dE \tag{2.1}$$

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

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. The density of state function given by Eq.(2.1) doesnt incorporate the non-parabolicity effect. Therefore, the parabolic density function N(E) is replaced by $N(z)$ in accordance with Kane model [11]. To describe the macroscopic density of state function, Kane assumed that if the variation in local electrostatic potential is sufficiently slow, the average density of states function for conduction band is expressed as:-

$$N(z) = \frac{m_n^{3/2}2^{3/4}\delta^{1/2}}{\pi^2\hbar^3}\gamma(z) \tag{2.2}$$

The variable $\gamma(z)$ in Eq.(2.2) as forwarded by Kane is given by:-

$$\gamma(z) = \frac{1}{\pi^{1/2}}\int_{-\infty}^{z}(z-\xi)^{1/2}\exp(-\xi)d\xi \tag{2.3}$$

In Eq.(2.3) the variable z implies the dimensionless energy expressed as:-

$$z = \frac{E}{\sqrt{2}\delta} \tag{2.4}$$

where δ is the standard deviation of a Gaussian distribution function for impurity potential energy which is expressed as:-

$$\delta = (\frac{2N_d\lambda q^4}{8\pi\epsilon^2})^{1/2} \tag{2.5}$$

where ϵ is the permittivity of silicon and λ is screening length in Thomas-Fermi model, where a higher carrier density requires the application of the Fermi-Dirac statistics.

The density of states function given by Eq.(2.2) is so complicated that one cannot use it to make any useful calculations. To avoid these complications, Slotboom [12] has suggested the following approximation for $\gamma(z)$:

$$\gamma(z) = z^{1/2}[1 - \frac{1}{8z^2}].For z > 0.601, vise - versa, E > 0.85 \tag{2.6}$$

and

$$\gamma(z) = \frac{1}{2\pi^{1/2}} \exp(-z^2)0.319 + 0.906 \exp(2z).For z \leq 0.601. \tag{2.7}$$

In heavily doped semiconductor one must integrate equations (2.6) and (2.7) to obtain the electron concentration n .

2.1.2 Density of States Effective Mass

The electron density (number of electron per volume) in the conduction band is obtained by integrating N(E)f(E)dE (density of states times probability of occupancy of states) from the bottom to top of the conduction band,

$$n = \int_{E_c} N(E)f(E)dE \tag{2.8}$$

Here there are two important quantities introduced in the above expression: N(E) is the number of states per unit energy per unit volume known as the density of states in the conduction band given in Eq.(2.1) and the function f(E) is the probability of an electronic state of energy E being occupied by an electron and is given by the Fermi-Dirac distribution function [13]

$$f(E) = \frac{1}{1 + \exp(\frac{E-E_F}{K_B T})} \tag{2.9}$$

The number of electron concentration n for both parabolic and non-parabolic band in degenerate and non-degenerate semiconductor can be obtained by performing Eq.(2.8).

If we suppose that $E - E_F >> K_B T$ (Parabolic Non-degenerate semiconductor), then Eq.(2.9) can be approximated as

$$f(E) \approx exp(-\frac{(E - E_F)}{K_B T}) \tag{2.10}$$

Thus, we can replace the Fermi-Dirac distribution by the Boltzmann distribution under the assumption that the number of electrons in the conduction band is far less than the number of available states in this band. The number of mobile electron for **non-degenerate** semiconductor can be obtained by performing the integration in Eq.(2.8), and is written as

$$n = N_C \exp(\frac{-(E - E_F)}{K_B T}) \tag{2.11}$$

where $N_C = 2(\frac{m_c^* K_B T}{2\pi\hbar^2})^{3/2}$ is the effective density of states for the edges of conduction band.

For Parabolic Degenerate case;

$$n = N_C \int_{E_C} \frac{(E - E_k)^{1/2} dE}{1 + \exp(\frac{E_k - E_F}{K_B T})} \tag{2.12}$$

Letting $\eta = \frac{E - E_k}{K_B T}$ and $\eta_F = \frac{E_F - E_k}{K_B T}$, Eq.(2.12) can be written as

$$n = N_C \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + \exp(\frac{\eta - \eta_F)}{K_B T})} \tag{2.13}$$

This can be reduced to

$$n = N_C F_{1/2}(\eta_F) \tag{2.14}$$

where $F_{1/2}(\eta_F) = \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + \exp(\frac{\eta - \eta_F)}{K_B T})}$ is the Fermi integral.

The number of electron concentration for Non-parabolic semiconductor is obtained by using Slotboom approximation discussed in section 2.1.1, and is given by

$$n = \int N(Z) f(Z) dZ \tag{2.15}$$

Substituting Eq.(2.2), this can be written as

$$n = \frac{m_n^{3/2} 2^{3/4} \delta^{1/2}}{\pi^2 \hbar^3} \int \gamma(Z) f(Z) dZ \tag{2.16}$$

Using Equations (2.6) and (2.7), one can obtain

$$n = \frac{m_n^{3/2} 2^{3/4} \delta^{1/2}}{\pi^2 \hbar^3} [\int_{-\infty}^{0.601} Z^{1/2} [1 - \frac{1}{8Z^2}] + \frac{0.319}{2\pi^{1/2}} \int_{0.601}^\infty \exp(-Z^2) + 0.906 \int_{0.601}^\infty \exp(2Z)] f(Z) dZ \tag{2.17}$$

Where z and δ are expressed respectively in Eq.(2.4) and Eq.(2.5).

2.1.3 Boltzmann Transport Equation in Relaxation Time Approximation

The conductivity of a substance is determined by the concentration and mobility of charge carriers. The probability of electrons occupying a unit volume of phase space with the center at point(x, k) at the moment of time t is f(x,k,t). That is to say that, f(x,k,t) is the distribution function for no equilibrium state will change with time. The nature of charge being dependent on which process predominates; the change due to the action of the electric field (E), and as a result of charge carrier collision. First, we assume that the electron is not subject to scattering and that the state is changed by an external force (electric field, magnetic field and so on). Then, after a time interval dt, the electron is changed into a new state with position r+$\dot{r}dt$ and wave vector k+$\dot{k}dt$. A particle that occupied a state r-$\dot{r}dt$ and k-$\dot{k}dt$ at a time t - dt will move into a state *f(k, r, t)* after a time interval dt (at time t). Therefore, the rate of change of the distribution function is given by

$$(\frac{df}{dt})_{drift} = \frac{[f(k-\dot{k}dt, r-\dot{r}dt, t-dt) - f(k,r,t)]}{dt} \tag{2.18}$$

The right-hand side of above equation is interpreted as follows. The first term of the right-hand side will change into *f(k, r, t)* after a time interval dt (increase in *f(k, r, t))* and the second term *f(k, r, t)* will change into another state after a time interval dt (decrease in *f(k, r, t)).* Since the scattering of a particle is not included in the present analysis, the above rate represents the continuous flow of a particle and thus the term is called a drift term.

Now, the Taylor expansion of the first term on the right-hand side in Eq.(2.18) gives

$$\begin{aligned} f(k-\dot{k}dt, r-\dot{r}dt, t-dt) =& f(k,r,t) - [\dot{k}...\frac{\partial f}{\partial k} + \dot{r}...\frac{\partial f}{\partial r} + \frac{\partial f}{\partial t}]dt + ... \\ \equiv& f(k,r,t) - [(\dot{k}.\nabla_k f) + (\dot{r}.\nabla_r f) + \frac{\partial f}{\partial t}]dt + ... \end{aligned} \tag{2.19}$$

where $\dot{k} = \frac{dk}{dt} = \frac{F}{\hbar}$ on the right hand side of the first term reflects the change in crystal momentum due to the total field force $F = q(E + v \times B)$, the second term $\dot{x} = \frac{dx}{dt} = v = \frac{\hbar k}{m^*}$ is the the electron velocity (i.e., change due to concentration gradients) and the last term is the local change in distribution function.

Keeping terms up to the second term in Eq.(2.19) and inserting it in to (2.18), the drift term is rewritten as

$$(\frac{df}{dt})_{drift} = -[\dot{k}.\nabla_k f + \upsilon.\nabla_r f + \frac{\partial f}{\partial t}] \tag{2.20}$$

This can be written as

$$(\frac{df}{dt})_{drift} = -[\frac{1}{\hbar}(F.\nabla_k f) + \upsilon.\nabla_r f + \frac{\partial f}{\partial t}] \tag{2.21}$$

On the other hand, a particle changes its state by scattering (collision) and we define the rate of change in the distribution function due to a collision by $(\frac{df}{dt})_{coll}$. Since the distribution function has to satisfy the equilibrium condition (steady state condition) or condition of balance, we have

$$(\frac{df}{dt})_{drift} + (\frac{df}{dt})_{coll} = 0 \tag{2.22}$$

Inserting (2.21) into this we obtain

$$(\frac{\partial f}{\partial t})_{coll} = \frac{1}{\hbar}(F.\nabla_k f) + \upsilon.\nabla_r f + \frac{\partial f}{\partial t} \tag{2.23}$$

The relaxation time approximation introduced in this work enables one to linearize the Boltzmann transport equation in that collision term is expressed in terms of the ratio of the perturbed distribution function (i.e., $f - f_o$) and the relaxation time. Let us further assume that if the electron distribution is distributed from the local equilibrium value f_o, then the effect of the collision is simply to restore f to the local equilibrium value f_o exponentially with a relaxation time τ which is the order of the time between electron collisions with ion. Any external perturbation drives the distribution function away from the equilibrium; the BTE governs the shift of the distribution function from equilibrium. It also assume that all the collision processes are elastic and can be treated in terms of a unique relaxation time. Elastic scattering requires that the charge of electron energy during the scattering process must be small compared to the energy of electrons. Considering the steady state case (the case that gives rise to $\frac{\partial f}{\partial t} = 0$), the collision term of BTE is written as

$$(\frac{\partial f}{\partial t})_{coll} = \dot{k}.\nabla_k f + \dot{r}.\nabla_r f \tag{2.24}$$

Evaluation of scattering rates $S(k, k')$ requires us to use one of the most useful results of time

dependent perturbation theory in quantum mechanics usually based on Fermi's Golden rule (FGR) which has derived by the time-dependent perturbation theory of the first order.

To evaluate the probability that state in state k to scatter in to any state k', we shall use the amplitude of that state and square it. Denoting the amplitude of the scattering state (or matrix element) as $|\langle k'|H|k\rangle| = H_{kk'}$, is given by [14]

$$H_{kk'} = \frac{1}{L^3}\int \phi^*_{k'} H' \phi_{k'} d^3r \tag{2.25}$$

where H' is the perturbing Hamiltonian, and $\phi_k(r)$ is the initial unperturbed electron wave function given by

$$\phi_k(r) = u_k(r)e^{ik.r} \tag{2.26}$$

where $u_k(r)$ is a Block function, which has the same periodicity as the crystal potential v(r) and $\phi^*_{k'}$ is the complex conjugate of the electron wave function $\phi_{k'}$.

Fermi's golden rule gives the transition rate from initial state to the final state which is expressed as

$$S(k,k') = \frac{2\pi}{\hbar}|\langle k'|H|k\rangle|^2 \delta[E_{k'} - E_k] \tag{2.27}$$

where E_k and $E_{k'}$ are the energies of the initial and final states respectively and δ-function indicates the energy conservation, which is equal to unity for $E_k = E_{k'}$ and vanishes otherwise. In fact, a generalized expression for the collision term given by Eq.(2.24) can be formulated in terms of the scattering rate $S(k,k')$ and the nonequilibrium distribution function f(k,r) which is given by

$$(\frac{df}{dt})_{coll} = \sum_{k'}\{S(k',k)f(k')[1-f(k)] - S(k,k')f(k)[1-f(k')]\} \tag{2.28}$$

Where $f(k')[1-f(k)]$ of $S(k',k)$ represents the probability of electron occupation in the initial state k' and of electron vacancy in the final state k. For simplicity, we consider the case where the Fermi level lies below the bottom of the conduction band in the band gap(then, the conditions $f(k) \ll 1$ and $f(k') \ll 1$ is hold).

At equilibrium, the principle of detailed balance balance enforces the condition

$$S(k',k)f_o(k')(1-f_o(k)) = S(k,k')f_o(k)(1-f_o(k')) \tag{2.29}$$

In the spacial case of elastic scattering ($\nabla_r f = 0$), $\varepsilon_k = \varepsilon_{k'}$, and as a result, $S(k', k) = S(k, k')$ irrespective of the nature of the distribution function. Using this, one can rewrites the collision term as

$$(\frac{df}{dt}) \mid_{coll} = \sum_{k'} S(k', k)(f(k') - f(k)) \tag{2.30}$$

Let us now assume that the external fields and gradients have been turned on for a long time. They have driven the distribution function to a steady state value f from f_o. The perturbation is assumed to be small, (i-e., distribution function is assumed not to deviate far from its equilibrium value of f_o). Under this condition, it is common practice to assume that

$$\frac{df}{dt} = \frac{df}{dt} \mid_{coll} = -\frac{(f - f_0)}{\tau} \tag{2.31}$$

Were τ is a time scale characterizing the relaxation of the distribution

and

$$f(k) = f_1 + f_0 \tag{2.32}$$

This is the relaxation time approximation which is crucial for getting a solution of the Boltzmann transport equation.

Rearranging Eq.(2.30), one can obtain

$$\frac{df}{dt} + \frac{f(k)}{\tau_q} = \sum_{k'} S(k, k') f(k') \tag{2.33}$$

where the quantum scattering time is defined as

$$\frac{1}{\tau_q} = \sum_{k'} S(k, k') \tag{2.34}$$

A particle (electron) prepared in state k at time t=0 by an external perturbation (electric field) will be scattered in to other state k' due to collisions and the distribution function in that state will approach the equilibrium distribution exponentially fast with the time constant τ_q may be viewed as a life time of the particle in the state k.

2.1.4 Solution of The Boltzmann Transport Equation

In this section, the expression for relaxation time which is heavily used in this paper for finding mobility further be used to obtain the electron conductivity is derived. The elastic and

anisotropic scattering assumption is used in the derivation. Together with this assumption and using relaxation time approximation, the Boltzmann transport equation is solved. In solving BTE, we have also used the time dependent perturbation theory in quantum mechanics.

Here we use the relaxation time approximation to the collision term in the absence of any concentration gradients. When the distribution function reaches a steady state, using the relaxation time approximation the BTE may be written as

$$\frac{\partial f}{\partial t} = -\frac{(f - f_o)}{\tau} + \frac{F}{\hbar}\nabla_k f + v.\nabla_r f = 0 \tag{2.35}$$

Defining the distribution function to be independent of position x (i.e., spatial uniformity results in $(\nabla_r f = 0)$, Eq.(2.35) is reduced to

$$f(k) = f_o(k) + \tau\frac{F}{\hbar}\nabla_k f \tag{2.36}$$

When the the external force $F = qE$ is applied in the x direction, this becomes

$$f(k) = f_o(k) + q\tau\frac{E_x}{\hbar}\nabla_k f \tag{2.37}$$

Using the definition of velocity $v = \frac{1}{\hbar}(\frac{\partial\varepsilon_k}{\partial k})$, eq.(2.37) can be written as

$$f(k) = f_o(k) + q\frac{\tau}{\hbar}E_x\frac{\partial f}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial k} = f_o(k) + q\tau E_x.v\frac{\partial f}{\partial\varepsilon} \tag{2.38}$$

and since the distribution function is assumed to be close to f_0, we can make the replacement $f(k) \longrightarrow f_o(k)$, hence the distribution function will become

$$f(k) = f_o + q\tau E_x v\frac{\partial f_0}{\partial\varepsilon} \tag{2.39}$$

Using this, for elastic scattering process one immediately obtains

$$f(k') - f(k) = q\tau\frac{\partial f_0}{\partial\varepsilon}E.v(1 - \frac{E.v'}{E.v}) \tag{2.40}$$

For parabolic band structure $(v = \frac{\hbar k}{m*})$, the collision term in the form of relaxation time approximation becomes

$$\frac{\partial f(k)}{\partial t} = \sum_{k'} S(k', k)(f(k') - f(k)) = -\frac{f(k) - f_o(k)}{\tau} \tag{2.41}$$

Where a new relaxation time is defined by

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')(1 - \frac{E.k'}{E.k}) \tag{2.42}$$

Let the vectors k, k' and E be directed along random directions in the 3D space. We fix the z-axis along k and the y-axis so that E lies in the y-z plane. From Figure 2.1, we get the relation

$$\frac{k'.E}{k.E} = \cos\theta + \sin\gamma \tan\alpha \tag{2.43}$$

where the angles are shown in the figure.

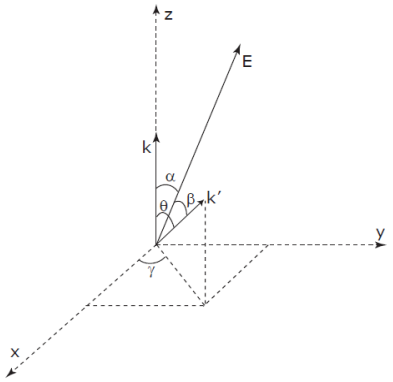

Figure 2.1: Angular relations between the vectors in Boltzmann transport equation.

When the sum over all k' is performed for the collision term, the $\sin\gamma$ sums to zero and the momentum relaxation time becomes

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')(1 - \cos\theta) \tag{2.44}$$

This can be written as

$$\frac{1}{\tau} = (\frac{L}{2\pi})^3 \int S(k,k')[1 - \cos\theta']d^3k' \tag{2.45}$$

where k_x and k'_x are the components of the electron wave vectors k and k' along the direction of the external force before and after scattering respectively, L^3 is the volume of the crystal and θ is the angle between k and k'.

This is the general form for scattering time that we use throughout this work. It is related to mobility by the Drude relation $\mu = \frac{q\langle\tau\rangle}{m*}$, where the scattering time have been averaged over all energies of electron. Thus the scattering time measures the average time spent by electron moving along the external field.

2.1.5 Differential Scattering Cross Section

Calculation of relaxation time can be simplified by introducing a differential scattering cross-section. It is noted that $\sigma(\theta', \phi')$ depends on θ' if the scattering process is anisotropic (i.e., independent of ϕ'). Under this condition, a simple relationship exists between $\sigma(\theta')$ and the scattering rate $S(k, k')$ [15].

In general, the differential scattering cross-section is defined as the total number of particle(electron) which make transitions from k-to-k' states per unit solid angle per unit time divided by the incident flux density.

$$\sigma(\theta', \phi') = \frac{(\frac{L}{2\pi})^3 S(k, k') \frac{d^3k'}{d\omega}}{\frac{\upsilon_k^2}{L^3}} = \frac{(L^3)^2 S(k, k') d^3k'}{(2\pi)^3 \upsilon_k^2 d\omega} \tag{2.46}$$

Where υ_k is the initial particle velocity, L^3 is the volume the crystal, and $d\omega = \sin\theta' d\theta' d\phi'$ is the solid angle between incident wave vector k and scattering wave vector k'.

Equation (2.46) can be written as

$$\sigma(\theta') = \frac{(L^3)^2 S(k, k') d^3k'}{(2\pi)^3 \upsilon_k^2 \sin\theta' d\theta' d\phi'} \tag{2.47}$$

Now, consider the case of anisotropic elastic scattering. Using Eq.(2.27) and Eq.(2.47), and using the relation $\upsilon_k = \upsilon_{k'}$, $k = k'$ and $d^3k' = k^2 \sin\theta' d\theta' d\phi' dk'$, one can obtain

$$\sigma(\theta') = \frac{(L^3)^2 k'^2 |H_{kk'}|^2}{(2\pi)^2 \hbar^2 \upsilon_{k'}^2} \tag{2.48}$$

The total scattering cross-section or integrated elastic cross section is obtained by integrating the differential cross section over all the solid angles, and is given by

$$\sigma_T = 2\pi \int_0^\pi \sigma(\theta')(1 - cos\theta') \sin\theta' d\theta' \tag{2.49}$$

Thus, the total differential scattering cross-section (σ_T) can be obtained from Eq.(2.49) provided that the perturbing Hamiltonian H' and hence $H_{kk'}$ is known.

Chapter 3

The Electron Scattering Mechanisms And Conductivity

3.1 Electron Scattering Mechanisms

In this chapter, we shall discuss the expressions that predicts the variation of electron conductivity with temperature and electron concentration due to different scattering mechanisms for both non-degenerate and degenerate case in semiconductor material (silicon). From many types of scattering mechanisms, one must know which type of scattering is predominant in a particular material under the prevalent condition of temperature and carrier concentration. In n-type Silicon, the important scattering mechanisms we focus in this paper for electron mobilities are mainly due to deformation potential acoustical phonon scattering and ionized impurity scattering for arbitrary value of temperature and concentrations. We will see these two scattering processes one by one in the preceding subsection, and at the end one can understand the affect of temperature and electron concentration on conductivity through electron drift mobility.

3.1.1 Ionized Impurity Scattering

In order to derive the differential scattering cross section and the relaxation time for ionized impurity scattering, the amplitude of the scattering event $H_{kk'}$ and the perturbing Hamiltonian H' must be determined first. The most popular models for ionized impurity scattering are Brooks and Herring [19-20].

In this work, the Brooks-Herring approach is employed and the screened Coulomb potential are used in the Hamiltonian. With this approach the perturbing Hamiltonian due to the screening potential is given by

$$H^{'} = qV'(r) = \frac{q^2 e^{-r/\lambda_D}}{4\pi\epsilon_0\varepsilon_s r}. \tag{3.1}$$

where $V'(r)$ is the screening Coulomb potential for ionized impurity atom given by

$$V'(r) = \frac{qe^{-r/\lambda_D}}{4\pi\epsilon_0\varepsilon_s r}. \tag{3.2}$$

and,

$$\lambda_D = \sqrt{\frac{\epsilon_0\varepsilon_s K_B T}{q^2 n_o}} \tag{3.3}$$

is the screening length.

The amplitude of the scattering event $H_{kk'}$ due to screening potential can be obtained by substituting equations (3.1) and (2.25) in to Eq.(2.26) and is

$$H_{kk'} = \frac{1}{L^3}\int e^{-ik'.r}(\frac{q^2 e^{-r/\lambda_D}}{4\pi\epsilon_o\varepsilon_s r})e^{ik.r}d^3r = \frac{q^2}{2L^3\epsilon_o\varepsilon_s}\int_0^{\pi}\int_0^{\infty} e^{-iK.r}(\frac{e^{-r/\lambda_D}}{r})r^2\sin\theta d\theta dr \tag{3.4}$$

where

$$d^3r = 2\pi r^2\sin\theta d\theta dr \tag{3.5}$$

is the volume element and

$$K = k' - k = 2|k|\sin(\frac{\theta'}{2}) \tag{3.6}$$

K is the reciprocal lattice vector.

Figure 3.1 shows the relationship between the incident and scattering wave vectors k and k' in the real space. By substituting Eq.(3.6) in to Eq.(3.4), we obtain

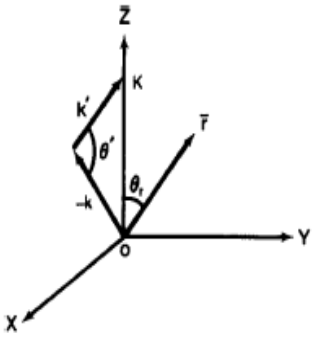

Figure 3.1: *Coordinates for computing the matrix element of scattering by an ionized impurity, where k is the wave vector of incident electron , k' is the wave vector of the scattered electron wave and* $K = k' - k = 2|k| \sin(\frac{\theta'}{2})$

$$H_{kk'} = \frac{q^2 \lambda_D^2}{L^3 \epsilon_o \varepsilon_s [1 + K^2 \lambda_D^2]} \tag{3.7}$$

The differential scattering cross section $\sigma(\theta')$ can be obtained by substituting Eq.(3.7) in to (2.48), which gives us

$$\sigma(\theta') = \frac{K^2 (q^2 \lambda_D^2)^2}{(2\pi\hbar\epsilon_0 \varepsilon_s)^2 [1 + K^2 \lambda_D^2]^2} \frac{1}{\upsilon_k^2} = \frac{(q^2 \lambda_D^2 m^*)^2}{(2\pi\hbar^2 \epsilon_0 \varepsilon_s)^2 [1 + K^2 \lambda_D^2]^2} \tag{3.8}$$

where $\upsilon_k = \frac{K\hbar}{m^*}$.

Using the Bohr radius a_B for the ground state of the impurity atom given by

$$a_B = \frac{4\pi\epsilon_0 \varepsilon_s \hbar^2}{q^2 m^*} \tag{3.9}$$

Equation (3.8) becomes

$$\sigma(\theta') = (\frac{q^2 m^*}{2\pi\hbar^2 \epsilon_0 \varepsilon_s})^2 . \frac{4\lambda_D^4}{[1 + K^2 \lambda_D^2]^2} = \frac{4\lambda_D^4}{a_B^2 [1 + K^2 \lambda_D^2]^2} \tag{3.10}$$

Now, by substituting Eq.(3.10) in to (2.49) and using Eq.(3.6), one can obtain the total scattering time σ_T, which reads

$$\sigma_T = \frac{8\lambda_D^4 \pi}{a_B^2} \int_0^\pi \frac{(1 - \cos\theta') \sin\theta' d\theta'}{[1 + 4\lambda_D^2 k^2 \sin^2(\frac{\theta'}{2})]^2} \tag{3.11}$$

Figure 3.2 shows the total scattering cross-section of silicon calculated by Eq.(3.11) for $N_I = 10^{-18} cm^{-3}$, where we assumed $n_o = N_I$. The result shows that the cross-section of high angle

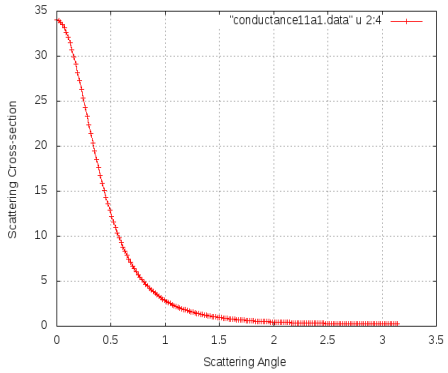

Figure 3.2: *Scattering cross-section as a function of scattering angle*

carrier is significantly degraded.

The relaxation time τ is related to the total scattering cross-section σ_T by

$$\frac{1}{\tau} = N_j \sigma_T \upsilon_{th} \tag{3.12}$$

where N_j is the density of a given scattering system (where j stands for a given scattering mechanism) and υ_{th} is the mean thermal velocity.

By substituting Eq.(3.11) in to (3.12), the relaxation time for ionizing impurity scattering τ_I can be written as

$$\frac{1}{\tau_I} = \frac{8\pi N_I \upsilon_{th} \lambda_D^4}{a_B^2} \int_0^{\pi} \frac{(1-\cos\theta')\sin\theta' d\theta'}{[1+4\lambda_D^2 k^2 \sin^2(\frac{\theta'}{2})]^2} \tag{3.13}$$

Letting $\sin(\frac{\theta'}{2}) = x, (1-\cos\theta') = 2x^2$ and $\sin\theta' d\theta' = 4x dx$, Eq.(3.13) can be written as

$$\frac{1}{\tau_I} = \frac{8\pi N_I \lambda_D^4 \upsilon_{th}}{a_B^2} \int_0^1 \frac{(8x^3)dx}{[1+4\lambda_D^2 k^2 x^2]^2} \tag{3.14}$$

Solving this integrals, we get

$$\frac{1}{\tau_I} = \frac{2\pi N_I \upsilon_{th}}{a_B^2 k^4} \ln[1+4k^2\lambda_D^4 - \frac{4k^2\lambda_D^4}{(1+4k^2\lambda_D^2)}] = \frac{2\pi N_I \upsilon_{th}}{a_B^2 k^4} \ln[1+\gamma^2 - \frac{\gamma^2}{(1+\gamma^2)}] = \frac{2\pi N_I \upsilon_{th}}{a_B^2 k^4} \ln[1+\gamma^2] \tag{3.15}$$

where $\gamma = 2K\lambda_D^2$ and $\ln[1+\gamma^2 - \frac{\gamma^2}{(1+\gamma^2)}] \cong \ln[1+\gamma^2]$ for $k\lambda_D^2 \ll 1$.

It is noted that $\ln(1+\gamma^2)$ is a slow varying function of temperature and electron density.

Multiplying the right hand side of Eq.(3.15) by $\frac{\lambda_D^4}{\lambda_D^4}$, we get

$$\frac{1}{\tau_I} = \frac{2\pi N_I \upsilon_{th} \lambda_D^4}{a_B^2} (\frac{1}{k^2\lambda_D^2})^2 \ln[1+\gamma^2] \tag{3.16}$$

Using the relation $k^2\lambda_D^2 = \frac{2m^*E\epsilon_o\varepsilon_s K_B T}{\hbar^2 q^2 n'}$, where $n' = n + n(1 - n/N_D)$ for $N_A^- = 0$ is the density of screening electrons surrounding the ionized donor impurity and, substituting equations (3.3) and (3.9) in to equation (3.16), it becomes

$$\frac{1}{\tau_I} = \frac{N_I q^4 \upsilon_{th}}{32\pi\epsilon_o^2\varepsilon_s^2 E^2} \ln[1+\gamma^2] \tag{3.17}$$

Substituting $\upsilon_{th} = \frac{k\hbar}{m^*}$, we get

$$\frac{1}{\tau_I} = \frac{N_I q^4 k\hbar}{32\pi\epsilon_o^2\varepsilon_s^2 m^* E^2} \ln[1+\gamma^2] \tag{3.18}$$

From the relation $E = \frac{\hbar^2 k^2}{2m^*}$, we can have $(2m^*E)^{1/2} = \hbar k$ and then substituting in to Eq.(3.18), we get

$$\frac{1}{\tau_I} = \frac{N_I q^4 \sqrt{2m^*E}}{32\pi\epsilon_o^2\varepsilon_s^2 m^* E^2} \ln[1+\gamma^2] = \frac{q^4 N_I \ln[1+\gamma^2]}{16\pi(2m^*)^{1/2}\epsilon_o^2\varepsilon_s^2 E^{3/2}} \tag{3.19}$$

Rearranging this, we get

$$\tau_I = \frac{16\pi(2m^*)^{1/2}\epsilon_o^2\varepsilon_s^2 E^{3/2}}{q^4 N_I \ln[1+\gamma^2]} \tag{3.20}$$

Eq.(3.20) shows that the relaxation time τ_I for ionized impurity scattering is directly proportional to $E^{3/2}$ and the temperature dependence of τ_I comes only from the variation of $\ln(1+\gamma^2)$ with T which is very small.

The electron mobility may be defined in terms of the conductivity effective mass m_c^* and the relaxation time τ (i.e., is directly proportional to the average relaxation time and varies inversely with conductivity effective mass).

Thus, the ionized impurity scattering mobility μ_I may be defined as

$$\mu_I = \frac{q\langle\tau_I\rangle}{m^*} \tag{3.21}$$

where $\langle\tau_I\rangle$ is the average relaxation time for ionized impurity scattering.

In general, the average relaxation time for conduction band $\langle\tau_c\rangle$ is defined as

$$\langle\tau_I\rangle = \frac{\int_0^\infty \tau_I \frac{\partial f_o}{\partial(E/K_BT)}(E/K_BT)^{3/2} d(E/K_BT)}{\int_0^\infty f_o(E/K_BT)^{1/2} d(E/K_BT)} \tag{3.22}$$

For Non-Degenerate semiconductor($\eta >> 1$), the ionized impurity scattering mobility μ_I^{ND} is derived as

$$\mu_I^{ND} = \frac{q}{m^*}.\left(\frac{16\pi(2m^*)^{1/2}\epsilon_o^2\varepsilon_s^2}{q^4 N_I} \frac{\int \frac{E^3 e^{-E/K_BT} dE}{\ln[8m^*\epsilon_o\varepsilon_s K_B T]}}{\int E^{3/2} e^{-E/K_BT} dE}\right) \tag{3.23}$$

Equation (3.23) gives us

$$\mu_I^{ND} = \frac{128\sqrt{2\pi}\epsilon_o^2\varepsilon_s^2(K_BT)^{3/2}}{N_I q^3\sqrt{m^*}} \tag{3.24}$$

For Degenerate case, the ionized impurity scattering mobility μ_I^D is given by

$$\mu_I^D = \frac{24\pi^3\varepsilon_s^2\hbar^3 n}{q^3 m^{*2} N_I} \tag{3.25}$$

which is weakly temperature dependent (through n), but now dependent on the number of carrier density.

These Equations shows that, the ionized impurity scattering mobility μ_I is directly proportional to $T^{3/2}$. Thus, the mobility due to ionized impurity scattering increases with temperature. We understood by considering that with increasing temperature, electrons can travel faster and this makes it easier to escape the ionized impurities.

3.1.2 Deformation Potential Acoustic Phonon Scattering

According to the deformation potential theory, the energy change is related to the volume change of crystal

$$\Delta E = \frac{\Delta V}{V} \tag{3.26}$$

where the ratio $\frac{\Delta V}{V}$ represents the change of crystal volume to the total crystal volume due to temperature change in a semiconductor.

Since $\frac{\Delta V}{V}$ can be expanded in terms of a Fourier series in displacement vector of acoustic phonon r_n, one can write

$$\frac{\Delta V}{V} = \nabla_r r_n \tag{3.27}$$

The lattice displacement r_n can be expressed in terms of the normal coordinates and normal frequencies in three-dimensional form (i.e., two transverse branches and one longitudinal branch).

In the present case, only the longitudinal-mode acoustic phonon scattering is assumed. Therefore, under this condition $\frac{\Delta V}{V}$ can be expressed by

$$\frac{\Delta V}{V} = \sum q_l r_l \tag{3.28}$$

where q_l is the wave vector of the longitudinal-mode acoustical phonon, and r_l represents the displacement due to longitudinal-mode acoustical phonons.

The perturbing Hamiltonian can be related to the change of crystal volume caused by the lattice phonons and the conduction band edge deformation potential D_{ac} by the expression

$$H' = D_{ac}(\frac{\Delta V}{V}) = D_{ac}\sum_{q} q_l r_l \tag{3.29}$$

And,

The matrix element due to the perturbing Hamiltonian can be expressed as

$$H_{kk'qq'} = \langle k', n_{q'}|H'|k, n_q\rangle = \int \phi^*_{k'}\varphi^*_{n_q}(D_{ac}\sum q_l r_l)\phi_k\varphi_{n_q}d^3r d^3r_l \tag{3.30}$$

where φ_{n_q} is the phonon wave functions and ϕ_k is the electron wave functions.

For phonon emission, the solution of Eq.(3.30) is

$$H_{kk'qq'} = D_{ac}q_l(\frac{\hbar}{L^3M})^{1/2}(\frac{\langle n_q\rangle}{2})^{1/2} \tag{3.31}$$

and

For phonon absorption it is given by

$$H_{kk'qq'} = D_{ac}q_l(\frac{\hbar}{L^3M})^{1/2}(\frac{(\langle n_q\rangle + 1)}{2})^{1/2} \tag{3.32}$$

Where M is the mass of the atom and $\langle n_q\rangle$ is the average phonon population density given by [12]

$$\langle n_q\rangle = \frac{1}{e^{\hbar\omega/K_BT} - 1} \approx \frac{K_BT}{\hbar\omega} \tag{3.33}$$

This is valid for long wave length acoustical phonons ($i.e., K_BT \gg \hbar\omega$) and $e^{\hbar\omega/K_BT} \approx 1 + \frac{\hbar\omega}{K_BT}$.

The square of the matrix element due to the deformation potential scattering is obtained from the summation of the square of Eqs.(3.31) and (3.32) and using the relation $\omega = \upsilon_s q_l$ (υ_s is velocity of sound) as follows:

$$\begin{aligned} |H_{kk'qq'}|^2 =& (D_{ac}q_l)^2(\frac{\hbar}{L^3M})[\frac{\langle n_q\rangle + 1}{2}] + (D_{ac}q_l)^2(\frac{\hbar}{ML^3})[\frac{\langle n_q\rangle}{2}] \\ =& \frac{D^2_{ac}K_BT}{ML^3\upsilon_s^2} \end{aligned} \tag{3.34}$$

Now, we can find the differential scattering cross section of acoustic phonon scattering σ_{ac} by substituting (3.34) in to Eq.(2.48) as follows:

$$\sigma_{ac} = \frac{(L^3)^2k^2}{(2\pi\hbar)^2}\frac{1}{\upsilon_k^2}\frac{D^2_{ac}K_BT}{M\upsilon_s^2L^3} \tag{3.35}$$

Using the relation $\upsilon_k = \frac{K\hbar}{m^*}$ and $\rho = M/L^3$ (ρ is the crystal density), we get

$$\sigma_{ac} = \frac{m^{*2} D_{ac}^2 K_B T}{4\pi^2 \hbar^4 \rho \upsilon_s^2} = \frac{m^{*2} D_{ac}^2 K_B T}{4\pi^2 \hbar^4 C_l} \tag{3.36}$$

The relaxation time due to the longitudinal-mode acoustical scattering time can be obtained by substituting Eq.(3.36) in to Eqs.(2.49) and (3.12), and we find

$$\frac{1}{\tau_{ac}} = 2\pi\upsilon \int_0^\pi \sigma_{ac}(1-\cos\theta')\sin\theta' d\theta' = \frac{m^{*2}\upsilon D_{ac}^2 K_B T}{\pi\hbar^4 C_l} = \frac{\upsilon}{l_{ac}} \tag{3.37}$$

where $l_{ac} = \frac{\pi\hbar^4 c_l}{m^{*2}\upsilon D_{ac}^2 K_B T}$ is the mean free path of electrons, which varies inversely with temperature.

Substituting $\upsilon = (\frac{2E}{m*})^{1/2}$ in to Eq.(3.37) yields

$$\frac{1}{\tau_{ac}} = \frac{m_n^{*3/2} K_B T D_{ac}^2 (2E)^{1/2}}{\pi\hbar^4 C_l} \tag{3.38}$$

This can be written as

$$\tau_{ac} = \frac{\pi\hbar^4 \rho \upsilon_s^2}{m_n^{*3/2} K_B T D_{ac}^2 (2E)^{1/2}} \tag{3.39}$$

which shows that for acoustical phonon scattering τ_{ac} varies with $E^{-1/2}$ and T^{-1}, where D_{ac} is the conduction edge deformation potential and ρ,υ_s are the mass density and the sound velocity in the material respectively. Using this, and the fact that $F_0(\zeta) = \ln(1+e^\zeta)$, the acoustic-phonon scattering limited drift mobility will be

$$\mu_{ac} = \frac{2q\hbar\rho\upsilon_s^2}{3\pi n m^* D_{ac}^2} \ln(1+e^\zeta) \tag{3.40}$$

where $\zeta = \frac{E_F}{K_B T}$. This expression holds for an arbitrary degeneracy at arbitrary temperatures and number of carriers concentration.

For strongly Non-Degenerate limit ($\zeta << 1$), equation Eq.(3.40) will become

$$\mu_{ac}^{ND} = \frac{2\sqrt{2\pi} q\hbar^4 C_l}{3 m_n^{*5/2} D_{ac}^2 (K_B T)^{3/2}} \tag{3.41}$$

with a temperature $T^{-3/2}$ dependence. On the other extreme, for a strongly Degenerate case, the mobility is

$$\mu_{ac}^{D} = \frac{(\pi/3)^{1/3} q\hbar^3 C_l}{m^{*2} K_B T D_{ac}^2 n^{1/3}} \tag{3.42}$$

which is different from the non-degenerate case in the temperature dependence and a carrier concentration dependence, (where $n^{1/3} = N_C F_{1/3} = N_C \int_0^\infty \frac{\eta^{1/3} d\eta}{1+\exp(\frac{\eta-\eta_F)}{K_B T})}$ is electron concentration in terms of Fermi integral).

Equation (3.42) predicts that the electron mobility due to acoustic phonon scattering μ_{ac} varies as $T^{-1.5}$. Thus, the effect of acoustic phonon (lattice) scattering is to reduce the mobility with increase in temperature.

3.2 Electron Conductivity in N-Type Silicon

Electrical conduction takes place as a result of the motion of the free electron under the action of an applied electric field. In this section, we shall derive an expression for conductivity of n-type silicon in which the conductivity is due to excess electron as a function of electron concentration using the solution of Boltzmann transport equation formulated in chapter 2.

3.2.1 Derivation of Electron Conductivity

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 [18]

$$J = -q \int_{Cb}^{\infty} \upsilon(k) g(k) f(k) d^3k \tag{3.43}$$

where g(k) is the total density of states in k-space which is given $1/4\pi^3$, f(k) is the distribution function from Eq.(2.39), $\upsilon(k)$ 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 (3.43) can be written as

$$J = -\frac{2q}{(2\pi)^3} \int \upsilon f(k) d^3k \tag{3.44}$$

Since no current flows in equilibrium, f_o does not contribute to the electric field current. Therefore, substituting Eq.(2.39) in to Eq.(3.44), we obtain

$$J = \frac{-2q^2}{(2\pi)^3} E \int \tau \upsilon_k^2 \frac{df_0}{d\varepsilon} d^3k \tag{3.45}$$

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

$$J_x = \frac{-2q^2}{(2\pi)^3} E_x \int \tau \upsilon_x^2 \frac{df_0}{d\varepsilon} d^3k \tag{3.46}$$

Using the relation

$$n = \frac{2}{(2\pi)^3} \int f_0 d^3k \tag{3.47}$$

Equation (3.48) is written as

$$J_x = -q^2 n E_x \frac{\int \tau \upsilon_x^2 \frac{df_0}{d\varepsilon} d^3k}{\int f_0 d^3k} \tag{3.48}$$

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

$$\frac{\partial f_0(\varepsilon)}{\partial \varepsilon} = \frac{-1}{K_B T} f_0 (1 - f_0) \tag{3.49}$$

Therefore, Eq.(3.48) becomes

$$J_x = \frac{q^2 n E_x}{K_B T} \frac{\int \tau \upsilon_x^2 f_0 (1 - f_0) d^3k}{\int f_0 d^3k} \tag{3.50}$$

Since the term $\tau(1 - f_0)$ in the integral of (3.50) is a function of the energy ε, we express it as $\phi(\varepsilon)$ and it is true that $\int \upsilon_x^2 \phi(\varepsilon) d^3k = \int \upsilon_y^2 \phi(\varepsilon) d^3k = \int \upsilon_z^2 \phi(\varepsilon) d^3k = \frac{1}{3} \int \upsilon^2 \phi(\varepsilon) d^3k$

We have

$$J_x = \frac{q^2 n E_x}{3 K_B T} \frac{\int \tau \upsilon^2 f_0 (1 - f_0) d^3k}{\int f_0 d^3k} \tag{3.51}$$

The integral with respect to d^3k is changed in to an integral with respect to ε by using the relation $\varepsilon = \frac{\phi^2 k^2}{2m^*}$, we obtain

$$d^3k = 4\phi k^2 dk = \frac{8\phi m^{*3/2}}{\sqrt{2}\hbar^3} \varepsilon^{1/2} d\varepsilon \tag{3.52}$$

Therefore Eq.(3.51) will be

$$J_x = \frac{q^2 n E_x}{3 K_B T} \frac{\int_0^\infty \tau \upsilon^2 \varepsilon^{1/2} f_0 (1 - f_0) d\varepsilon}{\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon} \tag{3.53}$$

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

$$J_x = \frac{2q^2 n E_x}{3K_B T m^*} \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0 (1 - f_0) d\varepsilon}{\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon} \tag{3.54}$$

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. Next, we carry out the calculation of Eq.(3.54) for the following two cases separately.

(i) **Degenerate Semiconductor**.

In this case the Fermi energy ε_F is located in the conduction band, and the term $-df_o/d\varepsilon = f_o(1 - f_o)/K_B T$ 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,

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

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

hold for the Fermi distribution function, and therefore we obtain

$$\frac{1}{K_B T} \int_0^\infty \tau(\varepsilon) \varepsilon^{3/2} f_0 (1 - f_0) d\varepsilon = -\int_0^\infty \tau(\varepsilon) \varepsilon^{3/2} \frac{df_0}{d\varepsilon} \cong \tau(\varepsilon_F) \varepsilon_F^{3/2} \tag{3.55}$$

$$\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon = \int_0^{\varepsilon_F} \varepsilon^{1/2} d\varepsilon = \frac{2}{3} \varepsilon_F^{3/2} \tag{3.56}$$

Inserting these relations into Eq.(3.54), we obtain

$$J_x = \frac{n e^2 \tau(\varepsilon_F)}{m^*} E_x \tag{3.57}$$

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 is obtained from Eqs.(3.46) and (3.54) is given by

$$\varepsilon_F = \frac{\hbar^2}{2m^*} (3\pi^2 n)^{2/3} \tag{3.58}$$

(ii) **Non-Degenerate semiconductor**.

This is a case where $f_0 \ll 1$ and $1 - f_0 \ll 1$. Thus, Eq.(3.53) becomes

$$J_x = \frac{2q^2 n E_x}{3K_B T m^*} \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0 d\varepsilon}{\int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon} \tag{3.59}$$

Integration by parts gives rise to

$$\int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon = \frac{3}{2} K_B T \int_0^\infty \varepsilon^{1/2} f_0 d\varepsilon \tag{3.60}$$

Using this relation we obtain

$$J_x = \frac{q^2 n E_x}{m^*} \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0 d\varepsilon}{\int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon} \tag{3.61}$$

Solving the integration, we get

$$J_x = \frac{q^2 n \langle \tau \rangle}{m^*} E_x \tag{3.62}$$

the relation $\langle \tau \rangle$ is given by

$$\langle \tau \rangle = \frac{\int_0^\infty \tau \varepsilon^{3/2} f_0 d\varepsilon}{\int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon} \tag{3.63}$$

and $\langle \tau \rangle$ represents the average of $\langle \tau \rangle(\varepsilon)$

When we define the average velocity of the electron by $\langle \upsilon_x \rangle$ in the presence of an electric field in the x direction, it is also calculated from Eq.(3.63). The average velocity is often referred to as the drift velocity. This is because the electron contributes to the current via drift motion along the electric field direction, suffering from collisions. The average time between the scattering events (collisions) or the scattering rate (collision rate) is given by the average value of the relaxation time $\langle \tau \rangle$.

Using the electron density n, the current density is written as

$$J_x = \sigma E_x = \frac{n q^2 \langle \tau \rangle}{m^*} E_x \tag{3.64}$$

where σ is the electron conductivity of a given material (silicon) defined as [9]

$$\sigma = \frac{J_x}{E_x} = \frac{n q^2 \langle \tau \rangle}{m^*} = n q \mu \tag{3.65}$$

For different scattering mechanisms, Eq.(3.65) can be written as

$$\sigma_T = n q \mu_T \tag{3.66}$$

And μ_T is the total electron mobility due to ionized impurity and acoustic phonon scattering and is obtained by using reciprocal sum formula which is given by

$$\mu_T^{-1} = \sum_i \mu_i^{-1} \tag{3.67}$$

This implies that

$$\mu_T^{-1} = (1/\mu_I + 1/\mu_{ac})^{-1} \tag{3.68}$$

where μ_I and μ_{ac} are ionized impurity scattering mobility and deformation potential acoustic phonon scattering mobility, respectively.

Chapter 4

Result and Discussion

4.1 Numerical Computations of Electrical Conductivity

In order to carry out the numerical calculations of the total electron conductivity in an n-type silicon as a function of temperature and total electron concentration n, we need to know the numerical values of ionized impurity scattering mobility μ_I and acoustic phonon scattering mobility μ_{ac} given respectively by Eqns.(3.24), (3.25), (3.41) and (3.42). In the calculation, we have used the constant values of various parameters like: deformation potential of acoustic phonon D_{AC}= 9.0eV, permittivity of Si ε_s= 11.7, etc.

As we have seen under each equation of electron mobilities discussed in chapter three that, the mobility depends on both temperature and dopant concentration. From eqns.(3.24) and (3.41), the approximate temperature dependence of mobility due to lattice scattering is $T^{-3/2}$, while the temperature dependence of mobility due to impurity scattering is $T^{+3/2}$. Thus, lattice scattering cause the mobility to decrease with increasing temperature and impurity scattering is typically only seen at low temperatures. These dependence comes from the scattering time τ which is the time between two scattering events.

To compute the relaxation time and temperature using *Eqs.*(3.20), the numerical computation gives the following results. Figure 4.1 shows the very small variation of relaxation time of

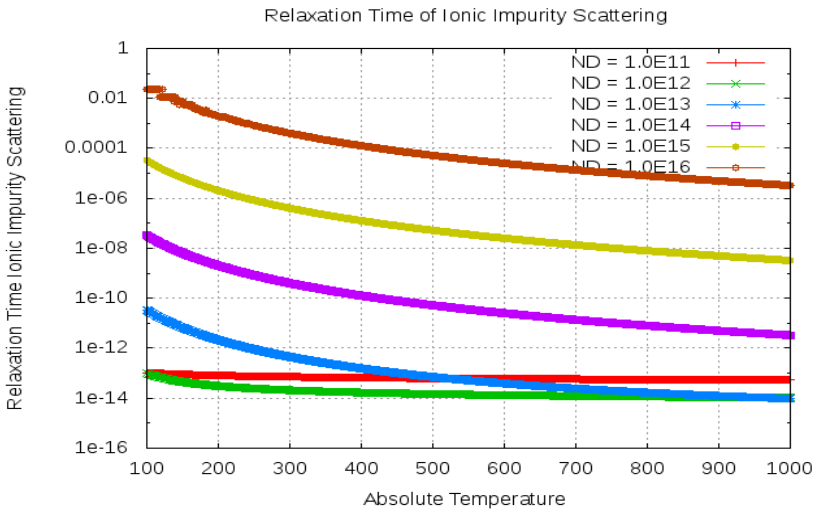

Figure 4.1: *Relaxation time of ionized impurity verses absolute Temperature (at* $10^{11} \leq N_D \leq 10^{16}\ cm^{-3}$.)

impurity scattering with temperature T. It can be seen from this figure that, at low temperatures carriers move more slowly, so there is more time for them to interact with charged impurities. This implies that, as temperature decrease the relaxation time increase. From eqn.(3.41) the drift mobility due to acoustic phonon deformation potential scattering μ_{ac} is proportional to the temperature. This means that electron conductivity due to this scattering mechanism also proportional to $T^{-3/2}$. The effect of acoustic phonon deformation potential scattering is therefore to reduce the conductivity with increasing temperature.

Ionized impurity scattering mobility μ_I is also directly proportional to temperature, the conductivity due to ionized impurity increases with temperatures opposite to the behavior observed with acoustical phonon deformation scattering mobility.

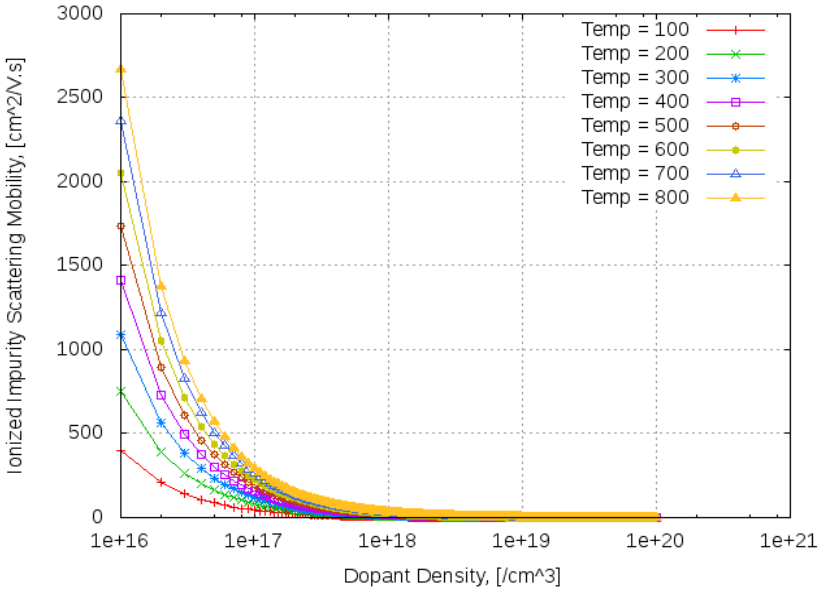

Figure 4.2: *Ionized impurity scattering mobility μ_I as a function of doping density N_D.*

Figure 4.2 shows the variation of particle (electron) mobility as a function of dopant density at temperature between $100 \leq T \leq 800$ using eqn.(3.25). One can see from the figure that as impurity scattering mobility 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.

At low temperatures conductivity actually increases with temperature since impurity scattering dominates, while at high temperature acoustic phonon scattering dominates. This is shown in figure 4.3 below.

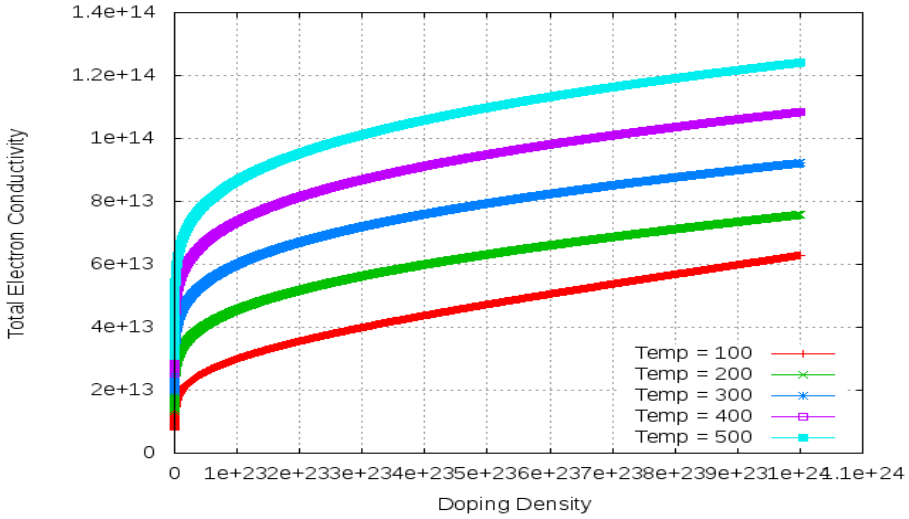

Figure 4.3: Total Electron Conductivity versus Donor Concentration for Temperature ranges from $100 \leq T \leq 500K$.

At low dopant concentrations acoustic phonon scattering potential dominates over the entire temperature range. With increasing dopant concentrations impurity scattering starts to dominate at low temperature. For low N_D conductivity increases with temperature, but as N_D increases at low temperature conductivity actually decreases.

Chapter 5

Conclusion

This work presents the investigation of how the electrical conductivity of n-type silicon depends on the electron concentration and temperatures at varies ranges. The expression for total electron conductivity as a function of dopant density and temperatures has been formulated for n-type silicon and calculated numerically by appropriately combining lattice and ionized impurity scattering combinations. We carried out a numerical computation of the equations to compute the variation of relaxation time, mobility and conductivity with dopant density and temperature. From the result of our simulation we have observed that, at low temperatures carriers move more slowly, so there is more time for them to interact with charged impurities.

Based on the data generated by the numerical computation, we have plotted the variation of total electron conductivity from combination of impurity scattering and acoustic phonon scattering as a function of electron concentration n and temperature T. As shown in the plots, as temperature increases the total:

(i) electron relaxation time decreases

(ii) electron mobility increases

(iii) electron conductivity decreases

Moreover, as the dopant density increases, the total:

(i) electron relaxation time increases

(ii) electron mobility decreases

(iii) electron conductivity increases

At low temperatures impurity scattering dominates, while at high temperature acoustic

phonon scattering dominates. At low dopant concentration acoustic phonon scattering dominates over the entire temperature range. With increasing dopant concentrations impurity scattering starts to dominate at low temperature. Therefore, one can see that the electron concentration and temperature can affect the conductivity of carriers.

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DECLARATION

I hereby declare that this master of science thesis is my original work and it has not presented for a degree in any other university and that all sources of material used for the thesis have been dully acknowledged.

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