THERMAL CONDUCTIVITY AND WIEDEMANN-FRANZ RATIO IN HEAVILY DOPED n-TYPE SILICON WITH MIXED SCATTERING

A Thesis Submitted to the
School of Graduate Studies
Addis Ababa University

In Partial Fulfillment
of the Requirements for the Degree
of Master of Science in Physics

By
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June 2003

Addis Ababa

ADDIS ABABA UNIVERSITY

SCHOOL OF GRADUATE STUDIES

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Acknowledgement

First of all I would like to express my profound appreciation to Prof. S. K. Sharma who let me work with him after too much time has passed and for his intensive and extensive assistance and helpful fatherly comments. The editing part- was totally left for him. I admire his tireless patience in reading, correcting and shaping the entire thesis. I am also grateful to Dr. Mulugeta Bekele for allowing the use of Ultra-Spark 5 Sun Station without which the present work would not have been possible and the university of Uppsala who had provided the computer. I am also indebted to Dr. Fesseha Kassahun, head of the department of physics, who arranged every thing for me to start working with Prof. S. K. Sharma.

Last but not least, I would like to extend my deepest thanks to my mother and brothers for their unreserved encouragement morally and financially to accomplish my studies at all.

Table of contents

Contents page

List of tables

List of figures

1. Introduction

Recently many workers have investigated the effect of heavy doping on transport properties and the band gap narrowing of silicon. Lee and Fossum [1], and Poortmans et al [2] have calculated the band gap narrowing in heavily doped silicon. Lee and Fossum have used simplified Kane's [3] density of state function to calculate the band gap narrowing of heavily doped n-type silicon and have obtained excellent agreement with the available experimental data. Poortmans et al have calculated band gap narrowing in p-type silicon. Sharma [4] has calculated D/μ in heavily doped n-type silicon and Elfagad et al [5] have calculated galvanomagnetic transport coefficients in heavily doped n-type silicon, using simplified Kane's density of states function. Both of these investigators have shown that using appropriate density of states function leads to significant changes in the calculation of transport coefficients in heavily doped n-type silicon. More recently Mulugeta Habte [6] has calculated the electron thermal conductivity and Wiedemann-Franz ratio in heavily doped n-type silicon considering ionized impurities scattering as the dominant electron scattering mechanism and has not included electron scattering by acoustic phonons and thus his theory is restricted to very heavily doped concentration, i.e. $N_d \geq 10^{19}/cm^3$. In the intermediate concentration range, i.e. $N_d \approx 10^{18} - 10^{19}/cm^3$, acoustic phonons scattering is no longer negligible and thus one must consider the mixed scattering of ionized impurities and acoustic phonons in the calculation of any transport coefficients of silicon having intermediate doping concentration. To the best of my knowledge no work has been reported in the calculation of Wiedemann-Franz ratio in heavily doped n-type silicon for the case of mixed scattering of ionized impurities and acoustic phonons.

In this thesis we derive the explicit expressions of electronic thermal conductivity and Wiedemann-Franz ratio in heavily doped n-type silicon using appropriate density of states function for the case of mixed scattering of electrons by ionized impurities as well as acoustic phonons. These explicit expressions are further used to calculate numerically the electronic thermal conductivity and Wiedemann-Franz ratio in heavily doped n-type silicon for various electron concentrations. For sake of comparison we have also calculated the corresponding values of electronic thermal conductivity and Wiedemann-Franz ratio when parabolic density of states function is used. It is seen from our calculations that taking into account the effect of band tails leads to significant change in the calculation of electronic thermal conductivity and Wiedemann-Franz ratio in heavily doped n-type semiconductors.

2. Density of states in heavily doped silicon

In lightly doped silicon the density of states $[D(E)]$, which is defined as number of electron states per unit volume per unit energy, is parabolic [7] and is given by

$$\frac{dn_s}{dE} = D(E) = \left(\frac{1}{2\pi^2}\right)\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}}[E - E_C]^{\frac{1}{2}}, \qquad 2.1$$

where n_s is the number of electron states per unit volume, m_n^* is the density of states effective mass, $\hbar$ is the reduced Planck's constant, E is energy of an electron and E_c is the bottom of the conduction band, usually assumed to be zero.

The parabolic density of states function D(E) given by equation (2.1) is sown below.

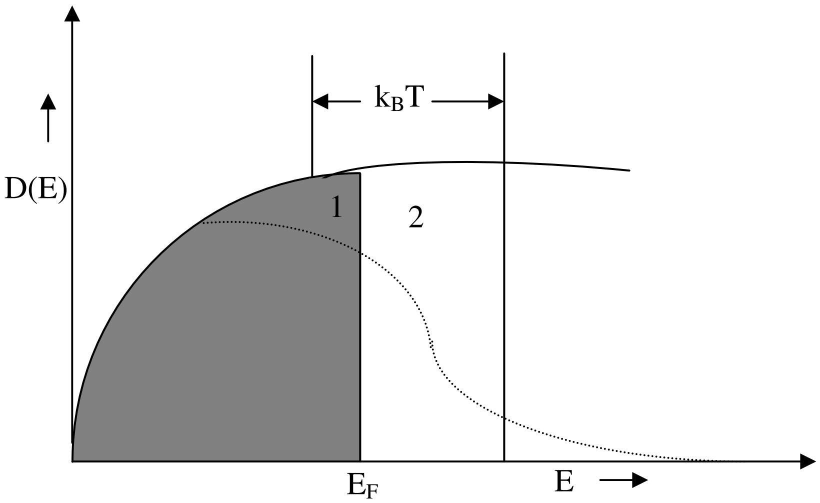

Figure 1: Density of single- particle states as a function of energy, for a free electron gas in three dimensions. The curve represents the density $f(E,T)D(E)$ of filled orbital at a finite temperature, but such that k_BT is small in comparison with E_F. The shaded area represents the filled orbital at absolute zero. The average energy is increased when the temperature is increased from 0 to T, for electrons are thermally exited from region 1 to region 2.

The high-density limit occurs when many impurity atoms are found within a volume characteristic of the "spread" or width of a typical wave function. Thus we do not, in the high density limit, think of a wave function as localized in a single impurity atom; the wave function is localized in a region in space in which many impurities are present, and no one impurity is very important. The high-density limit is in fact approached in semiconductors, where the average distance between impurities may be much smaller than the effective Bohr radius, yet large compared to the lattice spacing [8]. In a heavily doped n-type silicon, i.e. $N_d \geq 10^{18}/\text{cm}^3$, the density of states function is no longer parabolic for the simple reason that in a heavily doped semiconductor the impurity states and consequently electron states extend from well inside the forbidden gap to the conduction band, as a result of which the density of states function in heavily doped semiconductor shows tailing into the forbidden gap. In the following, we shall describe the density of states function with band tails.

Density of states function having band tails

Following Kane [3], the density of states function in heavily doped n-type silicon is given by

$$\frac{dn_s}{dE} = D(E) = \frac{m_n^{*\frac{3}{2}} 2^{\frac{3}{4}} \delta^{\frac{1}{2}}}{\pi^2 \hbar^3} y(z), \qquad 2.2$$

where

$$y(z) = \frac{1}{\pi^{\frac{1}{2}}} \int_{-\infty}^{z} (z-\xi)^{\frac{1}{2}} \exp\left(-\xi^2\right) d\xi \qquad 2.3$$

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

$\delta = \left(\frac{N_d e^4 a_s}{8\pi K^2} \right)^{\frac{1}{2}}$, is standard deviation of Gaussian distribution for impurity potential energy, a_s is

the Coulomb screening length and is given by $a_s = \left(\frac{\pi^{\frac{1}{3}} \hbar^2 K}{4 m_n^* e^2 (3N_d)^{\frac{1}{3}}} \right)^{\frac{1}{2}}$ [3], K is the dielectric constant of the crystal and N_d is the number of donor impurity ions per cm^3. From charge neutrality condition of a crystal i.e. $n + N_a^- = p + N_d^+$, if all the donor impurities are ionized, i.e. $N_d^+ = N_d$, in an n-type semiconductor where $n >> p$ and $N_d >> N_a, n_i$ then the charge neutrality implies $n = N_d$. This is justified in view of ionization energy (E_d=0) for $N_d \geq 10^{18} / cm^3$ [22].

The function y (z) occurring in Kane's density of states, i.e. equation (2.3), is so complicated that in this form, it can not be used for making any transport calculations in heavily doped n-type silicon. Slotboom has, however, suggested the following simplified form for y (z) [10]

$$y(z) \approx z^{\frac{1}{2}} \left(1 - \frac{1}{16z^2} \right) \qquad (for\ \infty > z > 0.601) \qquad 2.5$$

and

$$y(z) \approx \frac{1}{2\pi^{\frac{1}{2}}} \exp(-z^2)[0.319 + 0.906 \exp(2z)] \qquad (for\ -\infty < z \leq 0.601). \qquad 2.6$$

Electron concentration, i.e. number of electrons per unit volume, in the energy range $E \rightarrow E + dE$ [3] is then

$$dn = D(E) f\, dE, \qquad 2.7$$

where f is the Fermi-Dirac distribution function, given by the equation

$$f = \frac{1}{1+\exp(X-\eta)}, \qquad 2.8$$

where $X = \frac{E}{k_B T}$ and $\eta = \frac{E_F}{k_B T}$ are the dimensionless electron energy and Fermi energy respectively.

For parabolic density of states, substituting equation (2.1) into equation (2.7) and $dE = \sqrt{2}\delta\, dz$, the total electron concentration for parabolic density of states is

$$n = \frac{2^{\frac{1}{2}} m_n^{*\frac{3}{2}} (k_B T)^{\frac{3}{2}}}{\pi^2 \hbar^3} F_{\frac{1}{2}}(\eta), \qquad 2.9$$

where $F_b(\eta) = \int_0^{\infty} \frac{z^b dz}{[1+\exp(z-\eta)]}$ is the Fermi-Dirac integral of order b.

Following the same steps as above except replacing equation (2.1) by equation (2.2) and substituting the appropriate value of y (z), i.e. equations (2.5) and (2.6), electron concentration for density of states having band tails is then. Or we can get the equation for electron concentration, substituting $z^{\frac{1}{2}}$ by $y(z)$ in equation (2.9)

$$n = \frac{2^{\frac{5}{4}} m_n^{*\frac{3}{2}} \delta^{\frac{3}{2}}}{\pi^2 \hbar^3} \Psi_o \qquad 2.10$$

where

$$\Psi_o = \int_{-\infty}^{0.601} \frac{\exp(-z^2)[0.319+0.906\exp(2z)]dz}{2\pi^{\frac{1}{2}}\left[1+\exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right]} + \int_{0.601}^{\infty} \frac{z^{\frac{1}{2}}\left(1-\frac{1}{16z^2}\right)dz}{\left[1+\exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right]}. \qquad 2.11$$

It is more convenient to express electron concentration in the normalized form as

$$n_n = \frac{n}{10^{18}/cm^3} = \frac{2^{\frac{5}{4}} m_n^{*\frac{3}{2}} \delta^{\frac{3}{2}}}{10^{18} \pi^2 \hbar^3} \Psi_O \qquad 2.12$$

We shall use the density of states given by equations (2.2), (2.5) and (2.6) in chapter IV to derive the explicit expressions of K_e, σ and $\frac{K_e}{\sigma T}$.

3. Electron scattering mechanisms

Even though there are various carrier scattering mechanisms that are responsible for electrical resistivity of semiconductors, at room temperature and high electron concentrations in n-type silicon we need to consider only ionized impurities and acoustic phonons scattering mechanisms. It will therefore be appropriate for us to discuss both of these electron scattering mechanisms in some details.

3.1. Ionized impurities scattering

In a semiconductor, in which the number of electrons varies with varying impurity content, the change in number of electrons will be accompinished by changes in the scattering mechanism. For such conditions, of course, the relaxation time (τ), the time between any two successive collisions [11], will depend upon the impurity concentration and it will be impractical to change the electron concentration with out changing the relaxation time [12]. The scattering of electrons by ionized impurities is similar to the scattering of charged particles by nuclei, usually referred to as Rutherford scattering [13]. Following the works of Conwell and Weisskopf [14] we will, in this section, present the calculation of collision frequency of electrons scattered by ionized impurities ($\nu_I = \frac{1}{\tau_I}$).

In a homogeneous and isotropic medium, with uniform electric field ε_z applied in the z-direction. The Boltzmann transport equation [15] can be written as

$$\frac{-\varepsilon_Z e}{m_n^*}\frac{\partial f}{\partial u_z} = -\nu\left(f - f_o\right) = b - a, \qquad 3.1$$

where ‘ e ’ is charge of an electron, f is the total distribution function, f_o is the isotropic part of the distribution function, u_z is the electron velocity along z-axis, ‘b’ represents the number of particles entering a unit volume in unit time as a result of collisions and ‘a’ represents the corresponding number leaving in a similar manner.

Conwell and Weisskopf [14] made the following assumptions to simplify the calculation of the collision frequency of an electron by ionized impurities.

(1). Mass of the scattering center is infinite.

(2). Collisions are perfectly elastic.

(3). Scattering of an electron by one ion can be treated to a first approximation as independent of all other ions.

If 2d is the average distance between nearest neighbor impurity ions, then, according to assumption (3), an electron is scattered by a particular ion only when it comes within distance d of that ion. Therefore, one can express the number of electrons scattered out of unit volume in unit time into the solid angle $d\Omega'$ at $\theta' and\ \varphi'$ as

$$f\left(u,\theta.\varphi\right)N_d\sigma\left(\theta,\theta'\right)ud\Omega', \qquad 3.2$$

where u is the relative velocity of the electron and the scattering center, assumed to be the velocity of the electron, $\left(\theta-\theta'\right)$ is the angle between the scattered and incident directions, known as the scattering angle, σ(θ,θ') is the Rutherford scattering cross section, given by[16].

$$\sigma(\theta,\theta') = \left(\frac{e^2}{4KE}\right)^2 \frac{1}{\sin^4\left(\frac{\theta-\theta'}{2}\right)} \qquad 3.3$$

The term 'a' is the integral of the above expression, i.e. equation (3.2), over θ', φ'. It is apparent that the integration is not to be carried out over all θ'. The limitation on θ' can be expressed as [16]

$$\tan\left[\frac{(\theta'-\theta)}{2}\right] = \frac{e^2}{2KE\beta} = \frac{e^2}{Km_n^* u^2 \beta}, \qquad 3.4$$

where β is the impact parameter, the perpendicular distance between the center of force and the incident velocity, for maximum value of impact parameter $d\left(=1\big/2N_d^{\frac{1}{3}}\right)$ [1] the scattering angle is minimum, thus

$$\theta'-\theta = (\theta'-\theta)_{\min} = 2\tan^{-1}\left[\frac{e^2}{Km_n^* u^2 d}\right]. \qquad 3.5$$

Equation (3.5) gives the lowest limit for integration over θ'. According to assumption (2) it is possible to choose $\theta = 0$, then the expression for 'a' is

$$a = N_d u \int_{\theta'_{\min}}^{\pi} \int_{0}^{2\pi} f(u,0,\varphi)\sigma(\theta')d\Omega. \qquad 3.6$$

The term 'b', which determines the number of particles entering a unit volume in unit time, is evaluated in much the same manner as 'a'. Therefore, 'b - a' is given by

$$b - a = N_d u \int_{\theta'_{\min}}^{\pi} \int_{0}^{2\pi} [f(u,\theta',\varphi') - f(u,0,\varphi)]\sigma \, d\Omega'. \tag{3.7}$$

Using equation (3.7) in Boltzmann transport equation, i.e. equation (3.1), we get

$$-v(f - f_o) = N_d u \int_{\theta'_{\min}}^{\pi} \int_{0}^{2\pi} [f(u,\theta',\varphi') - f(u,0,\varphi)]\sigma \sin\theta' d\theta' d\varphi'. \tag{3.8}$$

Following Lorentz [17] the distribution function can be expanded as

$$\begin{aligned} f &= f_0 - u_z \chi(u) \\ &= f_0 - u\cos\theta\,\chi(u), \end{aligned} \tag{3.9}$$

where $u\chi(u)$ is the anisotropic part of the distribution of electron velocity. Using equation (3.9) it is possible to write the right hand side of equation (3.8) as

$$f(u,\theta',\varphi') - f(u,0,\varphi) = u\chi(u)(1 - \cos\theta). \tag{3.10}$$

Substituting equation (3.10) into equation (3.7), and after integrating over φ' we obtain

$$b - a = 2\pi N_d u^2 \chi(u) \left(\frac{e^2}{2Km_n^* u^2} \right)^2 \int_{\theta'_{\min}}^{\pi} \frac{(1 - \cos\theta')d(-\cos\theta')}{\left(\frac{1 - \cos\theta'}{2} \right)^2}. \tag{3.11}$$

Putting $x = 1 - \cos\theta'$, and $dx = d(-\cos\theta')$ equation (3.11) becomes

$$b - a = 8\pi N_d \chi(u) \left(\frac{e^2}{2Km_n^* u} \right)^2 \ln\left(\frac{2}{x_{\min}} \right). \tag{3.12}$$

Then $\theta'_{\min}$, the minimum angle of scattering can be obtained from equation (3.4) as

$$\theta'_{\min} = \cos^{-1}\left[\frac{2}{1 + t^2} - 1 \right] \tag{3.13}$$

where

$$t = \frac{e^2}{K m_n^* u^2 d}. \qquad 3.14$$

Using the calculated value of $\theta'_{\min}$, i.e. equation (3.13), the expression for $x_{\min}$ could be written as

$$x_{\min} = \frac{2t^2}{1+t^2}. \qquad 3.15$$

Substituting equations (3.14) and (3.15) into equation (3.12) '$b-a$' will be

$$b - a = 8\pi N_d \chi(u) \left(\frac{e^2}{2K m_n^* u} \right)^2 \ln\left[1 + \frac{K^2 m_n^{*2} u^4 d^2}{e^4} \right]. \qquad 3.16$$

Replacing the values of equations (3.10) and (3.16) into equation (3.8), and using $\frac{m_n^* u^2}{2} = E = k_B T X$, $d = \frac{1}{2N_d^{\frac{1}{3}}}$. The expression for collision frequency due to ionized impurities in terms of dimensionless electron energy becomes

$$\nu_I = \frac{1}{\tau_I} = \nu_{0I} X^{-\frac{3}{2}} \qquad 3.17$$

where,

$$\nu_{0I} = \frac{4\pi N_d e^4}{2^{\frac{5}{2}} m_n^{*\frac{1}{2}} K^2 (k_B T)^{\frac{3}{2}}} \ln\left[1 + \frac{K^2 E^2}{e^4 N_d^{\frac{2}{3}}} \right]. \qquad 3.18$$

Conwell and Weisskopf introduced this formula in calculating the effect of impurity scattering on mobility. For most of the cases of interest, the logarithmic function occurring in equation (3.18) is a slowly varying function of electron energy therefore one can treat ν_{oI} as a constant in the calculation of any transport coefficients.

3.2. Acoustic phonons scattering

Charge transport is, of course, by electrons; where as phonons, i.e. quanta of vibration energy, and all other mobile quasi-particles cause heat transport in solids that contain excess energy and interact with the lattice [13]. In semiconductors with low carrier density, and in the absence of light and electric field, the thermal energy transport is caused mainly by phonons [18]. In this part of chapter III we will derive the expression for electron collision frequency due to acoustic phonons, i.e. ordinary elastic waves [19], following the work of Weisskopf-Wigne [12]. The electron scattering transition in acoustic phonon scattering is shown below.

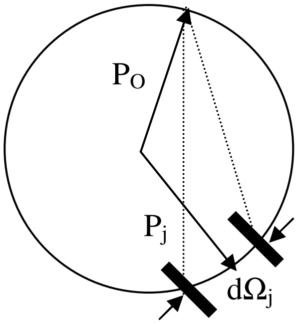

Figure 2: An electron initially in state P_o of the Brillouin zone makes transition to other states of the energy according to the classical model.

In the calculation of mean free time, made the following assumptions could be made [12].

(1). Probability that the electron (or holes) make a transition in any small interval dt of time is dt/τ is constant.

(2). The end state of the transition is independent of the initial state, and the probability of arriving at any particular end state is proportional to the probability that the end state would normally be occupied in the thermal equilibrium distribution.

Assumption (1) has two independent implications. (a) The probability of transition does not depend on the elapsed time since the last transition. (b) The probability of transition does not depend upon the quantum state occupied by the electron or hole. This assumption leads the matrix element for transition from state P_o to P_j be [12]

$$U_{oj} = \int \Phi_o^* u_1 \Phi_j d(all\, coordinates), \qquad 3.19$$

where Φ_o and Φ_j are the wave functions of the system corresponding to the states P_o and P_j in the Brillouin zone, here the Φ symbols are functions of the coordinates of the nuclei and of the position and spin of the excess electron.

The probability of transition per unit time will be proportional to the area and could be written as $W_{oj} d\Omega_j$ [12]. The total probability per unit time of making a transition from state P_o is then

$$W_o = \int_{\Omega(\varepsilon)} W_{oj} d\Omega_j, \qquad \Omega(\varepsilon) = \text{Energy surface.} \qquad 3.20$$

Here W_{oj} could be written as [12]

$$W_{oj} = \frac{|U_{jo}|^2}{\hbar} 2\pi\rho_j, \qquad 3.21$$

where ρ_j is the number of end states per unit energy per unit surface, it is a function of $\vec{P}_j$ given by $\rho_j = \frac{V}{h^3 u_j} = \frac{V}{h^3 u_0}$ since $u_j = u_0$. It must be noted that the density of end states is $\frac{V}{h^3}$.

The relaxation time due to acoustic phonons scattering is then

$$\frac{1}{\tau_A} = W_o = \int_{\Omega(\varepsilon_o)} W_{oj} d\Omega_j .$$

3.22

The value of the matrix element for transition from state P_o to P_j can be rewritten as [12]

$$\left|U_{oj}\right|^2 = \frac{AT}{V}, \qquad 3.23$$

where T is the absolute temperature, V the volume of the crystal, and A is a constant depending on the elastic properties of the crystal, the mass of the atoms, and a certain attributes of the wave functions but not upon P_o or P_j. From the isotropic approximation for all directions of propagation the value of A is given by the formula [12]

$$A = \frac{E_1^2 k_B}{VC_{11}}, \qquad 3.24$$

where E_1 is the deformation potential of the crystal, defined as the change in band gap per unit strain [18], $C_{11}\left(= \rho u^2\right)$ is the elastic stiffness constant [7] and ρ is the density of the crystal.

It is to be noted that $\left|U_{oj}\right|^2$ is independent of the change in direction of the electron's motion, so that, after being scattered, the electron is equally likely to have momentum in any direction. Since the values of W_{oj} do not depend on the direction of $\overrightarrow{P}_j$. The integration over $d\Omega_j$ in equation (3.22) reduces simply to multiplying by $4\pi P_o^2$, therefore

$$\frac{1}{\tau_A} = \frac{2\pi}{\hbar}\rho_j\left|U_{jo}\right|^2 4\pi P_o^2 = \frac{2\pi}{\hbar}\left[\frac{V}{h^3}.\frac{1}{u_o}\right]\frac{AT}{V}.4\pi P_o^2 = \frac{u_o}{l(T)}, \qquad 3.25$$

where $u_o = \frac{\left|P_o\right|}{m_n^*} = \left(\frac{2}{m_n^*}\right)^{\frac{1}{2}} E^{\frac{1}{2}}$, is the electron velocity.

This expression shows that the transition probability is proportional to u_o, corresponding to a mean free path $l(T)$ independent of velocity and is given by the formula

$$l(T)=\frac{E_1^2 k_B T m_n^{*2}}{\pi \hbar^4 u^2 \rho}. \qquad 3.26$$

Substituting equation (3.26) and $u_o=\left(\frac{2}{m_n^*}\right)^{\frac{1}{2}}(k_B TX)^{\frac{1}{2}}$ into equation (3.25), the collision frequency of electrons due to acoustic phonons is then

$$\nu_A=\frac{1}{\tau_A}=\nu_{OA}X^{\frac{1}{2}} \qquad 3.27$$

where

$$\nu_{oA}=\frac{2^{\frac{1}{2}} m_n^{*\frac{3}{2}} E_1^2 (k_B T)^{\frac{3}{2}}}{\pi \hbar^4 u^2 \rho}. \qquad 3.28$$

Whenever there are two or more scattering mechanisms, having collision frequencies of ν_1, ν_2, …, the collision frequency of the system can be written as [13]

$$\nu=\nu_1+\nu_2+\ldots\ldots. \qquad 3.29$$

For our case, where mixed scattering is considered, from equations (3.17) and (3.27) the collision frequency of the entire system becomes

$$\nu=\nu_{oA}\left(X^2+\frac{\nu_{oI}}{\nu_{oA}}\right)X^{-\frac{3}{2}}. \qquad 3.30$$

In chapter IV, in the calculation of transport coefficients, i.e. σ, K_e, $K_e/\sigma T$, we will use equation (3.30) for mixed scattering of electrons by ionized impurities and acoustic phonons.

4. Electrical and thermal conductivities and Wiedemann-Franz ratio for parabolic density of states

In this chapter we shall derive the expression for electrical conductivity, electronic contribution to thermal conductivity and Wiedemann-Franz ratio for n-type silicon having parabolic density of states.

4.1. Electrical conductivity for parabolic density of states

In calculating the electrical conductivity, first let we define and calculate the x-component of current density, dJ_x, due to electrons having their energy between E and $E + dE$

$$dJ_x = -eu_x dn, \qquad 4.1$$

where dn is the concentration of electrons having their energy in the above energy range which is given by equation (2.7).

Substituting density of states for lightly doped silicon given by equation (2.1) into equation (4.1) or using equation (2.1) directly, considering one dimensional motion, we get

$$dJ_x = -\frac{2m_n^{*3}e}{h^3} u_x f \, du_x du_y du_z . \qquad 4.2$$

In the presence of an external d.c electric field along x-axis, the distribution function can be expanded as $f = f_o + u_x f_x$. The current density dJ_x in the presence of an electric field $\vec{\varepsilon} = \varepsilon_x \hat{i}$ may be written as

$$dJ_x = -\frac{2m_n^{*3}e}{h^3}\left(f_o + u_x f_x\right)u^3 du \cos\theta\, d\left(-\cos\theta\right)d\varphi, \qquad 4.3$$

since f_o does not contribute to the current density (as the integral involving f_o vanishes due to the orthogonal properties of Legendre function), the expression for the current density dJ_x reduces to

$$dJ_x = -\frac{2m_n^{*3}e}{h^3} f_x u^4 du \cos^2\theta\, d(-\cos\theta)d\varphi. \qquad 4.4$$

After integrating over θ and φ, the total current density will then be

$$J_x = -\frac{8\pi m_n^{*3}e}{3h^3}\int_0^\infty f_x u^4 du, \qquad 4.5$$

where f_x is the anisotropic part of the distribution function and can be evaluated by solving Boltzmann transport equation. Now the Boltzmann transport equation in the presence of $\vec{\varepsilon} = \varepsilon_x \hat{i}$ ($\vec{B} = \vec{\nabla} f = 0$) may be written as

$$-\frac{e\varepsilon_x}{m_n^*}\frac{\partial f_o}{\partial u}\frac{u_x}{u} = -v\left(f - f_o\right) = -vu_x f_x. \qquad 4.6$$

Linearizing the Boltzmann equation and equating coefficients of u_x on both sides we get

$$f_x = \frac{e\varepsilon_x}{v}\frac{\partial f_o}{\partial E}. \qquad 4.7$$

Substituting equation (4.7) for f_x into equation (4.5) we obtain

$$J_x = -\frac{m_n^{*3}e^2\varepsilon_x}{3\pi^2\hbar^3}\int_0^\infty \frac{1}{v}\frac{\partial f_o}{\partial E}u^4 du. \qquad 4.8$$

After changing the variable of integration to E the electrical conductivity, $\sigma_{xx} = \frac{J_x}{\varepsilon_x}$ can be written as

$$\sigma_{xx} = -\frac{m_n^{*\frac{1}{2}} e^2 2^{\frac{3}{2}}}{3\pi^2\hbar^3}\int_0^\infty \frac{E^{\frac{3}{2}}}{\nu}\frac{\partial f_o}{\partial E}\, dE. \tag{4.9}$$

Substituting the value of the collision frequency for mixed scattering from equation (3.30), equation (4.9) could be rewritten as

$$\sigma_{xx} = \frac{m_n^{*\frac{1}{2}} e^2 2^{\frac{3}{2}}}{3\pi^2\hbar^3\nu_{OA}\left(k_B T\right)^{\frac{3}{2}}}\int_0^\infty \frac{E^3\left(-\frac{\partial f_o}{\partial E}\right)dE}{\left\{\left(\frac{E}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}}. \tag{4.10}$$

It is more convenient to change the variable of integration from E to z, given by equation (2.4), in equation (4.10). Thus we obtain the following expression for electrical conductivity

$$\sigma_{xx} = \frac{8 m_n^{*\frac{1}{2}} e^2 \delta^3}{3\pi^2\hbar^3\nu_{OA}\left(k_B T\right)^{\frac{3}{2}}}\int_0^\infty \frac{z^3\left(-\frac{\partial f_o}{\partial z}\right)dz}{\left\{\left(\frac{\sqrt{2}\delta z}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}} = \frac{2^{\frac{7}{2}} m_n^{*\frac{1}{2}} e^2 \delta^4}{3\pi^2\hbar^3\nu_{OA}\left(k_B T\right)^{\frac{5}{2}}}\Psi_3, \tag{4.11}$$

where

$$\Psi_3 = \int_0^\infty \frac{z^3 \exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\} dz}{\left\{0.59516 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2}. \tag{4.12}$$

For case of dominant ionized impurities scattering, i.e. $\nu_{OA} \to 0$, the expression for electrical conductivity reduces to

$$\sigma'_{xx} = \frac{2^{\frac{3}{2}} m_n^{*\frac{1}{2}} e^2 (k_B T)^{\frac{3}{2}}}{\pi^2 \hbar^3 \nu_{OI}} F_2(\eta), \qquad 4.13$$

where $F_2(\eta)$ is Fermi-Dirac integral of order 2.

4.2. Thermal conductivity for parabolic density of states

The thermal current density, C_x, due to electrons may be written as

$$C_x = \frac{2m_n^{*3}}{h^3} \iiint E u_x f \, du_x du_y du_z = \frac{2m_n^{*3}}{h^3} \iiint E u \cos\theta \, f u^2 du \sin\theta d\theta d\varphi. \qquad 4.14$$

In the presence of an external temperature gradient $\vec{\nabla} T$ and $\vec{\varepsilon}$ along x-direction f can be expanded as $f = f_o + u_x f_x$. After substituting for f into equation (4.14) and integrating over θ and φ we get

$$C_x = \frac{8\pi m_n^{*3}}{3h^3} \int_0^\infty E u^4 f_x du. \qquad 4.15$$

Thus to obtain the expression of thermal current density we need to evaluate f_x, the anisotropic part of distribution function in the presence of an external temperature gradient $\frac{dT}{dx}$ and E_x which is done by solving Boltzmann transport equation. Therefore Boltzmann transport equation in the presence of $\vec{\nabla} T = \frac{dT}{dx}\hat{i}$ and $\vec{\varepsilon} = \varepsilon_x \hat{i}$ can be written as

$$u_x \frac{\partial f_O}{\partial x} - \frac{e\varepsilon_x}{m_n^*} \frac{\partial f_O}{\partial u_x} = -\nu(f - f_O) = -\nu u_x f_x \qquad 4.16$$

but

$$\frac{\partial f_O}{\partial x} = -\frac{\partial f_O}{\partial E}\left[\frac{E}{T} + T\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right]\frac{dT}{dx}. \tag{4.17}$$

Therefore, substituting equation (4.18) into equation (4.17) gives

$$-u_x\frac{\partial f_O}{\partial E}\left[\frac{E}{T} + T\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right]\frac{dT}{dx} - \frac{e\varepsilon_x u_x}{m_n^* u}\frac{\partial f_O}{\partial u} = -vu_x f_x. \tag{4.18}$$

Solving equation (4.18) for f_x will give

$$f_x = \frac{1}{v}\frac{\partial f_O}{\partial E}\left[\left\{\frac{E}{T} + T\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right\}\frac{dT}{dx} + e\varepsilon_x\right]. \tag{4.19}$$

Therefore, the thermal current density will be

$$C_x = \frac{8\pi m_n^{*3}}{3h^3}\int_0^\infty \frac{Eu^4}{v}\frac{\partial f_O}{\partial E}\left[\left\{\frac{E}{T} + T\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right\}\frac{dT}{dx} + e\varepsilon_x\right]du. \tag{4.20}$$

Thermal conductivity K is defined as $K = -\dfrac{C_x}{\left(\dfrac{dT}{dx}\right)}$ with the boundary condition that $J_x = 0$

$$J_x = -\frac{8\pi m_n^{*3} e}{3h^3}\int_0^\infty \frac{u^4}{v}\frac{\partial f_O}{\partial E}\left[\left\{\frac{E}{T} + T\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right\}\frac{dT}{dx} + e\varepsilon_x\right]du = 0. \tag{4.21}$$

Using $J_x = 0$, i.e. equation (4.21), gives

$$e\varepsilon_x = -\frac{1}{T}\frac{dT}{dx}\left(\frac{\displaystyle\int_0^\infty \frac{Eu^4}{v}\frac{\partial f_O}{\partial E}du}{\displaystyle\int_0^\infty \frac{u^4}{v}\frac{\partial f_O}{\partial E}du} + T^2\frac{\partial}{\partial T}\left(\frac{E_F}{T}\right)\right). \tag{4.22}$$

Substituting equation (4.22) for ε_x into equation (4.20) the expression for thermal current density becomes

$$C_x = -\frac{8\pi m_n^{*3}}{3h^3 T}\frac{dT}{dx}\left\{ \frac{\left[\int_0^\infty \frac{Eu^4}{v}\frac{\partial f_O}{\partial E}du\right]^2}{\int_0^\infty \frac{u^4}{v}\frac{\partial f_O}{\partial E}du} - \int_0^\infty \frac{E^2 u^4}{v}\frac{\partial f_O}{\partial E}du \right\}. \qquad 4.23$$

In terms of energy of an electron, E, the electronic contribution to thermal conductivity K_e is given by

$$K_e = \frac{2^{\frac{3}{2}} m_n^{*\frac{1}{2}}}{3\pi^2\hbar^3 T}\left\{ \frac{\left[\int_0^\infty \frac{E^{\frac{5}{2}}}{v}\frac{\partial f_O}{\partial E}dE\right]^2 - \int_0^\infty \frac{E^{\frac{7}{2}}}{v}\frac{\partial f_O}{\partial E}dE \int_0^\infty \frac{E^{\frac{3}{2}}}{v}\frac{\partial f_O}{\partial E}dE}{\int_0^\infty \frac{E^{\frac{3}{2}}}{v}\frac{\partial f_O}{\partial E}dE} \right\}. \qquad 4.24$$

Now again substituting the value of collision frequency for mixed scattering, from equation (3.30), into equation (4.24) the electronic thermal conductivity becomes

$$K_e = \frac{2^{\frac{3}{2}} m_n^{*\frac{1}{2}}}{3\pi^2\hbar^3 T \nu_{OA}(k_B T)^{\frac{3}{2}}}\left\{ \frac{\left[\int_0^\infty \frac{E^4\left(\frac{\partial f_O}{\partial E}\right)dE}{\left\{\left(\frac{E}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}}\right]^2 - \int_0^\infty \frac{E^5\left(\frac{\partial f_O}{\partial E}\right)dE}{\left\{\left(\frac{E}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}} \int_0^\infty \frac{E^3\left(\frac{\partial f_O}{\partial E}\right)dE}{\left\{\left(\frac{E}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}}}{\int_0^\infty \frac{E^3\left(\frac{\partial f_O}{\partial E}\right)dE}{\left\{\left(\frac{E}{k_B T}\right)^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}}} \right\} \qquad 4.25$$

It is more convenient to transform all the variables of integration from E to the dimensionless energy variable z, given by equation (2.4). Thus for case of mixed scattering of acoustic phonons and ionized impurities, we obtain the following expression for electronic contribution to thermal conductivity

$$K_e = \frac{2^{\frac{9}{2}} m_n^{*\frac{1}{2}} \delta^6}{3\pi^2 \hbar^3 \nu_{OA} T (k_B T)^{\frac{5}{2}}} \left[\Psi_5 - \frac{\Psi_4^2}{\Psi_3} \right], \tag{4.26}$$

where Ψ_3 is defined by equation (4.12)

$$\Psi_4 = \int_0^\infty \frac{z^4 \exp\left\{ 0.77147 n_n^{\frac{5}{12}} z - \eta \right\} dz}{\left\{ 0.59516 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}} \right\} \left\{ 1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta \right) \right\}^2} \tag{4.27}$$

and

$$\Psi_5 = \int_0^\infty \frac{z^5 \exp\left\{ 0.77147 n_n^{\frac{5}{12}} z - \eta \right\} dz}{\left\{ 0.59516 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}} \right\} \left\{ 1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta \right) \right\}^2}. \tag{4.28}$$

For case of dominant ionized impurities scattering, K_e reduces to

$$K_e^{'} = \frac{2^{\frac{3}{2}} m_n^{*\frac{1}{2}} (k_B T)^{\frac{7}{2}}}{3\pi^2 \hbar^3 \nu_{OI} T} \left[5F_4(\eta) - \frac{16 F_3^2(\eta)}{3F_2(\eta)} \right], \tag{4.29}$$

where $F_3(\eta)$ and $F_4(\eta)$ are Fermi-Dirac integrals of order three and four respectively.

4.3. Wiedemann-Franz ratio for parabolic density of states

Using equations (4.11) and (4.26) we obtain the following expression for Wiedemann-Franz ratio, $\frac{K_e}{\sigma_{xx}T}$, for mixed scattering in n-type semiconductor having parabolic density of states

$$\frac{K_e}{\sigma_{xx}T} = \left(\frac{k_B}{e}\right)^2 \left(\frac{\sqrt{2}\delta}{k_B T}\right)^2 \left[\frac{\Psi_5}{\Psi_3} - \left(\frac{\Psi_4}{\Psi_3}\right)^2\right]. \qquad 4.30$$

Using equations (4.13) and (4.29), Wiedemann-Franz ratio in n-type semiconductor having parabolic density of states when ionized impurities scattering dominates is then

$$\frac{K_e^{'}}{\sigma_{xx}^{'}T} = \left(\frac{k_B}{e}\right)^2 \left[15\frac{F_4(\eta)}{F_2(\eta)} - 16\frac{F_3^2(\eta)}{F_2^2(\eta)}\right]. \qquad 4.31$$

5. Electrical and thermal conductivities and Wiedemann-Franz ratio for density of states having band tails

The expressions for the electrical conductivity, electronic contribution to thermal conductivity and Wiedemann-Franz ratio for heavily doped n-type silicon having density of states with band tails can be obtained from their corresponding expressions of these quantities derived in chapter IV, by assuming parabolic density of states, employing the procedure consisting of five steps given below.

Step1. Extend the limit of integration (i.e. from 0 to ∞), in all the integrals occurring in equations (4.11), (4.27) and (4.33), from -∞ to +∞ [1].

Step2. Express each integral $\int_{-\infty}^{+\infty} f(z)dz$ in these equations as $\int_{-\infty}^{+\infty} f(z)z^{\frac{1}{2}}dz$.

Step3. Break the entire range (i.e. from -∞ to +∞) of all the integrals in to two ranges (i) -∞ to 0.601 and (ii) 0.601 to +∞.

Step4. Substituting equation (2.6) for $z^{\frac{1}{2}}$ in the range of integration from -∞ to 0.601.

Step5. Substituting equation (2.5) for $z^{\frac{1}{2}}$ in the range of integration from 0.601 to +∞.

After following the procedures outlined above in steps 1 to 5, we obtain the following expressions for $K_e, \sigma, \frac{K_e}{\sigma T}$, for mixed scattering of acoustic phonons and ionized impurities for heavily doped n-type silicon having density of states with band tails

$$\sigma_{xx} = \frac{2^{\frac{7}{2}} m_n^{*\frac{1}{2}} e^2 \delta^4}{3\pi^2 \hbar^3 \nu_{OA} \left(k_B T\right)^{\frac{5}{2}}} \Psi_{\frac{5}{2}} \qquad 5.1$$

$$K_e = \frac{2^{\frac{9}{2}} m_n^{*\frac{1}{2}} \delta^6}{3\pi^2 \hbar^3 \nu_{OA} T \left(k_B T\right)^{\frac{5}{2}}} \left[\Psi_{\frac{9}{2}} - \frac{\Psi_{\frac{7}{2}}^2}{\Psi_{\frac{5}{2}}} \right] \qquad 5.2$$

$$\frac{K_e}{\sigma_{xx} T} = \left(\frac{K_B}{e} \right)^2 \left(\frac{\sqrt{2}\delta}{K_B T} \right)^2 \left[\frac{\Psi_{\frac{9}{2}}}{\Psi_{\frac{5}{2}}} - \left(\frac{\Psi_{\frac{7}{2}}}{\Psi_{\frac{5}{2}}} \right)^2 \right], \qquad 5.3$$

where

$$\Psi_{\frac{5}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{5}{2}} \{0.319 + 0.906 \exp(2z)\} \exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\} dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\} \left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2}$$

$$+ \int_{0.601}^{\infty} \frac{z^3 \left(1 - \frac{1}{16z^2}\right) \exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\} dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\} \left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \qquad 5.4$$

$$\Psi_{\frac{7}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{7}{2}} \{0.319 + 0.906 \exp(2z)\} \exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\} dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\} \left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2}$$

$$+ \int_{0.601}^{\infty} \frac{z^4 \left(1 - \frac{1}{16z^2}\right) \exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\} dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\} \left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \qquad 5.5$$

and

$$\Psi_{\frac{9}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{9}{2}}\{0.319+0.906\exp(2z)\}\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\}dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}\left\{1+\exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2}$$

$$+ \int_{0.601}^{\infty} \frac{z^5\left(1-\frac{1}{16z^2}\right)\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\}dz}{\left\{0.5951 n_n^{\frac{5}{6}} z^2 + \frac{\nu_{OI}}{\nu_{OA}}\right\}\left\{1+\exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \qquad 5.6$$

For case of dominant ionized impurities scattering these expressions for K_e, σ_{xx}, $\frac{K_e}{\sigma_{xx}T}$ reduces

to

$$\sigma'_{xx} = \frac{2^{\frac{7}{2}} m_n^{*\frac{1}{2}} e^2 \delta^4}{3\pi^2\hbar^3\nu_{OI}\left(k_B T\right)^{\frac{5}{2}}}\Psi'_{\frac{5}{2}} \qquad 5.7$$

$$K'_e = \frac{2^{\frac{9}{2}} m_n^{*\frac{1}{2}} \delta^6}{3\pi^2\hbar^3\nu_{OI} T\left(k_B T\right)^{\frac{5}{2}}}\left[\Psi'_{\frac{9}{2}} - \frac{\Psi'^{2}_{\frac{7}{2}}}{\Psi'_{\frac{5}{2}}}\right] \qquad 5.8$$

$$\frac{K'_e}{\sigma'_{xx}T} = \left(\frac{k_B}{e}\right)^2\left(\frac{\sqrt{2}\delta}{k_B T}\right)^2\left[\frac{\Psi'_{\frac{9}{2}}}{\Psi'_{\frac{5}{2}}} - \left(\frac{\Psi'_{\frac{7}{2}}}{\Psi'_{\frac{5}{2}}}\right)^2\right], \qquad 5.9$$

where

$$\Psi'_{\frac{5}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{5}{2}}\{0.319 + 0.906\exp(2z)\}\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} + \int_{0.601}^{\infty} \frac{z^3\left(1 - \frac{1}{16z^2}\right)\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \tag{5.10}$$

$$\Psi'_{\frac{7}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{7}{2}}\{0.319 + 0.906\exp(2z)\}\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} + \int_{0.601}^{\infty} \frac{z^4\left(1 - \frac{1}{16z^2}\right)\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \tag{5.11}$$

and

$$\Psi'_{\frac{9}{2}} = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \frac{|z|^{\frac{9}{2}}\{0.319 + 0.906\exp(2z)\}\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta - z^2\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} + \int_{0.601}^{\infty} \frac{z^5\left(1 - \frac{1}{16z^2}\right)\exp\left\{0.77147 n_n^{\frac{5}{12}} z - \eta\right\}dz}{\left\{1 + \exp\left(0.77147 n_n^{\frac{5}{12}} z - \eta\right)\right\}^2} \tag{5.12}$$

In the next chapter we shall use equations (5.1) to (5.3) to calculate numerical values of each of transport coefficients for various concentrations for mixed scattering of electrons by acoustic phonons and ionized impurities, for this it is more appropriate to express each of these transport coefficients in the dimensionless form as follows

$$\sigma^d = \frac{v_{OA}\sigma m_n^*}{ne^2} = \frac{2}{3}\left(\frac{\sqrt{2}\delta}{k_B T}\right)^{\frac{5}{2}} \frac{\Psi_{\frac{5}{2}}}{\Psi_o} \tag{5.13}$$

$$K_e^d = \frac{K_e v_{OA} m_n^*}{n k_B^2 T} = \frac{2}{3}\left(\frac{\sqrt{2}\delta}{k_B T}\right)^{\frac{9}{2}} \left[\frac{\Psi_{\frac{9}{2}}}{\Psi_o} - \frac{\Psi_{\frac{7}{2}}^2}{\Psi_o \Psi_{\frac{5}{2}}}\right] \tag{5.14}$$

and

$$WF^d = \frac{K_e e^2}{\sigma T k_B^2} = \left(\frac{\sqrt{2}\delta}{k_B T}\right)^2 \left[\frac{\Psi_{\frac{9}{2}}}{\Psi_{\frac{5}{2}}} - \left(\frac{\Psi_{\frac{7}{2}}}{\Psi_{\frac{5}{2}}}\right)^2\right], \tag{5.15}$$

where σ^d, $K^d{}_e$ and WF^d are the normalized electrical conductivity, electronic contribution to thermal conductivity and the Wiedemann-Franz ratio respectively.

For parabolic density of states with mixed scattering σ^d, K_e^d and WF^d could be written as

$$\sigma^d = \frac{v_{OA}\sigma m_n^*}{ne^2} = \frac{2}{3}\left(\frac{\sqrt{2}\delta}{k_B T}\right)^4 \frac{\Psi_3}{F_{\frac{1}{2}}(\eta)} \tag{5.16}$$

$$K_e^d = \frac{K_e v_{OA} m_n^*}{n k_B^2 T} = \frac{2}{3}\left(\frac{\sqrt{2}\delta}{k_B T}\right)^6 \left[\frac{\Psi_5}{F_{\frac{1}{2}}(\eta)} - \frac{\Psi_4^2}{\Psi_3 F_{\frac{1}{2}}(\eta)}\right] \tag{5.17}$$

$$WF^d = \frac{K_e e^2}{\sigma T k_B^2} = \left(\frac{\sqrt{2}\delta}{k_B T}\right)^2 \left[\frac{\Psi_5}{\Psi_3} - \left(\frac{\Psi_4}{\Psi_3}\right)^2\right]. \tag{5.18}$$

6. Calculation of Fermi energy, electrical and thermal conductivities and Wiedemann-Franz ratio in heavily doped n-type silicon having band tails

6.1. Numerical calculations

It is obvious from equations (5.4) to (5.6) that to calculate the transport coefficients one needs to know the numerical values of the normalized Fermi energy η for a given electron concentration. But as can be seen from equation (2.12) it is not possible to calculate η from this equation for a given value of n_n. However, one can numerically calculate the value of n_n from equation (2.12) for a given value of η using iteration method as follows. For a given value of n_n, we choose an arbitrary value of η as the first approximation and then calculate the right hand side (RHS) of equation (2.12). For the second approximation of η, we slightly increase or decrease the value of the first approximation and then recalculate the RHS of equation (2.12). Now if this value of RHS of equation (2.12) is closer to n_n than the value of RHS obtained using the first approximation value of η, then we continue to vary η in the same direction till the difference between the two sides of equation (2.12) becomes negligible, i.e., 1 in 10^6. However, if the second approximation of η yields a value which further moves away from the value of n_n, we vary η in the opposite direction and continue to change it in the same direction till we reach a value of η for which the value of n_n for the two sides of equation (2.12) matches almost exactly. This value of η is the dimensionless Fermi energy measured relative to the shifted parabolic conduction band edge E_C.

In calculating dimensionless Fermi energy and the various transport coefficients, in n-type silicon we have used the following values of various parameters.

$T=300^0K$, $K=11.8$, $E_1=9.5ev$, $m^*{}_n=6^{2/3}m^*{}_e$ and $m_e{}^*=0.36m_o$ (m_0 is free mass of an electron).

Using above values of various parameters and density of states having band tails we have numerically calculated η, σ^d, $K^d{}_e$ and WF^d for case of mixed scattering of electrons by ionized impurities and acoustic phonons for different concentrations of heavily doped n-type silicon. Various definite integrals occurring in the expressions of the transport coefficients have been evaluated on Ultra-Spark 5 Sun Station. We shall present the calculation of these transport coefficients in the form of figures (figures 1 to 4). We shall also present these transport coefficients along with various integrals in the form of tables (table 1 to 2). For sake of comparison we have also calculated K_e and $K_e/\sigma T$ for parabolic density of states when there is mixed scattering of electrons by ionized impurities and acoustic phonons.

Table 1: Different transport coefficients for parabolic density of states when there is mixed scattering of electrons by ionized impurities and acoustic phonons in n-type silicon.

n_n	η	ν_{OI}/ν_{OA}	ψ_3	ψ_4	ψ_5	σ^d	K^d_e	WF^d
1	-3.47099	6.23632	0.030153	0.116063	0.56533	1.62948	3.81401	2.34067
2	-2.76699	10.3354	0.014685	0.044727	0.170637	2.08778	5.18752	2.48471
6	-1.62504	21.7177	0.004566	0.009536	0.024639	2.83707	7.76944	2.73854
8	-1.31574	26.0283	0.003366	0.006365	0.01484	3.03709	8.51758	2.80452
10	-1.07102	29.8303	0.002664	0.004663	0.010037	3.1962	9.12172	2.85393
15	-0.61177	37.8598	0.001756	0.002674	0.00498	3.50296	10.29162	2.93798
20	-0.27053	44.5058	0.013179	0.001822	0.003063	3.7448	11.20104	2.99109
25	0.00595	50.2426	0.001062	0.001364	0.002121	3.95447	11.97331	3.02779
30	0.24139	55.3259	0.000896	0.001084	0.001583	4.14555	12.66155	3.05425
35	0.44845	59.9119	0.000785	0.000898	0.001244	4.32478	13.29319	3.07373
50	0.96257	71.5814	0.000573	0.000595	0.000732	4.82275	14.99308	3.10882
55	1.10995	74.9598	0.00053	0.000536	0.00064	4.98076	15.51795	3.11558
60	1.24883	78.1432	0.000495	0.000489	0.000568	5.13626	16.02897	3.12074
70	1.50611	84.0203	0.00044	0.000418	0.000464	5.44156	17.01991	3.12777
80	1.74201	89.3631	0.000399	0.000367	0.000392	5.74125	17.97869	3.13149
90	1.9614	94.2753	0.000368	0.00033	0.000341	6.03694	18.91568	3.13332
100	2.16763	98.832	0.000343	0.000301	0.000303	6.32963	19.8342	3.13361

Table 2: Different transport coefficients for density of states having band tails when there is mixed scattering of electrons by acoustic phonons and ionized impurities in n-type silicon.

n_n	η	ν_{OI}/ν_{OA}	ψ_0	$\psi_{5/2}$	$\psi_{7/2}$	$\psi_{9/2}$	σ^d	K^d_e	WF^d
1	-3.6239	6.23632	0.040217	0.0260908	0.099672	0.484519	2.33672	3.337	2.3667
2	-3.0323	10.3354	0.052155	0.0116688	0.0347408	0.13126	1.65896	4.19557	2.52905
6	-2.2094	21.7177	0.078745	0.00297597	0.0057876	0.0143086	1.84928	5.02574	2.71767
8	-1.8719	26.0283	0.098473	0.00229372	0.00401883	0.00892795	1.84329	5.10431	2.76912
10	-1.8651	29.8303	0.09537	0.00152304	0.00242364	0.00489062	1.82738	5.02969	2.7524
15	-1.5924	37.8598	0.111032	0.0008802	0.00120067	0.00206949	1.75636	4.89664	2.78795
20	-1.3902	44.5058	0.12368	0.00059193	0.000726827	0.00112463	1.68203	4.76635	2.8337
25	-1.2234	50.2426	0.134475	0.000433956	0.000492471	0.000702834	1.61536	4.66281	2.88654
30	-1.077	55.3259	0.14399	0.000336688	0.000358969	0.000480521	1.51113	4.58528	2.94217
35	-0.9464	59.9119	0.152559	0.00027203	0.000275532	0.000349885	1.51113	4.5302	2.99788
50	-0.6039	71.5814	0.174392	0.000168433	0.00015235	0.000172027	1.41797	4.46706	3.15031
55	-0.5012	74.9598	0.180738	0.000149065	0.00013099	0.000143472	1.40035	4.47292	3.19413
60	-0.4026	78.1432	0.186733	0.000133769	0.000114544	0.00012205	1.38827	4.48932	3.23376
70	-0.2152	84.0203	0.197845	0.000111467	0.000091266	0.000092660	1.37845	4.55102	3.30157
80	-0.0383	89.3631	0.208004	0.000096318	0.000075946	0.000073971	1.38481	4.64609	3.35565
90	0.1303	94.2753	0.217397	0.000085609	0.000065349	0.000061374	1.40457	4.77007	3.3961
100	0.29238	98.832	0.226159	0.000077808	0.000057737	0.000052494	1.43565	4.91941	3.42661

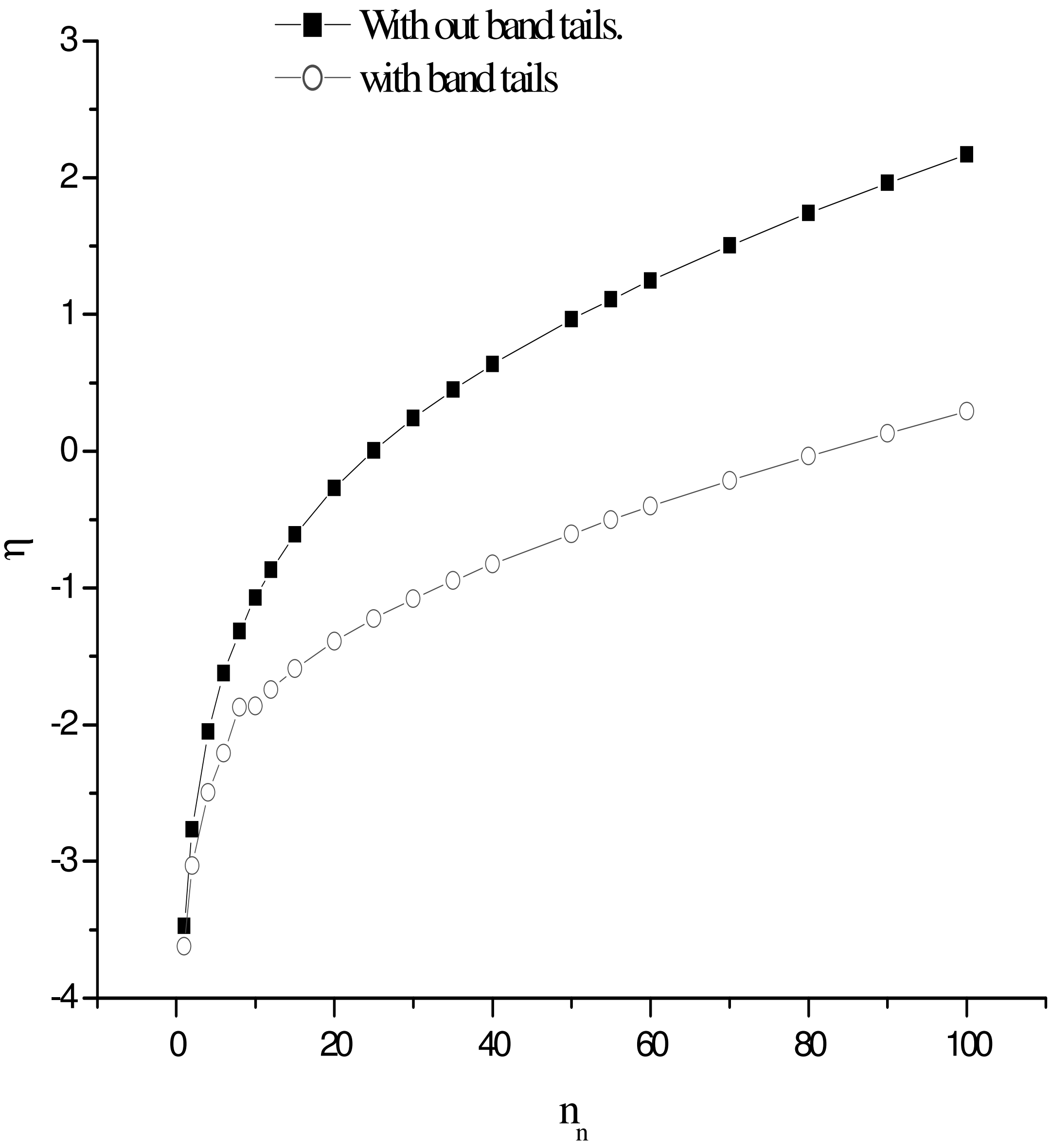

Figure 3:Graph of Dimensionless Fermi energy (η) versus normalized electron concentration (n_n) for parabolic density of states and density of sates having band tails in n-type silicon when there is mixed scattering of electrons by ionized impurities and acoustic phonons.

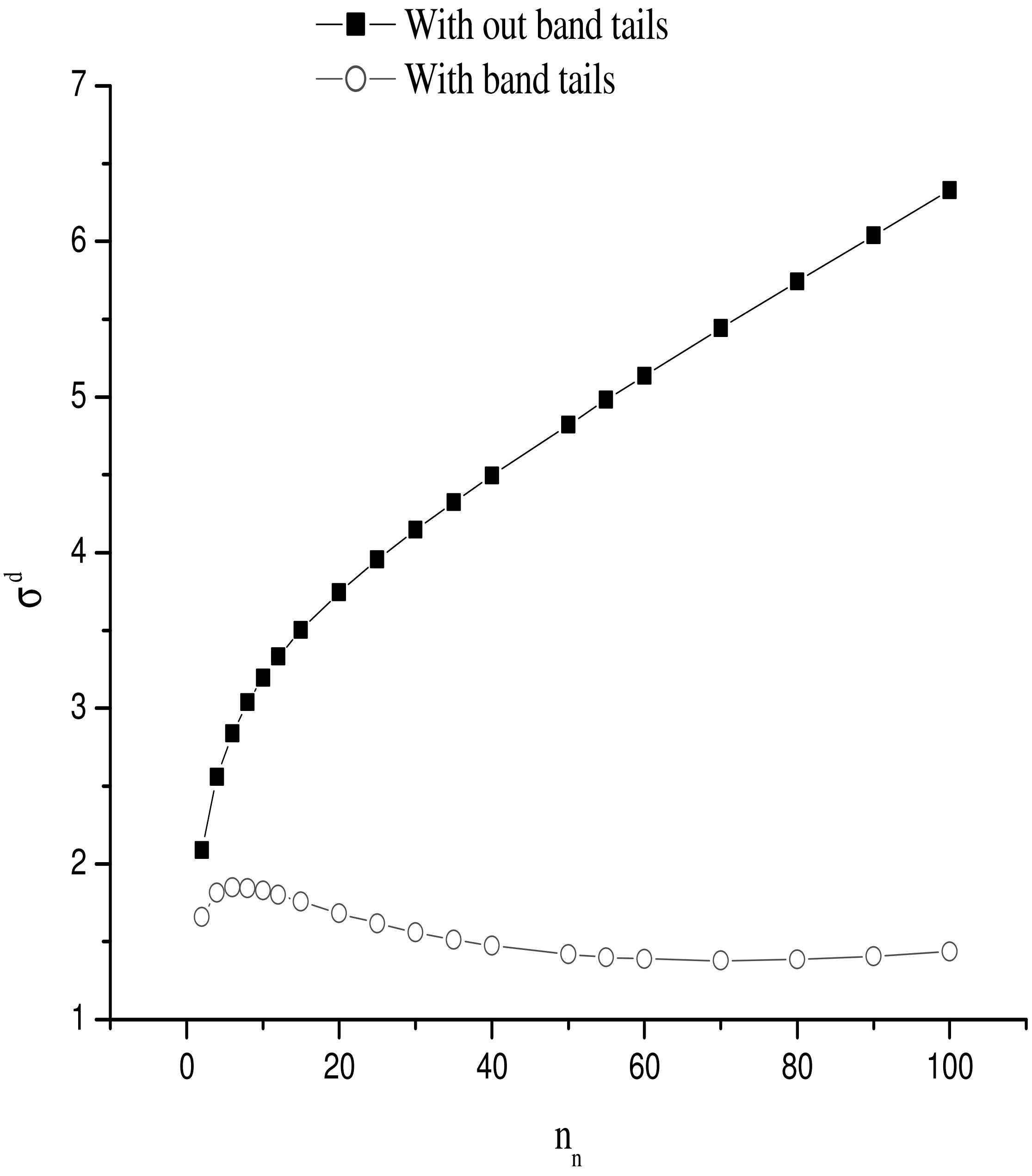

Figure 4: Graph of dimensionless electrical conductivity (σ^d) versus normalized electron concentration (n_n) for parabolic density of states and density of sates having band tails in n-type silicon when there is mixed scattering of electrons by ionized impurities and acoustic phonons.

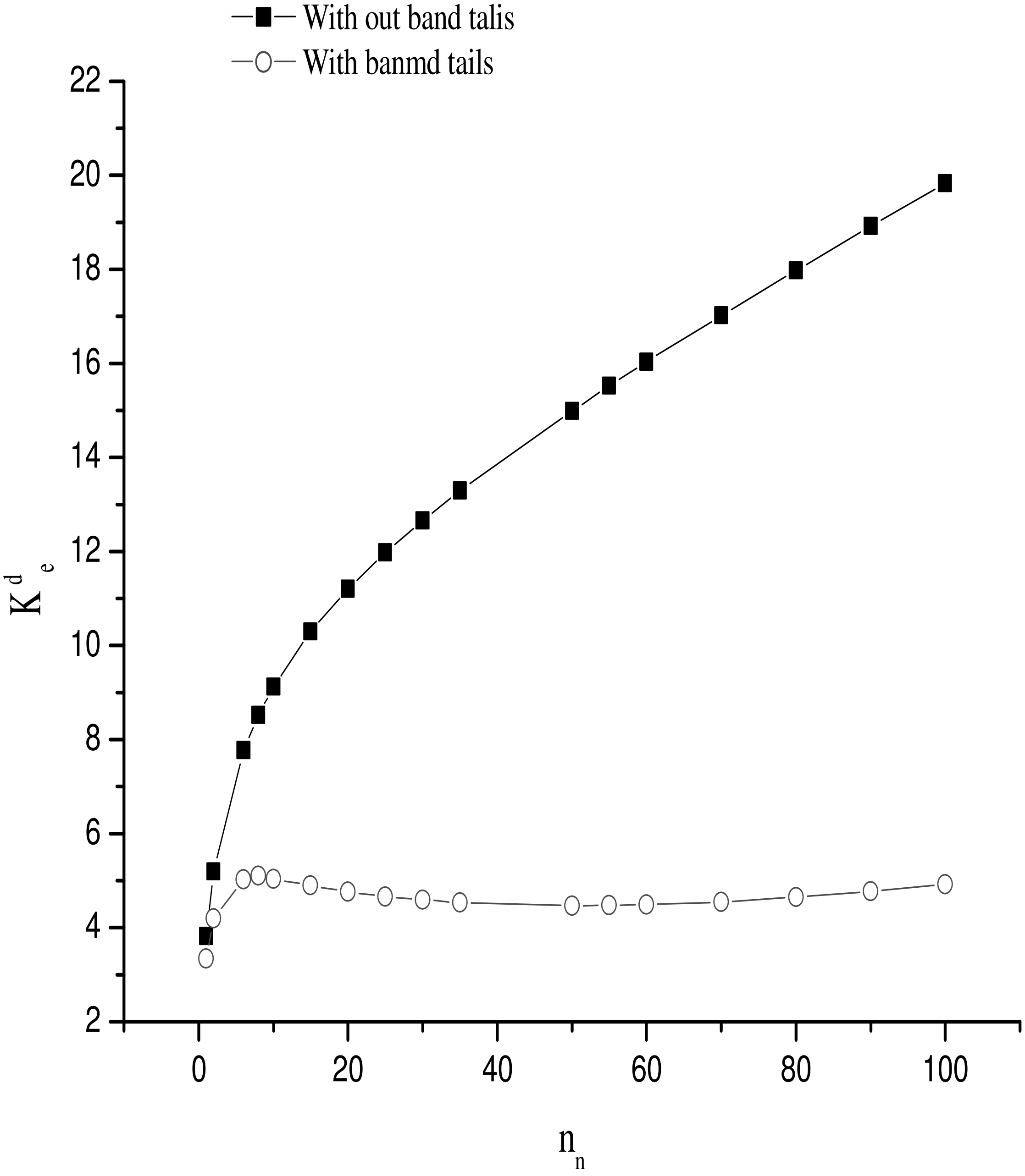

Figure 5:Graph of dimensionless thermal conductivity (K^d_e) versus normalized electron concentration (n_n) for parabolic density of states and density of sates having band tails in n-type silicon when there is mixed scattering of electrons by ionized impurities and acoustic phonons.

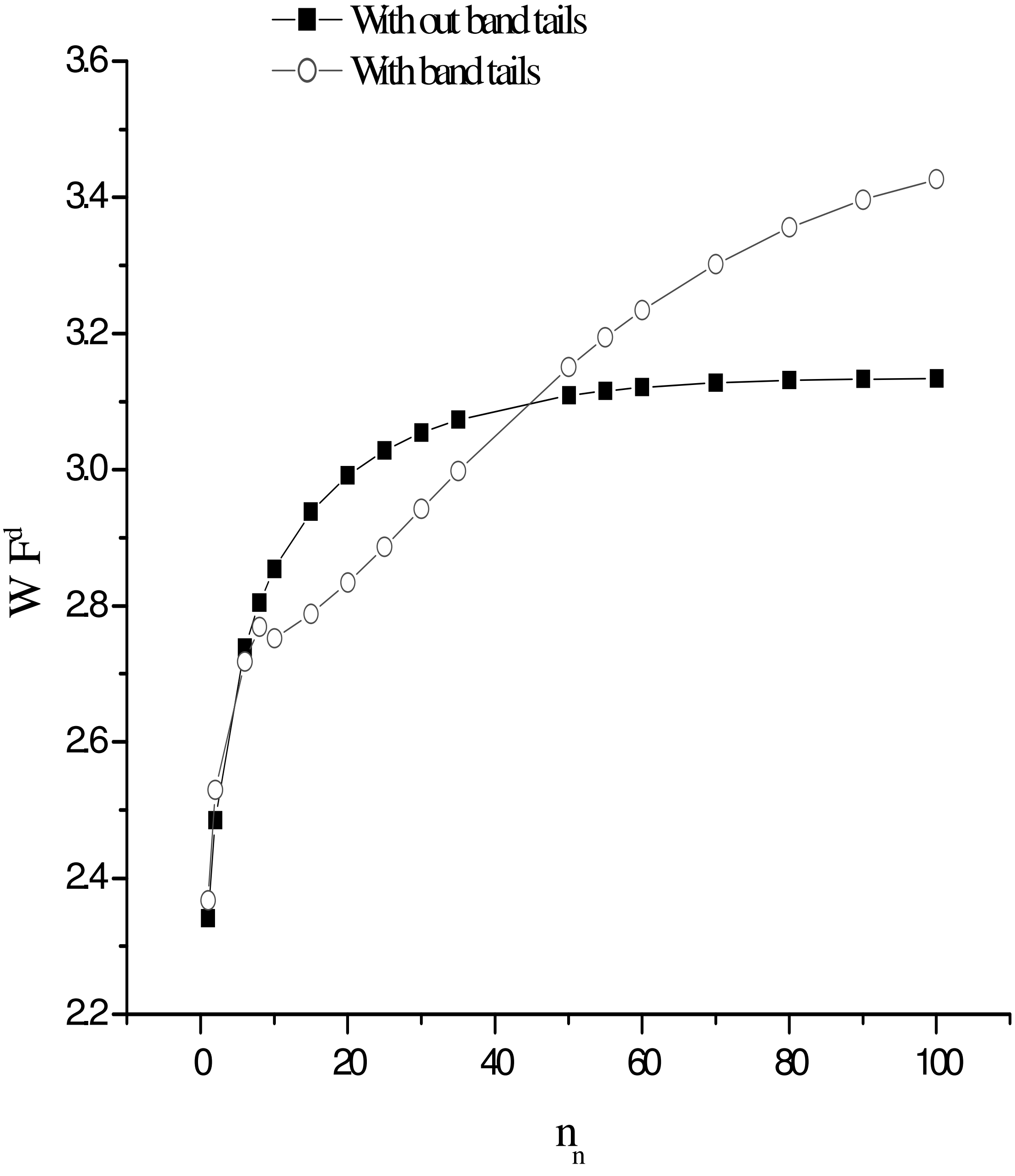

Figure 6: Graph of dimensionless Wiedemann-Franz ratio (WF^d) versus normalized electron concentration (n_n) for both parabolic density of states and density of states having band tails in n-type silicon when there is mixed scattering of electron by ionized impurities and acoustic phonons.

6.2. Discussion

Figure 3 shows the variation of dimensionless Fermi energy with normalized electron concentration for parabolic density of states as well as density of states having band tails. The square dots in figure 3 depict the calculation based on parabolic density of states where as the circles correspond to the calculation obtained by using density of states having band tails. It is seen from figure 3 that Fermi energy calculated by using density of states having band tails is always lower than that obtained by using parabolic density of states.

Figure 4 and 5 show the variation of dimensionless electrical and thermal conductivities respectively with normalized electron concentration. Both electrical and thermal conductivities increase with increase in electron concentration for parabolic density of states and these calculations are higher than corresponding calculations obtained by using density of states having band tails. However, both the electrical as well as thermal conductivities calculated by using density of states having band tails vary very little with increasing electron concentration and their variations with n_n in contrast to calculation based on parabolic density of states is insignificant in the entire range of electron concentration.

Figure 6 shows the variation of Wiedemann-Franz ratio with electron concentration. It is seen from figure 6 that $K_e/\sigma T$ based on density of states having band tails is lower than corresponding calculation obtained by using parabolic density of states for low values of electron concentration, i.e. 1to 50. However, for n_n>50, the values of $K_e/\sigma T$ obtained by using density of states having band tails is higher than the calculations obtained from parabolic density of states.

Conclusion

The results of this thesis show that.

1) It is very important to incorporate the effect of band tails with mixed scattering in the calculations of any thermal as well as galvanomagnetic transport coefficients in a heavily doped semiconductor when the carrier concentration is greater than 10^{18} /cm^3 at a temperature equal to 300^{0}K.

2) The quantity that v_{OI}/v_{OA} is of the order of ten for the electron concentration range of 1 to 10 which implies that, acoustic phonon scattering is not negligible in this region.

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