Some Transport Coefficients
in
Heavily Doped n-Type Silicon

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ABSTRACT

The Boltzmann transport equation has been solved applying the relaxation time approximation in the presence of weak electric and magnetic fields to obtain a general expression for the anisotropic part of the distribution function of the degenerate free electron gas in heavily doped n-type silicon. The isotropic part of the distribution function was assumed to be the Fermi-Dirac distribution function and the constant energy surfaces in k-space are considered to be ellipsoidal. The energy band distortion was taken into consideration by using the Slotboom's approximation for the general expression of the quantum density of states in heavily doped semiconductors given by Kane.

Employing the results of the Boltzmann transport equation expression have been derived for the electron drift mobility, the Hall coefficient, and the coefficient of transverse magnetoresistance valid for both the parabolic and non-parabolic density of states assuming ionized impurity scattering to be the dominant scattering mechanism.

Finally, a numerical calculation for the normalized Fermi energy, electron drift mobility, Hall coefficient , and coefficient of transverse magnetoresistance using the parabolic and the non-parabolic density of states in the impurity concentration range from $1x10^{18}$ to $2x10^{20}$ cm^{-3} at 300°K reavils that taking the band tail states in the quantum density of states reduces the magnitudes of these coefficients by as much as 37%, 59%, 54%, and 24%, respectively.

silicon using Mahan's [15] treatment to calculate many body shifts in both the conduction and valance bands and the non-parabolic density of states suggested by Slotboom [12] and from their calculations they obtained excellent agreement between the theoretical and the experimental values for both optical and electrical band gap narrowing in heavily doped n-type silicon for various doping concentrations.

Sharma [16] has calculated the diffusion mobility ratio, i.e., D/μ in a heavily doped n-type silicon using the non-parabolic density of states and has compared these results with those obtained by using the parabolic density of states. His calculations have shown that the difference between the two calculations can be as high as 20% . Moreover, from his calculations he also concluded that any serious calculation of the transport coefficients in heavily doped materials must incorporate the effect of band tails.

In light of these excellent agreements between theory and experiment, as confirmed by Lee and Fossum [14], one expects that the band tails arising due to the randomness of impurities should significantly modify the transport properties of highly doped materials. Therefore, it seems useful to calculate theoretically the various transport coefficients in heavily doped semiconductors taking into account the band tail density of states. However, to the best of our knowledge no theoretical calculation of any other transport coefficients in heavily doped silicon has been reported in the literature which take into account the band tails due to the random impurity distribution.

In this research wok, an attempt will be made to illustrate that taking the band tails into account can significantly affect the calculation of the transport coefficients in heavily doped n-type silicon having many-valley type energy band structure with ellipsoidal constant energy surfaces. In this thesis, we shall calculate the three most important transport coefficients, i.e., the drift mobility, the Hall coefficient, and the coefficient of magnetoresistance in heavily doped n-type silicon taking into account the anisotropy of the crystal structure, the degeneracy of the free carriers, and the distortion of the energy band structure. The impurities are considered to be donors and contribute a single electron to the conduction band. We also assumed that at $300^0 K$, all the impurities are ionized, and thus the electron concentration in the conduction band is equal to the donor concentration N_d.

In section (2.1) we discuss the energy band structure of lightly and heavily doped n-type silicon, and give the explicit expressions of the parabolic and the non-parabolic

density of states.

In section (2.2) we first formulate the Boltzman transport equation using the relaxation time approximation in the presence of dc electric and magnetic fields and then by linearizing this general equation, we solve it to obtain an expression for the anisotropic part of the electron distribution function.

In section (2.3), we derive a general expression of the electron current density $\vec{J}$ in terms of the conductivity coefficients using the anisotropic part of the distribution function derived in section (2.2). Next we evaluate the three conductivity coefficients assuming ellipsoidal constant energy surfaces. Finally, assuming a transverse orientation for the magnetic field and the current, it is seen that most of the components of these tensors will vanish and we are left only with a few of them. As a result of this assumption, the general expression for the current density will reduce to a simplified expression and thus we get an expression for the current density which is the modified form of that obtained by F. Seitz [1].

In chapter 3, we derive a general expression for the drift mobility, the Hall coefficient, and the coefficient of magnetoresistance using the parabolic as well as the non-parabolic density of states.

Finally, in chapter 4, we use the general expressions derived in chapter 3 to compute the drift mobility, the Hall coefficient, and the coefficient of magnetoresistance numerically in n-type silicon in the range of impurity concentration from 1×10^{18} to 2×10^{20} cm^{-3} at $300^{o}K$. We also plot the normalized drift mobility, Hall coefficient, and coefficient of magnetoresistance as a function of n_n. At the end we present a comparison of our results obtained by using the non-parabolic density of states with the corresponding values calculated by using the parabolic density of states.

2 Electron Transport Phenomena

In this chapter we shall briefly describe the band structure of silicon, the density of states in moderately as well as heavily doped n-type silicon. We shall then solve the Boltzmann transport equation in the presence of both electric and magnetic fields to obtain an expression for the anisotropic part of the electron distribution function. This will further be used to obtain an expression for the current density and the conductivity coefficients.

2.1. Energy Surfaces and Density of States (DOS) in n-type Silicon

In this section we shall discuss the constant energy surfaces, the density of states and the the energy band distorsion due to band tails and many body effects.

2.1.1. Eqi-energy surfaces and density of states in lightly doped n-type silicon

In lightly or moderately doped semiconductors, the concentration of the impurity atoms is strongly diluted and as a result, the wave functions associated with the electrons of the impurity atoms do not overlap. Therefore, the energy levels of the impurity atoms are discrete. In this case, the semiconductor still can be considered as having a perfect periodicity, and thus the conduction and valance-band edges as well as the donor and acceptor-state energies are well defined. These energies coincide with their respective positions in the intrinsic semiconductor, and as a result, the density of states versus energy obeys a square-root-law.

It is well known that the conduction band of silicon has six equivalent energy valleys or energy minima whose energy ellipsoids have the cubic crystal axes as axes of rotation as shown in Fig. (1).

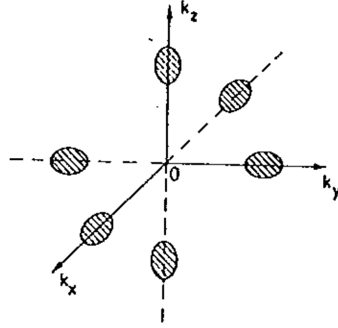

Fig. 1. Schematic diagram showing location of the six equivalent ellipsoidal conduction band valleys in silicon.

The energy function $\mathcal{E}(\vec{k})$ of electrons in the vicinity of each band edge, which are distinguished by an extreme value of the energy, $\mathcal{E}_c$, is simply obtained by a Taylor expansion about this edge value, i.e., about the wave vector $\vec{k} = \vec{k_0}$ at the edge of the conduction band $\mathcal{E}_c$:

$$\mathcal{E}(\vec{k}) = \mathcal{E}_c + \sum_{i=1}^{3} \frac{\hbar^2 (k_i - k_{i0})^2}{2m_i} + \cdots, \tag{2.1.1}$$

where $\mathcal{E}_c = \mathcal{E}(\vec{k_0})$ and m_i is the effective mass of electrons along the ellipsoid axes.

As can be seen from the above equation, the energy $\mathcal{E}$ can be represented by a quadratic function of the wave vector $\vec{k}$ if one stops the expansion after the second order term. However, the carriers, although behaving as free particles in the sense that the variation of $\mathcal{E}$ with $\vec{k}$ is parabolic for any direction of motion, have a different effective mass along each such direction. Geometrically, this means that the constant energy surfaces are ellipsoids. Moreover, as a result of the cubic symmetry of cubic crystals, $m_1 = m_2 \neq m_3$, where m_3 is the effective mass along the major axis of a given ellipsoid. Therefore, the constant energy surfaces in $\vec{k}$ space are ellipsoids of revolution about the main axes. Because one axis of these ellipsoids is distinguished, the values of the effective masses will be called longitudinal and transverse, m_L and m_T, respectively.

It follows from (2.1.5) that the surfaces of constant energy are spherical in $\vec{k}'$-space with an effective mass m^* which will disappear at the end. Using these relations one can easily show that the density of states in the νth energy ellipsoid is given by

$$\rho^{(\nu)}(\mathcal{E})d\mathcal{E} = \frac{(2m_T^2 m_L)^{1/2}}{\pi^2 \hbar^3}(\mathcal{E} - \mathcal{E}_C)^{\frac{1}{2}} d\mathcal{E}, \tag{2.1.6}$$

However, the conduction band of silicon contains six equivalent ellipsoids of revolution, and as a result, the total density of states in the conduction band for electrons becomes

$$\rho(\mathcal{E})d\mathcal{E} = \frac{1}{2\pi^2}\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}}(\mathcal{E} - \mathcal{E}_C)^{\frac{1}{2}} d\mathcal{E}, \tag{2.1.7}$$

where

$$m_n^* = M^{2/3}(m_T^2 m_L)^{\frac{1}{3}}, \tag{2.1.8}$$

is the electron density-of-states effective mass which accounts for all six conduction sub-bands in silicon and M is the number of equivalent energy minima.

2.1.2. Energy band distortion and density of states in heavily doped n-type silicon

A semiconductor is considered heavily doped for the impurity concentration in which the bound impurity states have disapeared. The situation in a heavily doped semiconductor is not as simple as that in a lightly or moderately doped semiconductor with regards to defining the band edge, $\mathcal{E}_c$ or $\mathcal{E}_v$, and to determining the degree of ionization for impurities. In a heavily doped semiconductor, therefore, we must take into account modifications introduced into the band structure by heavy impurity concentrations. The most important effects of heavy doping can be described as follows.

a) Shrinkage of the Band Gap Because of the Many Body Effects

The band gap in heavily doped semiconductors is substantially reduced. There are many reasons for the reduction of the band gap. The more important phenomena which influence the band gap at high doping densities ($N_d > 10^{18} cm^{-3}$) are due to many body effects. Using Mahan's [15] treatment to calculate many body shifts in the conduction and valance bands, Lee and Fossum [14] have identified and characterized the predominant many body

effects, i.e., carrier-carrier interactions, which are negligible when the majority electron density is low, that alter the energy band structure in highly doped n-type silicon from the fundamental structure in intrinsic and lightly doped silicon. Specifically the $\mathcal{E}$-k dispersion relations that characterize the allowed electron states are modified, and as a result, $\mathcal{E}_c$ and $\mathcal{E}_v$ are shifted away from their respective positions in intrinsic silicon, but the $\mathcal{E}$ -k curvature (dispersion relation) is unaltered.

According to them, the important may body effects which produce actual rigid shifts of the parabolic conduction and valance bands in energy-momentum ($\mathcal{E}$-k) space in heavily doped n-type silicon are the majority carrier (electrons) exchange energy and the minority carrier (hole) correlation energy. The electron exchange energy (electron -electron interaction) results in a down ward actual rigid shifts of the whole parabolic conduction band into the energy gap in $\mathcal{E}$- k space, and the hole correlation energy (electron-hole interaction) yields an actual upward rigid shift of the whole parabolic valance band into the band gap from its fundamental position in $\mathcal{E}$-k space.

b) Formation of impurity band

In lightly doped silicon, the impurity atoms create bound, discrete, and localized states all of which have the same discrete energy levels. However at high impurity concentrations approximately equal to $1 \times 10^{18}\ cm^{-3}$, the impurity atoms will interact with each other so that the wave functions of their associated electrons are going to overlap. This causes splitting of the impurity energy levels which at high impurity concentrations, greater than $1 \times 10^{18}\ cm^{-3}$, broadens to form a band known as the impurity band. The band was assumed to be symmetrical about the average impurity level which moves toward and ultimately into the the conduction band as the majority electron density increases. At the impurity concentration where the donor impurity band merges into the conduction band, the donor ionization energy is reduced to zero. Above this doping concentration the semiconductor is said to be heavily doped. Once the impurity band enters the conduction band, it is inconsequential because the bound impurity states have virtually disappeared. The donor ions are completely screened by the electrons and hence electrostatically indistinguishable from the silicon atoms. Hence in a heavily doped silicon, the free electron density n is approximately equal to the donor concentration N_d.

c) Tailing of the Band States into the Band Gap

The large number of statistically distributed impurity atoms also disturb the periodicity of the the lattice of the semiconductor. An impurity atom introduces a local variation in the potential energy of an electron because of the difference in the nuclear potentials of the impurity and host atom, and as a result, the lattice atoms surrounding the impurity atom relax into shifted positions. Such a local random variation in the potential energy modifies the positions of the band edges. As a result, the bands extend beyond their respective positions in the intrinsic semiconductor. This extended part of a band is called the band tailing.

The band tails represent, according to Kane [10], spatial averages of the quantum density of states in the conduction and valance bands, which vary because of fluctuations in the local electrostatic potential defined by the random distribution of the impurities. The fluctuation of the local potential in a highly doped semiconductor due to a random distribution of ionized impurities causes a spatially dependent distortion of the quantum density of states. Concomitantly the statistical average over the entire lattice of the density of states function, which defines the macroscopic properties of the semiconductor, shows "tailing" into the energy gap of both the conduction and valance band density of states; the bands are no longer parabolic near the extrema.

The general quantum density of states function, $\rho(\mathcal{E})$, based on the statistical average over the lattice is then quite complex in a highly doped semiconductor. This complexity is illustrated for n-type silicon in Fig.(3), which shows band tails and an impurity (donor) band superimposed on the parabolic conduction and valance bands.

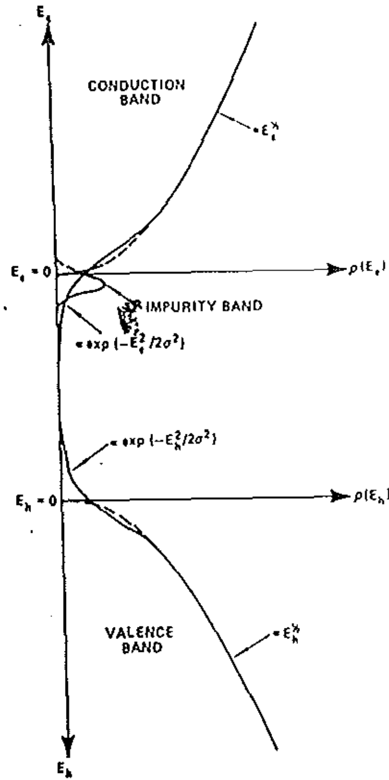

Fig. 3. Superimposed quantum density of states function for highly doped n-type silicon including the donor impurity band and the conduction - and valance- band tails. For simplicity the functions are described interms of the electron ($\mathcal{E}_e$) and hole ($\mathcal{E}_h$) energies defined in the figure.

To describe the macroscopic density of states function, Kane [10] assumed that the variation of the local potential were sufficiently slow that a local density of states Eq. (2.1.7), could be defined as if the local potential were constant. As a result, following Lee and Fossum [14], the simplified form of the general expression for the quantum density of states, which as shown by Kane [10] is the statistical average of the local density over the lattice, in the conduction band of heavily doped n-type silicon is given by:

$$\rho(\mathcal{Z}) = \frac{m_n^{*3/2} 2^{5/4} \sigma^{\frac{3}{2}}}{\pi^2 \hbar^3} Y(\mathcal{Z}), \tag{2.1.9}$$

where

$$Y(\mathcal{Z}) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\mathcal{Z}} (\mathcal{Z} - \zeta)^{\frac{1}{2}} \exp(-\zeta^2)\, d\zeta, \tag{2.1.10}$$

and

$$\mathcal{Z} \equiv \frac{\mathcal{E}}{\sqrt{2}\sigma}, \tag{2.1.11}$$

and σ is the standard deviation of the Gaussian distribution function for the potential energy, which is defined by the random impurity distribution.

To numerically account for the band tails in our model for the energy band structure in highly doped n-type silicon, we note that $Y(\mathcal{Z})$ in (2.1.9), which is defined in (2.1.10), can be approximated by [12]:

$$Y(z) \simeq z^{\frac{1}{2}}(1 - \frac{1}{16z^2}); \tag{2.1.12}$$

for $z > 0.601$,

$$Y(z) \simeq \frac{1}{2\pi^{\frac{1}{2}}} \exp(-z^2)[1.225 - 0.906[1 - \exp(2z)]], \tag{2.1.13}$$

for $z \leq 0.601$.

Now following Lee and Fossum [14], we can assume that all the N_d donors are ionized at $300^o K$, and as a result, the total mobile electron concentration n in the conduction band of a heavily doped n-type silicon is equal to the donor (dopant) concentration N_d, i.e.,

$$N_d \simeq n = \int_{-\infty}^{+\infty} \rho_e(\mathcal{E})\, f_0(\mathcal{E})\, d\mathcal{E}, \tag{2.1.14}$$

where $\rho_e(\mathcal{E})$ is now the non-parabolic density of states which is appropriate for the heavily doped semiconductor and is given by (2.1.9), and $f_0(\mathcal{E})$ is the Fermi-Dirac distribution function given by

$$f_0(\mathcal{E}) = \frac{1}{1 + \exp\left(\frac{\mathcal{E} - \mathcal{E}_F}{k_B T}\right)}, \tag{2.1.15}$$

where $\mathcal{E}_F$ is Fermi energy, k_B is the Boltzmann constant, and T is the absolute temperature. If the Coulomb potential of the ionized impurity atoms is only screened by the free carriers (electrons), the expression for σ [14] is given by:

$$\sigma = \left(\frac{N_d \lambda e^4}{8\pi\epsilon^2}\right)^{1/2} \tag{2.1.16}$$

where ϵ is the permitivity of silicon, and λ is the screening length in the Thomas-Fermi model, where a higher carrier density requires the application of the Fermi-Dirac statistics. In semiconductors mostly free electrons rather than ions provide screening, and thus we have the following expression for screening length [25]

$$\lambda = \left[\frac{\pi^{4/3}\epsilon\hbar^2}{3^{1/3}N_d^{1/3}m_n^* e^2}\right]^{1/2}. \tag{2.1.17}$$

Now substituting (2.1.17) into (2.1.16), we get:

$$\sigma = \frac{\pi^{7/12}e^{3/2}\hbar^{1/2}N_d^{5/12}}{\epsilon_d^{3/4}m_n^{*1/4}3^{1/12}}, \tag{2.1.18}$$

where ϵ_d is the dielectric constant of the given semiconductor.

On inserting (2.1.15) and (2.1.9) into (2.1.14) and taking into account (2.1.12) and (2.1.13), we get the following expression for the electron concentration in the conduction band of a heavily doped n-type silicon:

$$N_d = \frac{m_n^{*3/2}2^{5/4}\sigma^{3/2}}{\pi^2\hbar^3}\psi_0, \tag{2.1.19}$$

where

$$\psi_0 = \frac{1}{2\pi^{\frac{1}{2}}}\int_{-\infty}^{+0.601}\frac{\exp(-\mathcal{Z}^2)[0.319-(0.906)\exp(2\mathcal{Z})]}{\left(1+\exp[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta]\right)}\,d\mathcal{Z} + \int_{+0.601}^{+\infty}\frac{\mathcal{Z}^{1/2}(1-\frac{1}{(4\mathcal{Z})^2})}{\left(1+\exp[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta]\right)}\,d\mathcal{Z}, \tag{2.1.20}$$

where η is the dimensionless Fermi-energy and is given by

$$\eta = \frac{\mathcal{E}_F}{k_BT} \tag{2.1.21}$$

2.2. The Boltzmann Transport Equation (BTE)

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 the semiconductor.

A non vanishing macroscopic current density arises whenever the semiconductor is subjected to an external electric field, temperature and concentration gradients. Under the influence of these fields and gradients the equilibrium distribution of electrons in each region of the semiconductor is then deformed and becomes anisotropic because electrons move from filled states to adjacent empty states. The central problem of any transport theory is the calculation of the anisotropic part of the electron distribution function which determines the the magnitude of the macroscopic current density.

To obtain the expression of the anisotropic part of the electron distribution function, we shall solve Boltzman's transport equation in the presence of external electric, magnetic, and thermal fields.

2.2.1 Formulation of the Boltzmann transport equation

Conventionally, one uses an accounting procedure for carriers in phase space, i.e., in a six-dimensional space and momentum representation (x, y, z, k_x, k_y, k_z). The population of electrons in a region of phase space is given by the distribution function $f(\vec{k}, \vec{r}, t)$. It is also conventional to fix $f(\vec{k}, \vec{r}, t)$ so that it gives the probability that an electron will occupy a state with wave vector $\vec{k}$ and a given spin orientation in the neighborhood of the point $\vec{r}$ at time t. Since the distribution function changes with time, a group of electrons within a volume element of phase space will move and reside in different volume elements as time progresses. Considering the deformation due to the time dependence of $\vec{r}$ and $\vec{k}$ one obtains, using only the first term of a Taylor expansion:

$$\frac{\partial f}{\partial t} + \frac{d\vec{r}}{dt} \cdot \vec{\nabla}_r f + \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k f = \left(\frac{\partial f}{\partial t}\right)_c . \qquad (2.2.1).$$

The first term accounts for the local change of the distribution in time, the second term for the change in real space, the third term for the change in momentum space, and the term on the right hand side is the collision term which denotes the rate at which f changes at the point $(\vec{k}, \vec{r})$ as a result of collisions suffered by electrons.

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

$$\left(\frac{\partial f}{\partial t}\right)_c = \frac{d\vec{r}}{dt} \cdot \vec{\nabla}_r f + \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k f, \qquad (2.2.2).$$

where

$$\frac{d\vec{k}}{dt} = \frac{\vec{F}}{\hbar} = \frac{q}{\hbar}\left[\vec{E} + \frac{1}{c}(\vec{v} \times \vec{B})\right]. \tag{2.2.3}$$

Here $\vec{E}$ and $\vec{B}$ are the external dc electric and magnetic fields, respectively, q is charge of an electron, and $\vec{v}$ is the group velocity of the electron wave packet and is given by

$$\frac{d\vec{r}}{dt} = \vec{v} = \frac{1}{\hbar}\vec{\nabla}_k \mathcal{E}, \tag{2.2.4}$$

where $\mathcal{E}$ is the kinetic energy of electrons.

2.2.2 Boltzmann's transport equation in the relaxation time approximation

The important part for the carrier transport is the collision term of Eq. (2.2.2), which provid the 'friction' for the carrier transport. In the relaxation time approximation, the collision term is given by [25]:

$$\left(\frac{\partial f}{\partial t}\right)_c = -\left(\frac{f - f_0}{\tau}\right) \qquad (2.2.5),$$

where f is the total deformed distribution function, f_0 is the unperturbed distribution function, and τ is the relaxation time which depends only on the collision processes and not on the external fields. For most of the cases τ depends on the energy $\mathcal{E}$ of electrons.

Upon substituting Eqs. (2.2.3) and (2.2.5) into Eq. (2.2.2), the steady state Boltzmann transport equation, which describes the transport of electrons under the influence of external fields takes the form:

$$\vec{v} \cdot \vec{\nabla}_r f + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f = -\frac{f - f_0}{\tau} \tag{2.2.6}$$

2.2.3 Solution of the linearized Boltzmann transport equation

Now we proceed to seek the solution of Eq. (2.2.6) in the form of a series:

$$f(\vec{k},\vec{r}) = f_0(\vec{k},\vec{r}) + f_1(\vec{k},\vec{r}) + f_2(\vec{k},\vec{r}) + f_3(\vec{k},\vec{r}) + \cdots, \qquad (2.2.7),$$

where $f_0(\vec{k},\vec{r})$ is the isotropic part of the total deformed distribution function, i.e., the equilibrium distribution function of the particles and is assumed to be the Fermi- Dirac

distribution function, $f_1(\vec{k},\vec{r}); f_2(\vec{k},\vec{r})$ are the first, second, etc. order corrections to the equilibrium distribution function. Because of our assumption that the external fields are weak, $f_1(\vec{k},\vec{r}) + f_2(\vec{k},\vec{r}) + \cdots$ can be treated as a small perturbation. Therefore, in the first approximation, we shall retain only the first-order term $f_1(\vec{k},\vec{r})$ in Eq.(2.2.7), and all the higher orders would be neglected. Thus in the first order approximation we have the following expansion for f:

$$f(\vec{k},\vec{r}) = f_0(\vec{k},\vec{r}) + f_1(\vec{k},\vec{r}). \tag{2.2.8}$$

Substituting (2.2.8) into (2.2.6) we obtain the following equation for $f_1(\vec{k},\vec{r})$:

$$\vec{v}\cdot\vec{\nabla}_r\left[f_0(\vec{k},\vec{r}) + f_1(\vec{k},\vec{r})\right] + \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k\left[f_0(\vec{k},\vec{r}) + f_1(\vec{k},\vec{r})\right] = -\frac{f_1(\vec{k},\vec{r})}{\tau} \tag{2.2.9}$$

In the most general case T and $\mathcal{E}_F$ may depend on $\vec{r}$. Upon performing the differentiations and on taking into account (2.2.3), Eq. (2.2.9) reduces to:

$$\frac{\partial f_0}{\partial\mathcal{E}}\left(\vec{X}\cdot\vec{v}\right) + \vec{v}\cdot\vec{\nabla}_r f_1(\vec{k},\vec{r}) + \frac{q}{\hbar}\vec{E}\cdot\vec{\nabla}_k f_1(\vec{k},\vec{r}) + \frac{q}{\hbar c}\left(\vec{v}\times\vec{B}\right)\cdot\vec{\nabla}_k f_1(\vec{k},\vec{r}) = -\frac{f_1(\vec{k},\vec{r})}{\tau}, \tag{2.2.10}$$

where

$$\vec{X} = q\vec{E} - \vec{\nabla}_r\mathcal{E}_F - \left(\frac{\mathcal{E}-\mathcal{E}_F}{T}\right)\vec{\nabla}_r T. \tag{2.2.11}$$

Making use of the assumption that $\vec{\nabla}_r T$, $\vec{\nabla}_r\mathcal{E}_F$, as well as $\vec{E}$, are first order quantities, and the derivatives of f_1 are of the same order of magnitude as that of f_2, and on equating the first order terms in equation (2.2.10), we obtain

$$f_1(\vec{k},\vec{r}) = -\tau(\mathcal{E})\frac{\partial f_0}{\partial\mathcal{E}}\left(\vec{v}\cdot\vec{X}\right). \tag{2.2.12}$$

It follows from Eq. (2.2.12) that $f_1(\vec{k},\vec{r})$, to the first approximation, is independent of the magnetic field and thus the influence of a magnetic field can no longer be taken as a small perturbation. Therefore, the term proportional to the gradient of f_1 must also be taken into consideration, and as a result , we get the following expression for f_1.

$$f_1(\vec{k},\vec{r}) = -\tau\frac{\partial f_0}{\partial \mathcal{E}}\left(\vec{v}\cdot\vec{X}\right) - \frac{q\tau}{\hbar c}\left(\vec{v}\times\vec{B}\right)\cdot\vec{\nabla}_k f_1(\vec{k},\vec{r}). \tag{2.2.13}$$

Equation (2.2.13) is the linearized Boltzmann transport equation which can be solved by iteration. In order to obtain a more general solution for f_1, which is valid for any order of $\vec{B}$, we can rewrite (2.2.13) in a more convenient form by introducing a new variable Φ defined by

$$f_1(\vec{k},\vec{r}) = -\frac{\partial f_0}{\partial \mathcal{E}}\Phi(\vec{k},\vec{r}), \tag{2.2.14}$$

which remains to be determined. Substituting Eq. (2.2.14) into (2.2.13), one obtains

$$\Phi(\vec{k},\vec{r}) = \tau\left(\vec{X}\cdot\vec{v}\right) - \frac{q\tau}{\hbar c}\left(\vec{v}\times\vec{B}\right)\cdot\vec{\nabla}_k\Phi(\vec{k},\vec{r}) \tag{2.2.15}$$

Now the magnetic term of the above equation can be rewritten as:

$$\left(\vec{v}\times\vec{B}\right)\vec{\nabla}_k\Phi = -\left(\vec{B}\cdot\vec{\Omega}\right)\Phi, \tag{2.2.16}$$

where

$$\vec{\Omega} = \vec{v}\times\vec{\nabla}_k = \frac{1}{\hbar}\vec{\nabla}_k\mathcal{E}\times\vec{\nabla}_k, \tag{2.2.17}$$

is a vector differential operator in $\vec{k}$-space.

Finally, using Eq. (2.2.16), the expression for the unknown function takes the following form:

$$\Phi(\vec{k},\vec{r}) = \overline{X} + (\vec{B'}\cdot\vec{\Omega})\ \Phi(\vec{k},\vec{r}), \tag{2.2.18}$$

where

$$\vec{B'} = \frac{q\tau}{\hbar c}\vec{B}, \tag{2.2.19a}$$

$$\overline{X} = \tau(\vec{X}\cdot\vec{v}). \tag{2.2.19b}$$

We are therefore dealing with a linear partial differential equation of the first order for Φ, whose solution can be found. The corresponding integral expression, however, is very cumbersome. In practice, therefore, we content ourselves with an approximation for

magnetic fields that are not too strong. We do this by an iterative method, proceeding from the limiting case $\vec{B} = 0$ for which $\Phi = \overline{X}$. If this expression is substituted on the right hand side of Eq. (2.2.18), we obtain a first approximation and when the method is continued a solution in rising powers of the magnetic field is obtained.

$$\Phi(\vec{k}, \vec{r}) = \overline{X} + (\vec{B'} \cdot \vec{\Omega})\overline{X} + (\vec{B'} \cdot \vec{\Omega})(\vec{B'} \cdot \vec{\Omega})\overline{X} + \cdots \qquad (2.2.20)$$

This is the formal solution of the linearized BTE, Eq. (2.2.18). Substituting Eq. (2.2.20) into Eq.(2.2.14), we get the the following expression for the distribution function f_1:

$$f_1(\vec{k}, \vec{r}) = -\frac{\partial f_0}{\partial \mathcal{E}} \left[\overline{X} + (\vec{B'} \cdot \vec{\Omega})\overline{X} + (\vec{B'} \cdot \vec{\Omega})(\vec{B'} \cdot \vec{\Omega})\overline{X} + \cdots\right]. \qquad (2.2.21)$$

Equation (2.2.21) is a very general expression for the anisotropic part of the distribution function which takes into account the inhomogeneities on account of gradients in temperature and electron density.

In the following sections we shall consider a homogeneous semiconductor so that the spatial gradients of the temperature, Fermi-energy, electron concentration, etc. will vanish. On account of this assumption the expression for $\overline{X}$ reduces to:

$$\overline{X} = q\tau(\vec{v} \cdot \vec{E}). \qquad (2.2.22)$$

Since we are dealing with the effect of a uniform and time independent electric and magnetic fields, the differential operator $\vec{\Omega}$ does not act on them. Now on inserting Eq. (2.2.22) into Eq. (2.2.20), the expression for $\Phi(\vec{k})$ takes the form

$$\Phi(\vec{k}) = q\tau(\vec{E} \cdot \vec{v}) + \frac{q^2\tau}{\hbar c}\vec{B} \cdot \vec{\Omega}\left(\tau\vec{E} \cdot \vec{v}\right) + \frac{q^3\tau}{\hbar^2 c^2}\vec{B} \cdot \vec{\Omega}\left[\vec{B} \cdot \vec{\Omega}\left(\tau\vec{E} \cdot \vec{v}\right)\right] + \cdots \qquad (2.2.23)$$

As mentioned before, the relaxation time τ depends only on the energy. For most of the electron scattering mechanisms the energy dependence of τ can be expressed as follows:

$$\tau = \tau_0 \mathcal{E}^{\nu}, \qquad (2.2.24)$$

where τ_0 is a weak function of $\mathcal{E}$ and thus can be taken as a constant and ν is a parameter whose numerical value depends on the scattering mechanism.

It is convenient to use tensor notions. Thus the vector operator $\vec{\Omega}$ can be rewritten as:

$$\Omega_i = \epsilon_{ikl} v_k \frac{\partial}{\partial k_l}, \tag{2.2.25}$$

where ϵ_{ikl} is the usual permutation tensor defined as:

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = +1, \; \epsilon_{213} = \epsilon_{132} = \epsilon_{321} = -1, \tag{2.2.26}$$

all other components being zero, and

$$v_k = \frac{\hbar k_k}{m_k}. \tag{2.2.27}$$

Taking into account (2.2.25), we obtain the following expression for Φ:

$$\Phi(k) = q \sum_{l=1}^{3} \tau\, v_l\, E_l + \frac{q^2}{\hbar c} \sum_{l,m=1}^{l,m=3} \tau\, E_l B_m \epsilon_{mkj} v_k \frac{\partial}{\partial k_j}(\tau\, v_l) +$$
$$\frac{q^3}{\hbar^2 c^2} \sum_{l,m,n=1}^{l,m,n=3} \tau E_l B_m B_n \epsilon_{mkj} v_k \frac{\partial}{\partial k_j} \left(\epsilon_{nrs} v_r \frac{\partial}{\partial k_s} (\tau v_l) \right) + \cdots \tag{2.2.28}$$

2.3 Electrical Current Density and Conductivity Coefficients

In this section we will derive general expressions of the conductivity coefficients of the current density valid for both the parabolic and the non-parabolic density of states in a degenerate semiconductor, which will be used to derive the expressions of the various transport coefficients.

Since in an inter-valley scattering large change in $\vec{k}$ are necessary for the transitions, such scattering mechanisms are improbable. As a result of this we can usually limit ourselves to the intra-valley scattering. In this case each energy-valley can be treated independently, and thus the contributions made to the total current by the individual energy-valleys can be simply added, so that we can start with the calculation of the contribution made by a single energy-valley.

For a semiconductor having a cubic structure, the conductivity coefficients will remain scalar despite the complicated energy surfaces. However, if we take the contribution of a single energy valley with ellipsoidal energy surfaces, which will be denoted by a suffix (ν),

then this will give a tensorial conductivity because a single ellipsoid will not fit the cubic structure; this is only so if all ellipsoids and their arrangements are taken into account. To begin with we shall calculate the current density associated with a single ellipsoid, which we shall assume to be symmetric about the k_z-axis and to be centered on the point k_{z0}, as shown in Fig.(2).

The general expression for the electrical current density $\vec{J}$ may be rewritten as

$$\vec{J} = q \int_{cb} v(\vec{k})\, \rho(\vec{k})\, f(\vec{k})\, d^3k, \tag{2.3.1}$$

where $\rho(\vec{k})$ is the total density of states in $\vec{k}$-space which is given by $\frac{1}{4\pi^3}$, $f(\vec{k})$ is the modified distribution function which, in first order approximation, is given by Eq. (2.2.8), $v(\vec{k})$ is the group velocity the electron wave packet in $\vec{k}$-space and is given by Eq. (2.2.4), d^3k is the volume element in $\vec{k}$-space, and cb indicates that the integration is over the whole conduction band.

Since the isotropic part of the distribution function f_0 makes no contribution to the current, the total current is attributed to the anisotropic part of the distribution function. On account of this fact and using Eqs. (2.2.8) and (2.2.14), we get the following expression for the current density:

$$\vec{J} = -\frac{q}{4\pi^3} \int_{cb} \frac{\partial f_0}{\partial \mathcal{E}} v(\vec{k})\, \Phi(\vec{k})\, d^3k, \tag{2.3.2}$$

where Φ is given by Eq. (2.2.28).

Since $\frac{\partial f_0}{\partial \mathcal{E}}$ decreases exponentially with energy, the integration in Eq. (2.3.2) can be taken over the whole $\vec{k}$- space. On inserting Eq. (2.2.28) into Eq. (2.3.2), an expression for the current density in weak electric fields can be obtained in rising powers of the magnetic induction $\vec{B}$ in the $\nu^{(th)}$ ellipsoid. That is,

$$J_i^{(\nu)} = \sigma_{il}^{(\nu)} E_l + \alpha_{ilm}^{(\nu)} E_l B_m + \beta_{ilmn}^{(\nu)} E_l B_m B_n + \cdots, \tag{2.3.3}$$

where

$$\sigma_{il}^{(\nu)} = -\frac{q^2}{4\pi^3} \int_{cb(\nu)} \frac{\partial f_0}{\partial \mathcal{E}} v_i\, \tau\, v_l\, d^3k, \qquad (2.3.4),$$

$$\alpha^{(\nu)}_{ilm} = -\frac{q^3}{4\pi^3\hbar c}\int_{cb(\nu)} \frac{\partial f_0}{\partial \mathcal{E}} v_i\, \tau\, v_k \frac{\partial}{\partial k_j}(\tau\, v_l)\epsilon_{mkj} d^3k, \qquad (2.3.5)$$

and

$$\beta^{(\nu)}_{ilmn} = -\frac{q^4}{4\pi^3\hbar^2 c^2}\int_{cb(\nu)} \frac{\partial f_0}{\partial \mathcal{E}} v_i\, \tau\, v_k \frac{\partial}{\partial k_j}\left(\tau\, v_r \frac{\partial}{\partial k_s}(\tau\, v_l)\right)\epsilon_{nkj}\epsilon_{mrs} d^3k. \qquad (2.3.6)$$

Here $\sigma^{(\nu)}_{il}$, which is a tensor of rank II, is the usual zero-magnetic field conductivity tensor and it determines the current produced by the electric field in the absence of a magnetic field. $\alpha^{(\nu)}_{ilm}$, which is a tensor of rank III, is associated with the Hall effect, and $\beta^{(\nu)}_{ilmn}$ is a tensor of rank IV and is associated with the magnetoresistance effect. These coefficients are often called the conductivity coefficients.

As can be seen from their definitions, the tensorial form of the conductivity coefficients is caused by the crystal anisotropy and is independent of the magnetic field. In the evaluation of the above integrals, the simple model of spherical energy surfaces is no longer adequate since it always produces scalar values. The tensorial nature of the conductivity coefficients therefore requires anisotropic energy surfaces in $\vec{k}$-space. The anisotropy of the electron energy affects the relaxation time, but for the sake of simplicity it will further be assumed that the relaxation time depends on the energy only.

Any realistic theory of transport coefficients in silicon must incorporate the following assumptions.

1) The constant energy surfaces in the neighborhood of the energy minima
   are ellipsoids of revolution with the cubic axes as axes of rotation.
2) The $\vec{k}$ coordinate axes coincides with the cubic axes.
3) The electron energy $\mathcal{E}(\vec{k})$ is given by Eq.(2.1.1) in the vicinity of each band edge.

Now we proceed to evaluate these conductivity coefficients in a single energy- valley. Since τ and $\frac{\partial f_0}{\partial \mathcal{E}}$ are even functions of k_i and v_i is an odd function of k_i, the integrand in (2.3.4) is an odd function of k_i for $i \neq l$, and thus the integral vanishes when we integrate over the whole of $\vec{k}$-space. This means that $\sigma^{(\nu)}_{il} \neq 0$ only when $i = l$, and as a result of this $\sigma^{(\nu)}_{il}$ is a diagonal tensor, that is,

$$\sigma^{(\nu)}_{il} = \sigma^{(\nu)}_{i}\,\delta_{il}. \qquad (2.3.7)$$

where δ_{il} is the kronecker delta function. This integral can be computed by integrating first over a constant energy surface and then over the energy. We can express $d\vec{k}$ interms of energy $d\mathcal{E}(\vec{k})$ using the following relation:

$$d\mathcal{E} = \vec{\nabla}_k \mathcal{E} \cdot d\vec{k} = \hbar \mid \vec{v} \mid dk_n, \tag{2.3.8}$$

where dk_n is the projection of the vector $d\vec{k}$ on the normal to the constant energy surface. Introducing the element of the energy surface ds^ν for the νth energy-valley, the element of the volume has the form:

$$d^3k = ds^\nu dk_n \tag{2.3.9}$$

Taking into account Eqs. (2.2.27) and (2.3.8), we obtain

$$d^3k = \frac{d\mathcal{E} ds^\nu}{\hbar^2 \left(\sqrt{\sum_{l=1}^{3} \frac{k_l^2}{m_l^2}}\right)}. \tag{2.3.10}$$

For the evaluation of the above integrals, we shall transform the ellipsoidal energy surfaces into spherical energy surfaces by applying the transformation given by Eq. (2.1.4), and as a result, we get the following relation

$$d^3k = \left[\frac{m_T^2 m_L}{m^{*3}}\right]^{\frac{1}{2}} d^3k', \tag{2.3.11}$$

where d^3k is the volume element in $\vec{k}$-space, and d^3k' is the volume element in $\vec{k}'$-space. Now using (2.1.7) and (2.3.11), one can easily show that:

$$d^3k = \left[\frac{m_T^2 m_L}{2m^{*2}\hbar^2}\right]^{\frac{1}{2}} \frac{dS'^\nu d\mathcal{E}}{[\mathcal{E} - \mathcal{E}_C]^{1/2}}, \tag{2.3.12}$$

where dS'^ν is the element of the energy surface in $\vec{k}'$-space. From (2.1.4) and (2.2.27), the velocity components are given by:

$$v_i = \left(\frac{m^*}{m_i}\right)^{1/2} v_i', \tag{2.3.13a}$$

where

$$v_i' = \frac{\hbar k_i'}{m^*}. \tag{2.3.13b}$$

Therefore, interms of the new variables v_i' and k_i', the energy surfaces are once more spherical and the velocity satisfies the same relation as for spherical energy surfaces.
On inserting Eqs. (2.3.12) and (2.3.13) into (2.3.4), and on setting $\mathcal{E}_c = 0$, we obtain the following expression for the conductivity tensor $\sigma_{il}^{(\nu)}$:

$$\sigma_{il}^{(\nu)} = -\frac{q^2\hbar}{4\pi^3 m^{*2}}\left(\frac{m_T^2 m_L}{2m_i m_l}\right)^{1/2}\int_{\mathcal{E}^\nu}\tau\frac{\partial f_0}{\partial\mathcal{E}}\frac{d\mathcal{E}}{\sqrt{\mathcal{E}}}\int_{S'^\nu}k_i' k_l'\, dS'^\nu \tag{2.3.14}$$

Now the integral over a surface can be represented as an integral over a space angle using the following relation

$$dS'^\nu = k'^2 d\Omega', \tag{2.3.15}$$

where $d\Omega'$ is the element of the solid angle in $\vec{k}'$-space. On carrying out the surface integration using spherical coordinates along with Eq. (2.3.15), one readily obtains:

$$\sigma_{il}^{(\nu)} = -\frac{2q^2}{3}\frac{(2m_T^2 m_L)^{\frac{1}{2}}}{\pi^2\hbar^3}\frac{\delta_{il}}{(m_i m_l)^{\frac{1}{2}}}\int_{\mathcal{E}^\nu}\tau\frac{\partial f_0}{\partial\mathcal{E}}\mathcal{E}^{\frac{3}{2}}d\mathcal{E}, \tag{2.3.16}$$

where δ_{il} -is the kronecker delta function. Finally, on taking into account Eq. (2.1.6) the contribution made by a single energy-valley to the components of the conductivity tensor reduces to:

$$\sigma_{il}^{(\nu)} = \frac{q^2 n^{(\nu)} < \tau >}{m_i}\delta_{il}, \tag{2.3.17}$$

where

$$n^{(\nu)} = \int_{\mathcal{E}^\nu}\rho^{(\nu)}(\mathcal{E})f_0(\mathcal{E})\, d\mathcal{E}, \tag{2.3.18}$$

and

$$< \tau >= -\frac{2}{3}\frac{\int_{\mathcal{E}}\tau\mathcal{E}\rho(\mathcal{E})\frac{\partial f_0}{\partial\mathcal{E}}\, d\mathcal{E}}{\int_{\mathcal{E}}\rho(\mathcal{E})\, f_0(\mathcal{E})\, d\mathcal{E}}, \tag{2.3.19}$$

in which $\rho(\mathcal{E})$ is the density of states in the whole conduction band.

Next we proceed to evaluate $\alpha_{ilm}^{(\nu)}$ employing a similar procedure. For the case when τ is a function of $\mathcal{E}$ only, one can easily show that the term involving the derivative of τ gives zero contribution. As a result of this, Eq. (2.3.5) reduces to:

$$\alpha^{(\nu)}_{ilm} = -\frac{q^3}{4\pi^3 m_l c} \int_{cb(\nu)} \frac{\partial f_0}{\partial \mathcal{E}} \tau^2 \, v_i \, v_k \epsilon_{mkl} d^3k. \tag{2.3.20}$$

Now by following exactly the same procedure as in calculating $\sigma^{(\nu)}_{il}$, we obtain:

$$\alpha^{(\nu)}_{ilm} = \frac{q^3 n^{(\nu)} < \tau^2 >}{m_i m_l c} \epsilon_{mil}, \tag{2.3.21}$$

where

$$< \tau^2 > = -\frac{2}{3} \frac{\int_{\mathcal{E}} \tau^2 \mathcal{E} \rho(\mathcal{E}) \frac{\partial f_0}{\partial \mathcal{E}} d\mathcal{E}}{\int_{\mathcal{E}} \rho(\mathcal{E}) \, f_0(\mathcal{E}) \, d\mathcal{E}}. \tag{2.3.22}$$

Employing the relation $\epsilon_{mil} = \epsilon_{ilm}$, the above expression for $\alpha^{(\nu)}_{ilm}$ reduces to

$$\alpha^{(\nu)}_{ilm} = \frac{q^3 n^{(\nu)} < \tau^2 >}{m_i m_l c} \epsilon_{ilm} \tag{2.3.23}$$

From Eq. (2.3.23), we note that $\alpha^{(\nu)}_{ilm} \neq 0$ only when $i \neq l \neq m \neq i$.

Finally, we wish to evaluate $\beta^{(\nu)}_{ilmn}$. Up on performing the differentiation by applying a similar procedure as in the evaluation of the previous two conductivity coefficients, we obtain

$$\beta^{(\nu)}_{ilmn} = -\frac{q^4}{4\pi^3 m_l m j c^2} \int_{cb(\nu)} \frac{\partial f_0}{\partial \mathcal{E}} \tau^3 \, v_i \, v_k \epsilon_{nkj} \, \epsilon_{mjl} \, d^3k. \tag{2.3.24}$$

By following exactly the same steps as in calculating $\sigma^{(\nu)}_{il}$, one can show that:

$$\beta^{(\nu)}_{ilmn} = \frac{q^4 n^{(\nu)} < \tau^3 >}{m_i m_l m_j c^2} \epsilon_{jni} \epsilon_{jlm}, \tag{2.3.25}$$

where

$$< \tau^3 > = -\frac{2}{3} \frac{\int_{\mathcal{E}} \tau^3 \mathcal{E} \rho(\mathcal{E}) \frac{\partial f_0}{\partial \mathcal{E}} d\mathcal{E}}{\int_{\mathcal{E}} \rho(\mathcal{E}) \, f_0(\mathcal{E}) \, d\mathcal{E}}. \tag{2.3.26}$$

On account of the property of the unit anti-symmetrical tensor, the product $\epsilon_{jni}\epsilon_{jlm}$ summed over j is non-zero if and only if

$$n = l \; and \; i = m \neq l, or$$

$$n = m \; and \; i = l \neq m \tag{2.3.27}$$

The product is positive in the first case and negative in the second case. Consequently, on taking into account (2.3.27), we see that $\beta^{(\nu)}_{ilmn} \neq 0$ only when the indices are equal in pairs, that is,

$$i = l \ and \ m = n \ or \ i = m \ and \ l = n \qquad (2.3.28)$$

Thus, for cubic crystals a large number of the elements of the tensor $\beta^{(\nu)}_{ilmn}$ will vanish. Finally, using (2.3.17), (2.3.23), and (2.3.25), the contribution made by a single energy-valley (in our case the (100) ellipsoid in the conduction band of silicon) to the current density can be written as :

$$J_1^{(\nu)} = \sigma_{11}^{(\nu)} E_1 + \alpha_{123}^{(\nu)} E_2 B_3 + \alpha_{132}^{(\nu)} E_3 B_2 + \beta_{1122}^{(\nu)} E_1 B_2^2 + \beta_{1133}(\nu) E_1 B_3^2 + \beta_{1212}^{(\nu)} E_2 B_1 B^2 + \beta_{1313}^{(\nu)} E_3 B_1 B_3 \qquad (2.3.29a)$$

$$J_2^{(\nu)} = \sigma_{22}^{(\nu)} E_2 + \alpha_{231}^{(\nu)} E_3 B_1 + \alpha_{213}^{(\nu)} E_1 B_3 + \beta_{2211}^{(\nu)} E_2 B_1^2 + \beta_{2233}^{(\nu)} E_2 B_3^2 + \beta_{2121}^{(\nu)} E_1 B_2 B_1 + \beta_{2323}^{(\nu)} E_3 B_2 B_3 \qquad (2.3.29b)$$

$$J_3^{(\nu)} = \sigma_{33}^{(\nu)} E_3 + \alpha_{312}^{(\nu)} E_1 B_2 + \alpha_{321}^{(\nu)} E_2 B_1 + \beta_{3311}^{(\nu)} E_3 B_1^2 + \beta_{3322}^{(\nu)} E_3 B_2^2 + \beta_{3131}^{(\nu)} E_1 B_3 B_1 + \beta_{3232}^{(\nu)} E_2 B_3 B_2 \qquad (2.3.29c)$$

The non-zero terms of (2.3.17), (2.3.23), and (2.3.25) are given by

$$\sigma_{11}^{(\nu)} = \frac{q^2 n^{(\nu)} < \tau >}{m_1}; \quad \sigma_{22}^{(\nu)} = \frac{q^2 n^{(\nu)} < \tau >}{m_2}; \quad \sigma_{33}^{(\nu)} = \frac{q^2 n^{(\nu)} < \tau >}{m_3}; \qquad (2.3.30a)$$

$$\alpha_{123}^{(\nu)} = -\alpha_{213}^{(\nu)} = \frac{q^3 n^{(\nu)} < \tau^2 >}{m_1 m_2 c}; \quad \alpha_{231}^{(\nu)} = -\alpha_{321}^{(\nu)} = \frac{q^3 n^{(\nu)} < \tau^2 >}{m_2 m_3 c}; \quad \alpha_{312}^{(\nu)} = -\alpha_{132}^{(\nu)} = \frac{q^3 n^{(\nu)} < \tau^2 >}{m_3 m_1 c}; \qquad (2.3.30b)$$

$$\beta^{(\nu)}_{1212} = \beta^{(\nu)}_{1313} = \beta^{(\nu)}_{2121} = \beta^{(\nu)}_{2323} = \beta^{(\nu)}_{3131} = \beta^{(\nu)}_{3232}; \tag{2.3.30c}$$

$$\begin{aligned}
\beta^{(\nu)}_{1212} &= \frac{q^4 n^{(\nu)} < \tau^3 >}{m_1 m_2 m_3 c^2};\\
\beta^{(\nu)}_{1122} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_1^2 m_3 c^2};\\
\beta^{(\nu)}_{1133} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_1^2 m_2 c^2};\\
\beta^{(\nu)}_{2211} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_2^2 m_3 c^2};\\
\beta^{(\nu)}_{2233} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_2^2 m_1 c^2};\\
\beta^{(\nu)}_{3311} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_3^2 m_2 c^2};\\
\beta^{(\nu)}_{3322} &= -\frac{q^4 n^{(\nu)} < \tau^3 >}{m_3^2 m_1 c^2};
\end{aligned} \tag{2.3.30d}$$

Next we have to find the total current density by adding the contribution of all the energy-valleys. As stated in section (2.1.1), the conduction band of silicon consists of six equivalent ellipsoids of revolution with the cubic axes as the axes of revolution. If we take a given crystal axis there are always two axes of rotation in the same direction and four at right angles to it. Accordingly, two $J_i^{(\nu)}$ with mass m_L and four with mass m_T contribute to the current density components in this direction. The total current density components may then be expressed as:

$$J_i = \sum_{\nu=1}^{\nu=6} J_i^{(\nu)}, \; where \; i = x, y, z \tag{2.3.31}$$

Since all the ellipsoids are equivalent, the electron density $n^{(\nu)}$ per energy-valley in the conduction band of silicon is given by:

$$n^{(\nu)} = \frac{n}{6} \tag{2.3.32}$$

Note also that

$$m_1 = m_L \; and \; m_2 = m_3 = m_T; for \; the \; (100) \; and \; (\bar{1}00) \; ellipsoids;$$

$$m_2 = m_L \; and \; m_1 = m_3 = m_T; for \; the \; (010) \; and \; (0\bar{1}0) \; ellipsoids; \tag{2.3.33}$$

$$m_3 = m_L \; and \; m_1 = m_2 = m_T; for \; the \; (001) \; and \; (00\bar{1}) \; ellipsoids;$$

In view of (2.3.32) and (2.3.33), we have

$$J_x^{(100)} = J_x^{(\bar{1}00)}; \; J_x^{(010)} = J_x^{(0\bar{1}0)}; \; J_x^{(001)} = J_x^{(00\bar{1})}; \tag{2.3.34}$$

Employing these relations, the summation in Eq.(2.3.31) may be written as :

$$J_x = 2\left[J_x^{(100)} + J_x^{(010)} + J_x^{(001)}\right]. \tag{2.3.35a}$$

A similar relation holds for the other two components,

$$J_y = 2\left[J_y^{(100)} + J_y^{(010)} + J_y^{(001)}\right], \tag{2.3.35b}$$

$$J_z = 2\left[J_z^{(100)} + J_z^{(010)} + J_z^{(001)}\right], \tag{2.3.35c}$$

Now up on performing the summation over all ellipsoids one obtains the following expression for the components of the current density

$$J_x = \sigma_0 E_x + \alpha[E_y B_Z - E_z B_y] + \beta[B_y^2 + B_z^2]E_x + \gamma[E_y B_y + E_z B_z]B_x, \tag{2.3.36a}$$

$$J_y = \sigma_0 E_y + \alpha[E_z B_x - E_x B_z] + \beta[B_z^2 + B_x^2]E_y + \gamma[E_z B_z + E_x B_x]B_y, \tag{2.3.36b}$$

$$J_z = \sigma_0 E_z + \alpha[E_x B_y - E_y B_x] + \beta[B_x^2 + B_y^2]E_z + \gamma[E_x B_x + E_y B_y]B_z. \tag{2.3.36c}$$

Here after seting $q = (-e)$ for electrons we have

$$\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_0, \tag{2.3.37a}$$

$$\alpha_{123} = \alpha_{231} = \alpha_{312} = -\alpha_{213} = -\alpha_{321} = -\alpha_{132} = \alpha, \tag{2.3.37b}$$

$$\beta_{1212} = \beta_{1313} = \beta_{2121} = \beta_{2323} = \beta_{3131} = \beta_{3232} = \gamma, \tag{2.3.37c}$$

$$\beta_{1122} = \beta_{1133} = \beta_{2211} = \beta_{2233} = \beta_{3311} = \beta_{3322} = \beta, \tag{2.3.37d}$$

$$\sigma_0 = \frac{ne^2 < \tau >}{3}\left[\frac{2}{m_T} + \frac{1}{m_L}\right], \tag{2.3.38a}$$

$$\alpha = -\frac{ne^3 < \tau^2 >}{3c}\left[\frac{2}{m_L m_T} + \frac{1}{m_T^2}\right], \tag{2.3.38b}$$

$$\beta = -\frac{ne^4 < \tau^3 >}{3c^2}\left[\frac{1}{m_L m_T^2} + \frac{1}{m_T m_L^2} + \frac{1}{m_T^3}\right], \tag{2.3.38c}$$

$$\gamma = \frac{ne^4 < \tau^3 >}{m_L m_T^2 c^2} \tag{2.3.38d}$$

Eq.(2.3.36) can be rewritten in another form as:

$$J_x = \sigma_0 E_x + \alpha[E_y B_Z - E_z B_y] + \beta E_x B^2 + \gamma(\vec{E}\cdot\vec{B})B_x + \delta E_x B_x^2, \tag{2.3.39a}$$

$$J_y = \sigma_0 E_y + \alpha[E_z B_x - E_x B_z] + \beta E_y B^2 + \gamma(\vec{E}\cdot\vec{B})B_y + \delta E_y B_y^2, \tag{2.3.39b}$$

$$J_z = \sigma_0 E_z + \alpha[E_x B_y - E_y B_x] + \beta E_z B^2 + \gamma(\vec{E}\cdot\vec{B})B_z + \delta E_z B_z^2, \tag{2.3.39c}$$

where $\delta = -\beta - \gamma$, is a constant of the material and is given by:

$$\delta = -\frac{ne^4 < \tau^3 >}{3c^2}\left[\frac{2}{m_L m_T^2} - \frac{1}{m_T m_L^2} - \frac{1}{m_T^3}\right] \tag{2.3.40}$$

In an isotropic medium, where no direction is distinguished, the effective mass is no longer a tensor but is a scalar, i.e., it can be represented by a single effective mass, and thus δ will vanish. Therefore, δ accounts for the anisotropic terms, vanishing for an isotropic medium. It is only its presence that distinguishes a cubic medium from an isotropic medium. In cubic crystals, due to this term all directions are not equivalent.

The total current density $\vec{J}$ can be written in terms of its components given in Eq.(2.3.39) as follows:

$$\vec{J} = \sigma_0\vec{E} + \alpha(\vec{E}\times\vec{B}) + \beta\vec{E}B^2 + \gamma\vec{B}(\vec{E}\cdot\vec{B}) + \delta S\vec{E}, \tag{2.3.41}$$

where S is a diagonal tensor having elements B_x^2, B_y^2, B_z^2. F. Seitz [1] has derived a similar equation for anisotropic systems possessing cubic symmetry. His derivation was valid for non-degenerate semiconductors using the parabolic density of states and Boltzmann statistics.

Here we have modified Seitz's general equation in heavily doped n-type semiconductores using

1) Fermi-Dirac distrubution function to account for the degeneracy of the free electron gas.

2) non-parabolic density of states to account for the distorsion of the energy band structure.

We have also derived general expressions for the conductivity coefficients taking into account the degeneracy, anisotropy, and energy band distorsion of heavily doped n-type silicon

This equation, i.e., Eq. (2.3.41) or (2.3.39) is the basic equation in our analysis of transport coefficients. This is because all the transport coefficients that we are going to deal with are expresed interms of the conductivity coefficients.

In order to obtain the galvanomagnetic coefficients in accordance with their usual definition, Eq. (2.3.41) must be inverted, i.e., we should obtain an expression for $\vec{E}$ interms of $\vec{J}$ up to terms of second order in $\vec{B}$. By iterating Eq. (2.3.41), we obtain that:

$$\vec{E} = \rho_0 \vec{J} - R_0(\vec{J} \times \vec{B}) + \rho_0[b\vec{J}B^2 + c\vec{B}(\vec{B} \cdot \vec{J}) + dS\vec{J}], \tag{2.3.42}$$

where

$$\begin{aligned} \rho_0 &= {\sigma_0}^{-1}; \\ R_0 &= \frac{\alpha}{{\sigma_0}^2}; \\ b &= -\rho_0(\beta + \rho_0\alpha^2); \\ c &= -\rho_0(\gamma - \rho_0\alpha^2); \\ d &= -\rho_0\delta; \end{aligned} \tag{2.3.43}$$

in which ρ_0 is the resistivity in the absence of a magnetic field, R_0, which will be discussed in section (3.2), is the low field Hall coefficient, and the last three terms are called the magneto-resistance coefficients.

As can be seen from Eq. (2.3.39), the relation between the current and the electric field is a tensor because each current component depends now not only on the corresponding field component but also on other components. This of course has nothing to do with the crystal anisotropy but must be attributed to the influence of the magnetic field which deflects the electrons at right angles to their direction of motion and thus leads to an electrical field in this direction. The conductivity tensor in a magnetic field which can be taken from the coefficients of the components of the electric field strength in (2.3.39),

also appears in isotropic medium. This must be distinguished from the tensorial form of the normal conductivity coefficients, which is caused by the crystal anisotropy and is independent of the magnetic field. In general these two effects are superimposed. However, in a cubic crystal only the magnetic field leads to a tensorial conductivity, as can be seen from (2.3.41), but the crystal structure itself does not.

3 Transport Coefficients in Heavily Doped n-Type Silicon (HDNS)

In heavily doped semiconductors, band tails arising because of the randomness of the impurity distribution can significantly modify the density of states function by introducing additional states in the band gap. As a result of this both the conduction and the valence bands are no longer parabolic near the extrema, and thus the parabolic density of states function given in Eq. (2.1.7), is no longer valid at high impurity concentrations. Therefore, any meaningful theory of transport coefficients in heavily doped semiconductors must use the appropriate expression for the density of states, and as a result, we are obliged to modify our transport equations which are appropriate for heavily doped semiconductors.

In this research work, we shall study only the three most important transport coefficients, that is, the electron drift mobility, the Hall coefficient, and the coefficient of magneto-resistance. In this chapter we shall derive general expressions of these transport coefficients which is valid for both parabolic and non-parabolic density of states in heavily doped n-type silicon.

3.1 The Electron Drift Mobility (EDM)

The electron drift mobility μ_e in the conduction band of a semiconductor is related to the conductivity σ_e by the well known relation [25]:

$$\sigma_e = en\mu_e, \tag{3.1.1}$$

n is the electron concentration in the whole conduction band, e is the magnitude of the electron charge. However, as we have shown in section (2.3.1), the conductivity associated with a single valley is a diagonal tensor of rank II, and as a result, the mobility associated with a single valley must also be a diagonal tensor of rank II. Therefore, the electron drift mobility associated with a single energy valley is anisotropic rather than isotropic.

Therefore, in view of (3.1.1), the tensorial components of the electron drift mobility $\mu_{il}^{(\mu)}$ in a semiconductor are related to the components of the conductivity tensor $\sigma_{il}^{(\nu)}$ in the $\nu^{(th)}$ ellipsoid by the following relation:

$$\sigma_{il}^{(\nu)} = en^{(\nu)}\mu_{il}^{(\nu)}, \tag{3.1.2}$$

On inserting (2.3.17) into (3.1.1), we get the following expression for the components of the electron drift mobility tensor:

$$\mu_{il}^{(\nu)} = \frac{e}{m_i} < \tau > \delta_{il} \tag{3.1.3}$$

where $< \tau >$ is the average relaxation time given by (2.3.19), and m_i isthe effective mass associated with the major axes of ellipsoids. Therefore, the drift mobility of electrons associated with a single energy-valley is a diagonal tensor.

The total mobility of electrons in the conduction band of silicon is obtained by summing the contribution of the six ellipsoids just in a similar procedure as in section (2.3), and as a result, we get

$$\mu_{ii} = \frac{e}{m_c^*} < \tau >, \tag{3.1.4}$$

where m_c^* is the conductivity effective mass, and is given by

$$\frac{1}{m_c^*} = \frac{1}{3}\left[\frac{2}{m_T} + \frac{1}{m_L}\right] = \frac{2k+1}{3m_L}, \tag{3.1.5}$$

and k is the anisotropy factor which is given by

$$k = \frac{m_L}{m_T}. \tag{3.1.6}$$

As can be seen, the diagonal elements μ_{ii} of the mobility tensor are all equal; this means that the total mobility of cubic semiconductors, having ellipsoids of revolution as the constant energy surfaces, is a scalar quantity. The only effect of taking into account ellipsoidal energy surfaces is that the density of states effective mass is replaced by the conductivity effective mass in the expression for the mobility. Thus we have

$$\mu_{11} = \mu_{22} = \mu_{33} = \mu_e, \tag{3.1.7}$$

where

$$\mu_e = \frac{e}{m_c^*} < \tau >, \tag{3.1.8}$$

Now this equation, with $< \tau >$ given by Eq. (2.3.19), is valid in both parabolic and non-parabolic band models of the conduction band of a degenerate electron gas.

3.1.1 The electron drift mobility in HDNS with parabolic DOS

In the absence of band tails, the parabolic density of states in the conduction band is given by Eq. (2.1.7). Using the parabolic density of states and taking into account (2.3.19) with $\mathcal{E}_C = 0$, we obtain the following expression for the electron drift mobility.

$$\mu_e = -\frac{2e}{3m_c^*}\frac{\int_0^\infty \tau \mathcal{E}^{\frac{3}{2}} \frac{\partial f_0}{\partial \mathcal{E}} d\mathcal{E}}{\int_0^\infty \mathcal{E}^{\frac{1}{2}} f_0(\mathcal{E})\, d\mathcal{E}}. \tag{3.1.9}$$

In heavily doped silicon ($N_d > 3 \times 10^{18} cm^{-3}$) the acoustic phonon scattering becomes insignificant and one can safely assume that the ionized impurity scattering is the dominant scattering mechanism in the temperature range 100 to $300^0 K$. Thus τ is given by:

$$\tau = \tau_0 x^{\frac{3}{2}}, \tag{3.1.10}$$

where x is the dimensionless energy given by:

$$x = \left(\frac{E}{k_B T}\right), \tag{3.1.11}$$

and τ_0 is a weak function of energy and therefore can be treated as a constant.

On inserting (3.1.10) into (3.1.9), and changing the variable of integration from $\mathcal{E}$ to x and then performing integration by parts, one gets

$$\mu_e = 2\frac{e\tau_o}{m_c^*}\frac{\int_0^\infty x^2 f_0(x) dx}{\int_0^\infty x^{\frac{1}{2}} f_0(x) dx}, \tag{3.1.12}$$

where $f_0(x)$ is given by Eq. (2.1.15).

For the purpose of numerical calculation it is more convenient to express the EDM in dimensionless form by normalizing it with $\frac{e\tau_o}{m_L}$. Thus dimensionless electron drift mobility μ_n in n-type silicon is given by:

$$\mu_n = \mu_e/(\frac{e\tau_o}{m_L}) = \frac{2(2k+1)}{3}\frac{\int_0^\infty x^2 f_0(x) dx}{\int_0^\infty x^{\frac{1}{2}} f_0(x) dx}. \tag{3.1.13}$$

3.1.2 The electron drift mobility in HDNS with non-parabolic DOS

The expression for the drift mobility of a degenerate electron gas given by Eq. (3.1.8) is valid for both parabolic and non-parabolic band models provided that $<\tau>$ defined by Eq. (2.3.19) is evaluated using the appropriate expression of the density of states. In a heavily doped n-type silicon, as shown in Fig.(3), the density of states is no longer parabolic, since the conduction band density of states show tailing into the energy gap. As a result, with the electron energy defined as in Fig.(3), the lower integration limit in (2.3.19) must be $-\infty$ because additional states are available for electrons in the energy gap below the shifted parabolic conduction band edge $\mathcal{E}_c$.

With these modifications, the general expression for η in Eq. (3.18) in the distorted conduction band can be rewritten as:

$$<\tau>= -\frac{2}{3}\frac{\int_{-\infty}^{+\infty} \tau(\mathcal{E}_e)\mathcal{E}_e\rho(\mathcal{E})\frac{\partial f_0}{\partial \mathcal{E}}\, d\mathcal{E}}{\int_{-\infty}^{+\infty} \rho(\mathcal{E})\, f_0(\mathcal{E})\, d\mathcal{E}}. \tag{3.1.14}$$

$\rho(\mathcal{E})$ is now the non-parabolic density of states appropriate for distorted bands as illustrated in Fig.(3). Following Slotboom we have already discussed this distorted density of states in section (2.1.2), and it was given by Eq. (2.1.9) for a heavily doped n-type silicon. $\mathcal{E}$ is the total energy of electrons relative to the shifted parabolic conduction band edge, and $\mathcal{E}_e$ is the kinetic energy of electrons in the distorted conduction band. As shown in Fig. (3), for convenience we set the origin of the energy at the shifted parabolic conduction band edge $\mathcal{E}_c$ and we measure the electron energy $\mathcal{E}$ relative to $\mathcal{E}_c$. It is more convenient to use the dimensionless energy $\mathcal{Z}$ in the expression for $<\tau>$ in Eq. (3.1.14). Thus we obtain:

$$<\tau>= -\frac{2}{3}\frac{\int_{-\infty}^{+\infty} \tau(\mathcal{Z}_e)\mathcal{Z}_e\rho(\mathcal{Z})\frac{\partial f_0}{\partial \mathcal{Z}}\, d\mathcal{Z}}{\int_{-\infty}^{+\infty} \rho(\mathcal{Z})\, f_0(\mathcal{Z})\, d\mathcal{Z}}, \tag{3.1.15}$$

On inserting Eqs. (2.1.9), (2.1.15) into (3.1.15), we get the following expression for $<\tau>$:

$$<\tau>= \frac{2\tau_0}{3}\left(\frac{\sqrt{2}\sigma}{k_B T}\right)^{5/2}\frac{\psi_{5/2}}{\psi_0}, \tag{3.1.16}$$

where ψ_0 is given by Eq. (2.1.20), and

$$\psi_{\frac{5}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{+0.601} \frac{|\mathcal{Z}|^{\frac{5}{2}}[0.319 - (0.906)\exp(2\mathcal{Z})]}{\left(1+\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z} - \eta\right]\right)^2} \times$$

$$\exp\left(\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z} - \eta - \mathcal{Z}^2\right) d\mathcal{Z} +$$

$$\int_{+0.601}^{+\infty} \frac{\mathcal{Z}^3\left(1 - \frac{1}{(4\mathcal{Z})^2}\right)\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z} - \eta\right]}{\left(1+\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z} - \eta\right]\right)^2} d\mathcal{Z}. \tag{3.1.17}$$

Substituting (3.1.16) into (3.1.8), we get the following expression for the electron drift mobility in heavily doped n-type silicon:

$$\mu_e = \frac{e\tau_0}{m_L} \frac{2(2k+1)}{9} \left(\frac{\sqrt{2}\sigma}{k_BT}\right)^{\frac{5}{2}} \frac{\psi_{\frac{5}{2}}}{\psi_0}, \tag{3.1.18}$$

The normalized dimensionless electron drift mobility then becomes

$$\mu_n = \frac{\mu_e}{(e\tau_0/m_L)} = \frac{2(2k+1)}{9} \left(\frac{\sqrt{2}\sigma}{k_BT}\right)^{\frac{5}{2}} \frac{\psi_{\frac{5}{2}}}{\psi_0}, \tag{3.1.19}$$

3.2 The Hall Coefficient (HC)

The physical phenomena which take place in a substance placed in the combined electric and magnetic fields in the presence of electric current due to the action of the electric field are termed galvanomagnetic phenomena. The effect of these fields is quite different. Whilst an electric field accelerates the electrons in the direction of the current, a magnetic field deflects them from their direction with out altering their energy. Of all the transport coefficients of the galvanomagnetic phenomena, we shall consider only the two most important ones, that is, the Hall coefficient and the coefficient of magneto-resistance. In this section we shall deal with the Hall effect, which is described by the Hall coefficient, where as the coefficient of magneto-resistance will be discussed in the next section.

Now we proceed to describe the Hall effect by considering the usual experimental

arrangement shown below in Fig.(4).

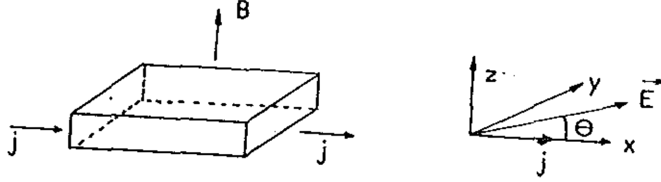

Fig. 4. The Hall geometry

Consider a finite semiconductor sample in the form of a parallelpiped with its edges directed along the coordinate axes as shown in Fig. (4). An electric field E_x is applied to a semiconductor extending in the x-direction and a current density J_x flows in it. Now we switch on a magnetic field induction $\vec{B}$ acting in the z-direction. As a result, due to the Lorentz force, the following force will act on electrons.

$$\vec{F_L} = -\frac{e}{c}[\vec{v} \times \vec{B}]. \tag{3.2.1}$$

Electrons are deflected in the positive y-direction by this force. However, since electrons are constrained by the sides of the semiconductor slab, they will accumulate near the back side of the slab. As a result an electric field will be generated in the positive y-direction that opposes their further motion and accumulation. In equilibrium this transverse field, E_y, which is usually called the Hall field, will balance the Lorentz force, and no current will flow in the y-direction. For such arrangements, the Hall coefficient is conventionally defined by the relation

$$R = \frac{E_y}{J_x B} \tag{3.2.2}$$

For the case of weak magnetic fields, only terms linear in $\vec{B}$ need be retained for the Hall effect in Eq. (2.3.39). As a result of this assumption we get the following expression for the components of the current density:

$$J_x = \sigma_0 E_x + \alpha E_y B,$$

$$J_y = \sigma_0 E_y - \alpha E_x B, \tag{3.2.3}$$

$$J_z = 0.$$

The Hall field E_y is determined by the requirement that there will be no transverse current J_y. Using (3.2.2), (3.2.3), and Setting $J_y = 0$ in (3.2.3), one can easily show that:

$$R = \frac{\alpha}{\sigma_0^2}\left[\frac{1}{1+\frac{\alpha^2 B^2}{\sigma_0^2}}\right]. \tag{3.2.4}$$

In view of (2.3.38a) and (2.3.38b), we get:

$$R = -\frac{1}{nec}\frac{<\tau^2>}{<\tau>^2}\frac{3k(k+2)}{(2k+1)^2}\left[\frac{1}{1+\frac{e^2B^2}{m_L^2c^2}\frac{<\tau^2>^2}{<\tau>^2}(\frac{k(k+2)}{2k+1})^2}\right], \tag{3.2.4}$$

where k is given by (3.1.6). Here it can be easily seen that the second term in the denominator of the square brackets is of the order of $w_c^2\tau^2$, and thus by our assumption of weak magnetic fields, can be neglected. Thus our expression for R simplifies to:

$$R = -\frac{1}{nec}\frac{<\tau^2>}{<\tau>^2}\frac{3k(k+2)}{(2k+1)^2}. \tag{3.2.5}$$

This expression is valid for both parabolic and non-parabolic bands with the appropriate choice of the density of states. In the next section we shall derive an explicit expression for the R using the parabolic and the non-parabolic density of states in a heavily doped n-type silicon.

3.2.1 The Hall coefficient in HDNS with parabolic DOS

Here we shall assume that the quantum density of states have the square-root dependence on energy and use the Fermi-Dirac statistics to describe the degenerate electron gas in the conduction band. In this case density of states function is given by Eq. (2.1.7) and $<\tau^2>$ is given by (2.3.22). For reasons mentioned before we shall consider ionized impurity scattering as the dominant scattering mechanism so that the relaxation time is given by (3.1.8). Using these assumptions along with setting $\mathcal{E}_c = 0$ and on performing the integration by parts, we obtain the following expression for the Hall coefficient of a degenerate electron gas in heavily doped n-type silicon:

$$R = -\frac{1}{nec}\frac{9k(k+2)}{4(2k+1)^2}\frac{[\int_0^{+\infty} x^{7/2} f_0(x)\,dx][\int_0^{+\infty} x^{1/2} f_0(x)\,dx]}{[\int_0^{+\infty} x^2 f_0(x)\,dx]^2}, \tag{3.2.6a}$$

The normalized hall coefficient is then given by

$$r = \frac{R}{1/(nec)} = -\frac{9k(k+2)}{4(2k+1)^2} \frac{[\int_0^{+\infty} x^{7/2} f_0(x)\, dx][\int_0^{+\infty} x^{1/2} f_0(x)\, dx]}{[\int_0^{+\infty} x^2 f_0(x)\, dx]^2}, \tag{3.2.6b}$$

3.2.2 The Hall coefficient in HDNS with non-parabolic DOS

Here, since the conduction band in the vicinity of the energy extrema is distorted due to band tail formation, additional states are available for electrons below the shifted parabolic conduction band edge and thus the lower limit of integration can be set to $-\infty$. Therefore, we have to use the non-parabolic density of states for the quantum density of states which is given by Eq (2.1.9). By applying the non-parabolic density of states for the quantum density of states, we get the following expression for $< \tau^2 >$:

$$< \tau^2 > = \frac{2\tau_0^2}{3} \left(\frac{\sqrt{2}\sigma}{k_B T}\right)^4 \frac{\psi_4}{\psi_0}, \tag{3.2.7}$$

where ψ_0 and $\psi_{5/2}$ are given by Eqs. (2.1.20) and (3.1.16), respectively and ψ_4 is given by

$$\psi_4 = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{+0.601} \frac{\mathcal{Z}^4[0.319 - (0.906)\exp(2\mathcal{Z})]}{(1+\exp[\frac{\sqrt{2}\sigma}{k_B T}\mathcal{Z} - \eta])^2} \times \exp(-\mathcal{Z}^2 + \frac{\sqrt{2}\sigma}{k_B T}\mathcal{Z} - \eta)\, d\mathcal{Z} +$$

$$\int_{+0.601}^{+\infty} \frac{\mathcal{Z}^{\frac{9}{2}}(1 - \frac{1}{(4\mathcal{Z})^2})\exp[\frac{\sqrt{2}\sigma}{k_B T}\mathcal{Z} - \eta]}{(1+\exp[\frac{\sqrt{2}\sigma}{k_B T}\mathcal{Z} - \eta])^2} d\mathcal{Z}. \tag{3.2.8}$$

Now substituting Eqs. (3.1.16), and (3.2.7) into (3.2.5), we get the following expression for R.

$$R = -\frac{1}{nec} \frac{9k(k+2)}{2(2k+1)^2} \frac{k_B T}{\sqrt{2}\sigma} \frac{\psi_0 \psi_4}{\psi_{\frac{5}{2}}{}^2}, \tag{3.2.9}$$

The normalized Hall coefficient r is given by:

$$r = \frac{R}{(1/nec)} = -\frac{9k(k+2)}{2(2k+1)^2} \frac{k_B T}{\sqrt{2}\sigma} \frac{\psi_0 \psi_4}{\psi_{\frac{5}{2}}{}^2}, \tag{3.2.10}$$

3.3. The Coefficient of Magneto-resistance(CMR)

In this section we shall discuss the change in the resistivity ρ in a magnetic field and also derive the expression of the coefficient of transverse magnetoresistance. In a magnetic field the resistivity ρ becomes magnetic field dependent and increases with increasing magnetic field. Since the longitudinal magnetoresistance reacts particularly sensitively to the band structure, it cannot be described by the simple model of spherical energy surfaces. This means we must take into account the real band structure of the material which is in most cases anisotropic. Here also we shall assume that the magnetic field is weak, and thus we shall neglect all higher order terms greater than B^2. Since magnetoresistance is highly dependent on the relative orientation of the magnetic field and the current, we consider the two special cases, i.e., the longitudinal and the transverse orientations. If $\vec{E}$ is the electric field and $\vec{J}$ is the electric current, then the resistivity measured in the direction of the current $\vec{J}$ is given by:

$$\rho = \frac{\vec{E} \cdot \vec{J}}{J^2} \tag{3.3.1}$$

Therefore, on using Eq.(2.3.42), we get a general expression for the resistivity in the presence of a magnetic field.

$$\rho(\vec{B}) = \rho_0 + \frac{\rho_0}{J^2}[bB^2J^2 + c(\vec{B} \cdot \vec{J})^2 + dSJ^2], \tag{3.3.2a}$$

or

$$\rho(\vec{B}) = \rho_0 + \frac{\rho_0}{J^2}[bB^2J^2 + c(\vec{B} \cdot \vec{J})^2 + d(J_x^2B_x^2 + J_y^2B_y^2 + J_z^2B_z^2)]. \tag{3.3.2b}$$

where ρ_0 is the resistivity in the absence of a magnetic field, and $\rho(\vec{B})$ is the resistivity in the presence of a magnetic field.

a) The Longitudinal Magneto – resistance (LMR)

The LMR is measured with $\vec{B}$ parallel to $\vec{J}$. When $\vec{J}$ is parallel to any of the cubic axes it yields:

$$\rho(\vec{B}) = \rho_0 + \rho_0[b + c + d]B^2. \tag{3.3.3}$$

But in cubic semiconductors, for which the constant energy surfaces are ellipsoids of revolution, the term in the square bracket is zero. Thus,

$$\rho(\vec{B}) = \rho_0,$$
$$\sigma(\vec{B}) = \sigma_0, \tag{3.3.4}$$

and from this it follows that

$$J_i = \sigma_0 E_i. \tag{3.3.5}$$

As can be seen from Eq. (3.3.5), a magnetic field applied in the direction of the current $\vec{J}$ does not affect the current $\vec{J}$. This means that there is no LMR along any of the $< 100 >$ directions of a cubic crystal whose constant energy surfaces are ellipsoids of revolution. As a result of this the coefficient of LMR which is defined by the relation,

$$H = \frac{\rho(\vec{B}) - \rho_0}{\rho_0 B^2}, \tag{3.3.6}$$

is zero along any of the cubic axes. Therefore, the coefficient of LMR in cubic semiconductors, having ellipsoids of revolution as the constant energy surfaces, is non-zero only when the current does not coincide with any of the crystallographic directions.

b) The Transvers Magneto – resistance (TMR)

On inserting Eq. (3.3.2b) into Eq. (3.3.6), we obtain the following expression for the coefficient of TMR:

$$H_t = b + \frac{c(\vec{B}\cdot\vec{J})^2}{J^2 B^2} + \frac{d(J_x^2 B_x^2 + J_y^2 B_y^2 + J_z^2 B_z^2)}{J^2 B^2}. \tag{3.3.7}$$

As can be seen from Eq.(3.3.7), the coefficient of TMR is strongly dependent on the angle between the current $\vec{J}$ and the magnetic field $\vec{B}$, and thus MR varies with crystal orientation.

The TMR is defined when $\vec{B}$ is perpendicular to $\vec{J}$. If $\vec{J}$ is parallel to any of the cubic axes, the coefficient of TMR depends only on b, that is,

$$H_t = b, \tag{3.3.8}$$

For other orientations of $\vec{J}$, H_t depends on both b and d. On account of Eq. (2.3.43), the expression for the coefficient of TMR in Eq. (3.3.8) becomes

$$H_t = -\left(\frac{\beta}{\sigma_0} + \frac{\alpha^2}{\sigma_0^2}\right), \tag{3.3.9}$$

so that on taking into account Eqs. (2.3.38a), 2.3.38b), and (2.3.38c) along with (3.3.9), we get the following expression for the coefficient of TMR:

$$H_t = \frac{e^2}{m_L^2 c^2}\left[\frac{k(k^2+k+1)}{(2k+1)}\frac{<\tau^3>}{<\tau>} - \left(\frac{k(k+2)}{(2k+1)}\right)^2 \frac{<\tau^2>^2}{<\tau>^2}\right]. \tag{3.3.10}$$

This formula for the coefficient of TMR is valid in both parabolic and non-parabolic band models. In the following sections we will analyze this formula in the two band models.

3.3.1 The coefficient of transverse magnetoresistance (CTMR) in HDNS with parabolic density of states

As we have previously mentioned, in the rigid band approximation the quantum density of states in a heavily doped silicon retains the square-root dependence on energy that describes the quasi free electrons in the coduction band for intrinsic silicon. Therefore, for the parabolic $\mathcal{E}$ - $|\vec{k}|$ relation, the density of states is given by Eq. (2.1.7). Following a similar procedure as in section (3.2.1), we obtain the following expression for the CTMR:

$$H_t = \frac{e^2\tau_0^2}{m_L^2 c^2}\left(\frac{2k(k^2+k+1)}{(2k+1)}\frac{\int_0^{+\infty} x^5 f_0(x)\,dx}{\int_0^{+\infty} x^2 f_0(x)\,dx} - \frac{9}{4}\left(\frac{k(k+2)}{(2k+1)}\right)^2 \frac{\left[\int_0^{+\infty} x^{7/2} f_0(x)\,dx\right]^2}{\left[\int_0^{+\infty} x^2 f_0(x)\,dx\right]^2}\right). \tag{3.3.11a}$$

The normalized CTMR is given by:

$$h_t = \frac{H_t}{e^2\tau_0{}^2/(m_L^2c^2)} = \left(\frac{2k(k^2+k+1)}{(2k+1)}\frac{\int_0^{+\infty} x^5 f_0(x)\,dx}{\int_0^{+\infty} x^2 f_0(x)\,dx} - \frac{9}{4}\left(\frac{k(k+2)}{(2k+1)}\right)^2 \frac{\left[\int_0^{+\infty} x^{7/2} f_0(x)\,dx\right]^2}{\left[\int_0^{+\infty} x^2 f_0(x)\,dx\right]^2}\right). \tag{3.3.11b}$$

3.3.2 The coefficient of transverse magnetoresistance (CTMR) in HDNS with non-parabolic density of states

To calculate the CTMR using the non-parabolic density of states, we shall evaluate $<\tau^3>$ in a manner similar to the one used in evaluating $<\tau>$ and $<\tau^2>$ for the calculation of Hall coefficient in section (3.2). Thus, we obtain the following expression for $<\tau^3>$ using the non-parabolic density of states:

$$<\tau^3>=\frac{2\tau_o^3}{3}\left(\frac{\sqrt{2}\sigma}{k_BT}\right)^{11/2}\frac{\phi_{11/2}}{\phi_0}, \tag{3.3.12}$$

where ψ_0 is given by Eq.(3.1.20), and

$$\psi_{\frac{11}{2}}=\frac{1}{2\pi^{\frac{1}{2}}}\int_{-\infty}^{+0.601}\frac{|\mathcal{Z}|^{\frac{11}{2}}\exp\left(-\mathcal{Z}^2+\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta\right)[0.319-(0.906)\exp(2\mathcal{Z})]}{\left(1+\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta\right]\right)^2}d\mathcal{Z}+$$

$$\int_{+0.601}^{+\infty}\frac{\mathcal{Z}^6\left(1-\frac{1}{(4\mathcal{Z})^2}\right)\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta\right]}{\left(1+\exp\left[\frac{\sqrt{2}\sigma}{k_BT}\mathcal{Z}-\eta\right]\right)^2}d\mathcal{Z}. \tag{3.3.13}$$

On substituting Eqs. (3.1.16), (3.2.7), and (3.3.12) into the general Eq. (3.3.10), we may write the CTMR for a heavily doped n-type silicon having band tails in the conduction band in the following form:

$$H_t=\frac{e^2\tau_0{}^2}{m_L^2c^2}\left(\frac{\sqrt{2}\sigma}{k_BT}\right)^3\left[\frac{k(k^2+k+1)}{(2k+1)}\frac{\psi_{\frac{11}{2}}}{\psi_{\frac{5}{2}}}-\left(\frac{k(k+2)}{(2k+1)}\right)^2\frac{\psi_4^2}{\psi_{\frac{5}{2}}{}^2}\right]. \tag{3.3.14}$$

Finally the normalized dimensionless CTMR is given by:

$$h_t=\frac{H_t}{\frac{e^2\tau_0{}^2}{m_L^2c^2}}=\left(\frac{\sqrt{2}\sigma}{k_BT}\right)^3\left[\frac{k(k^2+k+1)}{(2k+1)}\frac{\psi_{\frac{11}{2}}}{\psi_{5/2}}-\left(\frac{k(k+2)}{(2k+1)}\right)^2\frac{\psi_4^2}{\psi_{\frac{5}{2}}{}^2}\right], \tag{3.3.15}$$

4 Numerical Calculation of Transport Coefficients and Discussion of Results

In this section, we shall first discuss the procedure to compute the drift mobility, the Hall coefficient, and the coefficient of magnetoresistace numerically as a function of doping density N_d in an n-type Si in the impurity concentration range from approximately 1×10^{18} to $2 \times 10^{20} cm^{-3}$. When the doping density N_d exceeds the effective level density N_c at the lower edge of the conduction band, the Fermi level moves from the band gap into the conduction band. In such a case one has to use Fermi-Dirac distribution function for the carriers.

This requires the knowledge of the Fermi energy as a function of carrier concentration. Therefore, we have to calculate the position of the Fermi energy $\mathcal{E}_F$ relative to the shifted parabolic conduction band edge $\mathcal{E}_c$ using the parabolic as well as the non-parabolic density of states in a heavily doped n-type silicon. The relative position of $\mathcal{E}_F$ is determined by equating the density of the occupied states in the conduction band n to the doping concentration N_d as we did in section (2.1.2).

$$n = N_d = \frac{m_n^{*3/2}\, 2^{5/4}\, \sigma^{3/2}}{\pi^2\, \hbar^3}\, \psi_0, \tag{4.1}$$

where ψ_0 from (2.1.20) is given by:

$$\psi_0 = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{+0.601} \frac{\exp(-\mathcal{Z}^2)[0.319 - (0.906)\exp(2\mathcal{Z})]}{(1+\exp[1.4939\; n_n^{5/12}\mathcal{Z} - \eta])}\, d\mathcal{Z} + \int_{+0.601}^{+\infty} \frac{\mathcal{Z}^{1/2}(1 - \frac{1}{(4\mathcal{Z})^2})}{(1+\exp[1.4939\; n_n^{5/12}\mathcal{Z} - \eta])}\, d\mathcal{Z}, \tag{4.2}$$

In the given range of doping concentration from $1\times10^{18} cm^{-3}$ to $2\times10^{20} cm^{-3}$, we increased n continuously in certain steps starting from 1×10^{18} up to 2×10^{20} cm^{-3}. Now since Fermi energy is very sensitive to doping and temperature of semiconductors, its value is different at different doping densities at a given temperature.

As can be seen from Eq. (4.1), it is not possible to calculate the Fermi energy from this relation for a given value of electron density n. Consequently, we cannot calculate the μ_n, R, and H_t for given values of n. However, the reverse is possible, i.e., one can calculate the electron density n using the parabolic as well as the non-parabolic density of states for various values of Fermi energy numerically using the following procedure.

For the given value of n, the left hand side (LHS) of Eq. (4.1), we choose an arbitrary value of the normalized Fermi-energy η as a first approximation and then calculate the right hand side (RHS) of Eq. (4.1). Then we change the value of η slightly from its previous value, and we call this value of η as second approximation, and again calculate the RHS of Eq. (4.1) and then compare it with the given value n. Now if this value is closer to the given value of n than the previous one, we continue to vary η in the same direction until the value of the integral on the RHS of Eq. (4.1) and the given value of n match. If the second approximation of η gives a value of the RHS of Eq. (4.1) which is further away from the given value of n, we choose the second value of η in opposite direction and continue to change η till we match the two sides of Eq. (4.1). That value of η for which both sides of Eq. (4.1) are equal is taken as the actual value of η which corresponds to the given values of n. Following this procedure, we have calculated the variation of the normalized Fermi-energy with the normalized electron concentration (n_n) and the result is plotted in Fig. (5).

For the purpose of numerical calculations, it is convenient to express the the electron density n as a dimensionless quantity by normalizing it with 10^{19} cm^{-3} as:

$$n_n = \frac{N_d}{10^{19} cm^{-3}}. \tag{4.3}$$

We can now use Eq. (4.5) to obtain the value of the dimensionless Fermi-energy η for a given value of n by using the procedure mentioned above.

For the numerical calculation we have used the following values:

$$m_n^* = 1.18 m_0,$$
$$\epsilon_d = 11.7. \tag{4.4}$$

To evaluate the normalized EDM, HC, and CTMR in the non-parabolic band model we will use Eqs. (3.1.21), (3.2.9) and (3.3.15), respectively. For the numerical calculations these equations can be simplified by substituting the numerical values of the various parameters given before. Thus, the simplified expression for the normalized transport coefficients of in the heavily doped n-type silicon with non-parabolic DOS are given by:

$$\mu_n = (6.9992273) n_n^{\frac{25}{24}} \frac{\psi_{\frac{5}{2}}}{\psi_0}, \tag{4.5}$$

$$r = -(0.8685184)\, n_n^{\frac{-5}{12}}\, \frac{\psi_0\, \psi_4}{{\psi_{\frac{5}{2}}}^2}, \tag{4.6}$$

$$h_t = \left[(51.840291)\, \frac{\psi_{\frac{11}{2}}}{\psi_{\frac{5}{2}}} - (36.953728) \frac{{\psi_4}^2}{{\psi_{\frac{5}{2}}}^2}\right]\, n_n^{15/12}, \tag{4.7}$$

where ψ_0 is given by Eq.(4.2), and

$$\psi_{\frac{5}{2}} = (0.282) \int_{-\infty}^{+0.601} \frac{|\, \mathcal{Z}\, |^{\frac{5}{2}} [0.319 - (0.906) \exp(2\mathcal{Z})]}{\left(1 + \exp\left[(1.4939)\, n_n^{(5/12)}\, \mathcal{Z} - \eta\right]\right)^2} \times$$
$$\exp\left((1.4939)\, n_n^{(5/12)}\, \mathcal{Z} - \eta - \mathcal{Z}^2\right)\, d\mathcal{Z} +$$

$$\int_{+0.601}^{+\infty} \frac{\mathcal{Z}^3 (1 - \frac{1}{(4\mathcal{Z})^2}) \exp\left[(1.4939)\, n_n^{(5/12)}\, \mathcal{Z} - \eta\right]}{\left(1 + \exp\left[(1.4939)\, n_n^{(5/12)}\, \mathcal{Z} - \eta\right]\right)^2}\, d\mathcal{Z}, \tag{4.8}$$

$$\psi_4 = (0.282) \int_{-\infty}^{+0.601} \frac{\mathcal{Z}^4 [0.319 - 0.906 \exp(2\mathcal{Z}))]}{\left(1 + \exp\left[(1.4939)\ n_n^{\frac{5}{12}} \mathcal{Z} - \eta\right]\right)^2} \times$$
$$\exp\left((1.4939) n_n^{\frac{5}{12}}\, \mathcal{Z} - \eta - \mathcal{Z}^2\right)\, d\mathcal{Z} +$$
$$\int_{+0.601}^{+\infty} \frac{\mathcal{Z}^{\frac{9}{2}} (1 - \frac{1}{(4\mathcal{Z})^2}) \exp\left[(1.4939) n_n^{\frac{5}{12}} \mathcal{Z} - \eta\right]}{\left(1 + \exp\left[(1.4939) n_n^{\frac{5}{12}} \mathcal{Z} - \eta\right]\right)^2} d\mathcal{Z}, \tag{4.9}$$

$$\psi_{\frac{11}{2}} = (0.282) \int_{-\infty}^{+0.601} \frac{|\, \mathcal{Z}\, |^{\frac{11}{2}}\ \exp\left[(1.4939)\, n_n^{\frac{5}{12}} \mathcal{Z} - \eta - \mathcal{Z}^2\right] [0.319 - (0.906) \exp(2\mathcal{Z})]}{\left(1 + \exp[(1.4939)\, n_n^{5/12}\, \mathcal{Z} - \eta]\right)^2}\, d\mathcal{Z} +$$

$$\int_{+0.601}^{+\infty} \frac{\mathcal{Z}^6 (1 - \frac{1}{(4\mathcal{Z})^2}) \exp\left[(1.4939)\, n_n^{\frac{5}{12}}\, \mathcal{Z} - \eta\right]}{\left(1 + \exp\left[(1.4939)\, n_n^{\frac{5}{12}}\, \mathcal{Z} - \eta\right]\right)^2} d\mathcal{Z}. \tag{4.10}$$

As we can see from the above equations once the value of η is known, one can easily calculate ψ_0, $\psi_{\frac{5}{2}}$, ψ_4, and $\psi_{\frac{11}{2}}$ and thus μ_n, r, and h_t can be calculated as a function of N_d.

We have also performed the corresponding calculations based on a simple degenerate parabolic model for the sake of comparison with our calculations. In a degenerate parabolic band the electron concentration n is given by [14]:

$$n = N_c\, F_{\frac{1}{2}}(\eta), \tag{4.11}$$

where $N_c = 3.2 \times 10^{19}\ cm^{-3}$ for n-type Si at $T = 300^0 K$ and η is the dimensionless effective Fermi-energy. For a given value of n and T one can easily calculate η using relation (4.11) in a similar procedure used for the non-parabolic case and the corresponding values of n_n and η are plotted in Fig. (5) along with the corresponding values calculated based on the degenerate non-parabolic band. The corresponding expressions for μ_n, r, and h_t based on the simple parabolic band model are given by:

$$\mu_n = (7.69782) \frac{\int_0^\infty \frac{x^2}{1+\exp(x-\eta)} dx}{\int_0^\infty \frac{x^{\frac{1}{2}}}{1+\exp(x-\eta)} dx}, \qquad (4.12)$$

$$r = -(0.6487398) \frac{\int_0^{+\infty} \frac{x^{\frac{7}{2}}}{1+\exp(x-\eta)} dx \int_0^{+\infty} \frac{x^{\frac{1}{2}}}{1+\exp(x-\eta)} dx}{\left[\int_0^{+\infty} \frac{x^2}{1+\exp(x-\eta)} dx\right]^2}, \qquad (4.13)$$

$$h_t = \left[(31.098028) \frac{\int_0^{+\infty} \frac{x^5}{1+\exp(x-\eta)}\, dx}{\int_0^{+\infty} \frac{x^2}{1+\exp(x-\eta)}\, dx} - (24.938838) \left(\frac{\int_0^{+\infty} \frac{x^{\frac{7}{2}}}{1+\exp(x-\eta)}\, dx}{\int_0^{+\infty} \frac{x^2}{1+\exp(x-\eta)}\, dx} \right)^2 \right], \qquad (4.14)$$

and the variation of the normalized Fermi energy, EDM, HC, and CTMR with doping concentration are shown in Figs. (5), (6), (7), and (8), respectively.

In Fig.(5), we have plotted the normalized Fermi-energy η at $300^o K$, calculated using the parabolic density of states (solid line) and the non-parabolic density of states (broken line) as a function of the normalized carrier concentration n_n in the impurity concentration range from 1×10^{18} to $2 \times 10^{20} cm^{-3}$ in n-type Si. The positions of the Fermi-energy have been evaluated relative to the parabolic conduction band edge. As one can see from Fig. (5), the normalized Fermi energy increases with increasing normalized doping concentration for both cases. From the comparision of the two curves, we see that the value of η calculated from a non-parabolic density of states almost coincides with that calculated from a parabolic density of states for impurity concentrations approximately below 1×10^{18} cm^{-3}. This may be attributed to the fact that, below this doping concentration the conduction band is only slightly distorted from the parabolic shape, and thus the total density of states in the conduction band can be approximated by the ordinary parabolic density of states. Therefore, one can neglect the effect of band tails. However, for doping concentrations above 1×10^{18} cm^3, the value of η calculated using the parabolic density of states, at a given doping concentration is always greater than the corresponding value calculated from a non-parabolic density of states. moreover as, as can be seen from Fig.(5),

the deviation between the two curves increases as n_n increases. From our calculations it is observed that using the non-parabolic density of states reduces the magnitude of the normalized Fermi-energy by as much as 37% from the corresponding value calculated by using the parabolic density of states at the doping concentration $2 \times 10^{20}\ cm^{(-3)}$

In Fig. (6), we plot the normalized electron drift mobility μ_n calculated using the parabolic as well as the non-parabolic density of states as a function of the normalized doping concentration n_n in the doping concentration range from 1×10^{18} to $2 \times 10^{20} cm^{-3}$ in n-type silicon. From Fig.(6), we note that the value of μ_n calculated from a non-parabolic density of states near the impurity concentration approximately $1 \times 10^{18} cm^{-3}$ almost coincides with that calculated from a parabolic density of states. Since, below this doping concentration, the values of η obtained from these two calculations are remarkably close, the parabolic density of states is valid in this range of doping concentration, and thus one can neglect the effect of band tails in the calculation of the EDM. However, as can be seen from Fig.(6), above this doping concentration the normalized electron drift mobility obtained using the non-parabolic density of states (Broken line+) shows substantial deviation from that obtained using the parabolic density of states (solid line). The value of μ_n calculated using the parabolic density of states increases almost linearly with increasing n_n, where as that obtained from the non-parabolic density of states first decreases rapidly with increasing n_n in the doping concentration range approximately from 1×10^{18} to $4 \times 10^{19}\ cm^{-3}$, and it is seen that at the doping concentration nearly equal to 4×10^{19} it reaches a minimum value and then begins to increase slowly with increasing doping concentrations for all doping concentrations above this value.

From our calculations, it is seen that the deviation of μ_n calculated using the non-parabolic density of states from that obtained using the parabolic density of states increases with increasing n_n and the value of the normalized electron drift mobility calculated using the non-parabolic density of states is found to yield as high as 59% deviation from that calculated using the parabolic density of states at the doping concentration $2 \times 10^{20}\ cm^{(-3)}$. Therefore, as a result of this, at higher impurity concentrations, approximately greater than 1×10^{18}, the parabolic density of states is no longer valid, and thus one must use the non-parabolic density of states which takes into account the band tails to describe a highly distorted semiconductor.

In Fig.(7), we plot the normalized Hall coefficient r calculated using the parabolic density of states (solid line) and the non-parabolic density of states (doted line) as a function of the normalized doping concentration n_n in the range of doping concentration from 1×10^{18} to $2 \times 10^{20} cm^{-3}$ in n-type silicon. For electrons we have assumed that the Hall coefficient is negative. As shown in Fig. (7), the value of r calculated using the non-parabolic density of states is very nearly the same as that calculated using the parabolic density of states for impurity concentrations approximately below $1 \times 10^{18} cm^{-3}$. Therefore, for all doping concentrations below 1×10^{18} cm^{-3} the parabolic density of states is a good approximation of the conduction band density of states and the effect of band tails can be neglected in the quantum density of states. For the impurity concentrations above 1×10^{18} cm^{-3}, the normalized Hall coefficient r calculated using the parabolic density of states is seen to increase slowly with increasing normalized doping concentration. On the other hand the value of the normalized Hall coefficient r calculated using the non-parabolic density of states decreases slowly as the normalized doping concentration increases from 0.1 to 5, and it is seen that at the doping concentration nearly equal to $5 \times 10^{19} cm^{-3}$ it reaches a minimum value. Above this doping concentration, however, it begins to increase slowly with increasing normalized doping concentration n_n in the range of doping concentration in which our calculations are valid. Our results also show that the values of the normalized Hall coefficient calculated using the non-parabolic density of states are reduced by 54% than those calculated using the parabolic density of states at the doping concentration 6×10^{20} cm^{-3}. As a result, for all impurity concentrations, in which our calculations are valid, the parabolic density of states is no longer valid and thus one must use the non-parabolic density of states to take into account the effect of band tails.

In Fig.(8), we present a plot of the normalized coefficient of transverse magnetoresistance h_t calculated using the non-parabolic density of states (doted line) and the parabolic density of states (solid line) in the doping range from 1×10^{18} to $2 \times 10^{20} cm^{-3}$ in n-type silicon. The values of the normalized coefficient of transverse magnetoresistance are so close that lines drawn separately cannot be distinguished at the impurity concentration, approximately equal to $1 \times 10^{18} cm^{-3}$. Consequently, the value of the normalized coefficient of transverse magnetoresistance (h_t) can be calculated with sufficient accuracy using the parabolic density of states, without taking into account the density of states in

the band tail. This coincidence of the two models for impurity concentration of about $1 \times 10^{18} cm^{-3}$ also shows that the number of occupied states in the band tail is much less than the total number of electrons, and thus one can neglect it. However in the impurity concentration range from 1×10^{18} to $2 \times 10^{20} cm^{-3}$, in which our calculation is valid, it is seen that the deviation between the values of h_t obtained from the two models increases with increasing normalized doping concentration, n_n. The values of the normalized coefficient of transverse magnetoresistance calculated using the parabolic density of states increases smoothly (slowly) with increasing normalized doping concentration n_n in the range of impurity concentration in which our calculations are valid. The results of our calculations also show that, the values of h_t obtained from the non-parabolic density of states decreases slowly as n_n increases from 0.1 to 1.0, and at the normalized doping concentration approximately equal to $1 \times 10^{19} cm^{-3}$, it is seen that, h_t reaches its minimum value, and then it begins to increase slowly with increasing doping concentrations. From the results of our calculations we have observed that the difference between the two calculations can be as high as 24%, i.e., taking into account the band tails in the quantum density of states reduces the value of h_t calculated using the parabolic density of states by 24% at the doping concentration $2 \times 10^{20}\ cm^{-3}$. Therefore, in calculating the normalized coefficient of magnetoresistance at all impurity concentrations greater than $1 \times 10^{18} cm^{-3}$, the parabolic density of states is no longer valid, and thus one must use the non-parabolic density of states which takes into account the band tail density of states.

5 Summary and Conclusion

In this thesis the three most important transport coefficients, i.e., the electron drift mobility, the Hall coefficient, and the coefficient of transverse magnetoresistance have been studied using the parabolic and non-parabolic density of states in heavily doped n-type silicon. The Boltzmann transport equation has been solved to calculate the anisotropic part of the deformed distribution function of the degenerate electron gas. We have used ellipsoids of revolution for the constant energy surfaces in $\vec{k}$-space to account for the anisotropy of the crystal structure.

The non-parabolicity of the energy bands was taken into consideration by using Slotboom's approximation for the general expression of the quantum density of states in heavily doped semiconductors given by Kane.

Moreover, at higher doping concentrations, ionized impurity scattering was assumed to be the dominant scattering mechanism and the relaxation time was assumed to be dependent only on the energy.

Taking all these assumptions into consideration, we have derived general expressions for the conductivity coefficients valid for both parabolic and non-parabolic density of states, taking into account both the anisotropy of the crystal structure and the non-parabolicity of the energy bands.

These conductivity coefficients have been used to derive general expressions for the above mentioned transport coefficients for the first time that takes into account the band tails in the density of states of both the conduction and valance bands.

Finally, the normalized transport coefficients, i.e., μ_n, r, h_t have been calculated numerically by using both the parabolic and non-parabolic density of states in the doping concentration range from 1×10^{18} to $2 \times 10^{20}\, cm^{-3}$ at $300^o K$.

On the basis of our calculations it is concluded that the total number of occupied states in the band tail is small compared with the total number of electrons occupying the parabolic portion of the conduction band at all doping concentrations approximately below $1 \times 10^{18}\, cm^{-3}$, and as a result, one can neglect the effect of band tail states in the quantum density of states and apply the usual classical parabolic quantum density of states.

However, for doping concentrations above $1 \times 10^{18}\, cm^{-3}$, the deviation between the

values of the normalized transport coefficients calculated by using the parabolic and non-parabolic density of states increases with increasing n_n. The calculation of η, μ_n, r, and h_t by using the non-parabolic density of states are found to reduce the corresponding values obtained by using the parabolic density of states as much as 37%, 59%, 54%, and 24%, respectively. This means that, at higher doping concentrations, taking the band tails into account in heavily doped semiconductors significantly changes the values of the electron drift mobility, the Hall coefficient, and the coefficient of transverse magnetoresistance. Therefore, it is very important to take into account the effect of band tails in the calculation of any transport coefficient in heavily doped semiconductors.