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RESEARCH ARTICLE

A New Study on Calculation of Electron Transport Characteristics in Semiconductor Materials

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ABSTRACT

We introduce a new calculation method to compute the electron transport properties in semiconductor devices. Using the relaxation-time approximation, the Boltzmann transport equation for electrons has been solved to calculate the thermal energy flux, electrical conductivity, seebeck coefficient and thermal conductivity.

KEYWORDS: *Semiconductor device; Boltzmann transport equation; seebeck coefficient.*

INTRODUCTION

To carry out calculations of the electronic transport properties of in semiconductor material and devices it is necessary to solve the Boltzmann transport equation. There are many different techniques for the solution of the Boltzmann equation when the applied field is sufficiently low. The use of numerical calculation to solve the Boltzmann equation has been described and reviewed elsewhere [1-3].However, in more general cases the Boltzmann transport equation is often exceedingly difficult to solve directly. By contrast, it is relatively easy, although computionally intensive, to simulate the trajectories of individual carriers as they move through a semiconductor under the influence of the applied field and the random scattering processes. Indeed, much of our understanding of high field transport in bulk semiconductors and in devices has been obtained through the use of such a method, Monte Carlo simulation [4-7]. The Monte Carlo method allows the Boltzmann transport equation to be solved using a statistical numerical approach, by following the transport history of one or more carriers (particles), subject to the action of external forces, such as an applied electric field, and the intrinsic scattering mechanisms. In this communication we present calculations of electron transport charactersitics in low electric field application. We demonstrate the effect of low electric field on the electron transport properties in these materials.

CALCULATION METHOD

Consider the distribution function of electrons is f, and the number of electrons with an energy between E and E+dE is f D(E)dE. Since the electric field, temperature gradient and concentration gradient are small, these electrons will have almost the same probability to move toward any direction. Also because the solid angle of a sphere is 4π, the probability for an electron to move in the (θ,φ) direction within a solid angle $d\Omega = \sin\theta d\theta d\phi$) will be dΩ/4π. A charge q (= -e for electrons and +e for holes) moving in the (θ,φ) direction within a solid angle dΩcauses a charge flux of qvcosθ and energy flux Evcosθ in the Z direction, where dΩ is defined as the angel between the velocity vector and the positive Z direction with a range between 0 to π. Hence, the charge flux and energy flux in the Z direction carried by all electrons moving toward the entire sphere surrounding the point are respectively,

$$J_z = \int_{4\pi} \frac{d\Omega}{4\pi} \int_{E=0}^{\infty} (fD(E))(qv\cos\theta)dE = \int_{\phi=0}^{2\pi} \frac{1}{4\pi} d\phi \int_{\theta=0}^{\pi} \sin\theta \cos\theta d\theta \int_{E=0}^{\infty} fD(E)qvdE \qquad (1)$$

$$J_{E_Z} = \int_{4\pi} \frac{d\Omega}{4\pi} \int_{E=0}^{\infty} (fD(E))(Ev\cos\theta)dE = \int_{\phi=0}^{2\pi} \frac{1}{4\pi} d\phi \int_{\theta=0}^{\pi} \sin\theta\cos\theta d\theta \int_{E=0}^{\infty} fD(E)EvdE \tag{2}$$

With the relaxation-time approximation, the Boltzmann Transport Equation for electrons take the following form,

$$\frac{\partial f}{\partial t} + \vec{v} \bullet \nabla f + q\vec{E} \bullet \frac{\partial f}{\partial \vec{p}} = \frac{f_0 - f}{\tau} \tag{3}$$

where q=-e for electrons and +e for holes. For the steady state case with small temperature/concentration gradient and electric field in the Z direction only, the variation of the distribution function in time is much smaller than that in space, or $\frac{\partial f}{\partial t} << \vec{v} \bullet \nabla f$, so that we can assume $\frac{\partial f}{\partial t}$~0. The temperature gradient and electric field is small so that the deviation from equilibrium distribution f_0 is small, i.e. $f_0 - f << f_0, \nabla f \approx \nabla f_0$, and $\frac{\partial f}{\partial \vec{p}} \approx \frac{\partial f_0}{\partial \vec{p}} = \frac{\partial f_0}{\partial E}\frac{dE}{d\vec{p}} = \vec{v}\frac{\partial f_0}{\partial E}$. With these assumptions, eqationn 3 becomes

$$\vec{v} \bullet [\nabla f_0 + q\vec{E}\frac{\partial f_0}{\partial E}] = \frac{f_0 - f}{\tau} \tag{4}$$

The equilibrium distribution of electrons is the Fermi-Dirac distribution

$$f_0(\vec{k}) = \frac{1}{\exp(\frac{E(\vec{k}) - \mu}{k_B T}) + 1} = \frac{1}{\exp(\eta) + 1};\ \eta \equiv \frac{E - \mu}{k_B T} \tag{5}$$

where μ is the chemical potential that depends strongly on carrier concentration and weakly on temperature. Both E and μ are measured from the band edge (e.g. E_C for conduction band). This reference system essentially sets E_C = 0 at different locations although the absolute value of E_C measured from a global reference varies at different location. In this reference system the same quantum state $\vec{k}$ = (k_x, k_y, k_z) has the same energy $E(\vec{k}) = E(\vec{k}) - E_C = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}$ at different locations. Hence this reference system yields the gradient $\nabla E(\vec{k}) = 0$, simplifying the following derivation. If we use a global reference level as our zero energy reference point, the same quantum state $\vec{k}$ = (k_x, k_y, k_z) has different energy $E(\vec{k}) = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m} + E_C$ because E_C changes with locations. In this case, $\nabla E(\vec{k}) = \nabla E_C \neq 0$, making the following derivation somewhat inconvenient. However, both reference systems will yield the same result.

From equation 5,

$$\frac{\partial f_0}{\partial E} = \frac{df_0}{d\eta}\frac{\partial \eta}{\partial E} = \frac{df_0}{d\eta}\frac{1}{k_B T} \quad ; \text{ or } \quad \frac{df_0}{d\eta} = k_B T \frac{\partial f_0}{\partial E} \tag{6}$$

From equation 6,

$$\nabla f_0 = \frac{df_0}{d\eta}\nabla\eta = k_B T \frac{\partial f_0}{\partial E}\nabla\eta \tag{7}$$

Also because $\nabla E(\vec{k}) = 0$ for the reference system that we are using

$$\nabla\eta = \frac{1}{k_B T}(\nabla E(\vec{k}) - \nabla\mu) - \frac{E - \mu}{k_B T^2}\nabla T = -\frac{1}{k_B T}\nabla\mu - \frac{E - \mu}{k_B T^2}\nabla T \tag{8}$$

From equations 7 and 8,

$$\nabla f_0 = -\frac{\partial f_0}{\partial E}(\nabla \mu + \frac{E-\mu}{T}\nabla T) \tag{9}$$

Combine equations 4 and 9, we obtain

$$\vec{v} \bullet [-\nabla \mu - \frac{E-\mu}{T}\nabla T + q\vec{E}]\frac{\partial f_0}{\partial E} = \frac{f_0 - f}{\tau} \tag{10}$$

Note that

$$\vec{E} = -\nabla \varphi_e \tag{11}$$

where φ_e is the electrostatic potential (also called electrical potential, which is the potential energy per unit of charge associated with a time-invariant electric field $\vec{E}$);
From equations 10 and 11, we obtain

$$\vec{v} \bullet [-\nabla \mu - \frac{E-\mu}{T}\nabla T - q\nabla \varphi_e]\frac{\partial f_0}{\partial E} = \frac{f_0 - f}{\tau} \tag{12}$$

From equation 12, we obtain

$$f = f_0 - \tau\vec{v} \bullet [-\nabla \Phi - \frac{E-\mu}{T}\nabla T]\frac{\partial f_0}{\partial E} \tag{13}$$

where $\Phi = \mu + q\varphi_e$, is the electrochemical potential that combines the chemical potential and electrostatic potential energy. This definition of the electrochemical potential is the definition in Chen's text multiplied by a factor of q. Both definitions are used in the literature, with the definition here are used more widely. Electrochemical potential is the driving force for current flow, which can be caused by the gradient in either chemical potential (e.g. due to the gradient in carrier concentration) or the gradient in electrostatic potential (i.e. electric field). When you measure voltage ΔV across a solid using a voltmeter, you actually measured the electrochemical potential difference $\Delta\Phi$ per unit charge between the two ends of the solid, i.e. $\Delta V = \Delta\Phi / q$. If there is no temperature gradient or concentration gradient in the solid, the measured voltage equals $\Delta\varphi_e$.

In the current case all the gradients and $\vec{E}$ are in the Z direction, so from equation 13,

$$f = f_0 - \tau v \cos\theta[-\frac{d\mu}{dZ} - \frac{E-\mu}{T}\frac{dT}{dZ} + qE_z]\frac{\partial f_0}{\partial E} = f_0 - \tau v \cos\theta[-\frac{d\Phi}{dZ} - \frac{E-\mu}{T}\frac{dT}{dZ}]\frac{\partial f_0}{\partial E} \tag{14}$$

Combine equations 1 and 14, we obtain the charge flux and energy flux respectively

$$\begin{aligned} J_Z = & \int_{\phi=0}^{2\pi}\frac{1}{4\pi}d\phi \int_{\theta=0}^{\pi}\sin\theta\cos\theta d\theta \int_{E=0}^{\infty} f_0 D(E) q v dE \\ & + \int_{\phi=0}^{2\pi}\frac{1}{4\pi}d\phi \int_{\theta=0}^{\pi}\sin\theta\cos^2\theta d\theta \int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E) q v^2 \tau(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z)dE \end{aligned} \tag{15}$$

&

$$\begin{aligned} J_{E_Z} = & \int_{\phi=0}^{2\pi}\frac{1}{4\pi}d\phi \int_{\theta=0}^{\pi}\sin\theta\cos\theta d\theta \int_{E=0}^{\infty} f_0 D(E) E v dE \\ & + \int_{\phi=0}^{2\pi}\frac{1}{4\pi}d\phi \int_{\theta=0}^{\pi}\sin\theta\cos^2\theta d\theta \int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E) E v^2 \tau(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z)dE \end{aligned} \tag{16}$$

Note that the first term in the right hand of equation 15 side is zero and the second term yields

$$J_Z = \frac{1}{3}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E) q v^2 \tau(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z)dE \tag{17}$$

$$J_{E_Z} = \frac{1}{3}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E) E v^2 \tau(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z)dE \tag{18}$$

Note that

$$E = \frac{1}{2} m v^2 \tag{19}$$

Use equation 17 to eliminate v in equation 19, we obtain

$$\begin{aligned} J_z &= \frac{2q}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE \\ &= \frac{2q}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E \tau \left(\frac{d\Phi}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ}\right) dE \end{aligned} \tag{20}$$

$$J_{E_z} = \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E^2 \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE \tag{21}$$

The energy flux from equation 21 can be broken up into two terms as following

$$\begin{aligned} J_{E_z} &= \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E^2 \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE \\ &= \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E (E-\mu) \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE \\ &+ \mu \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE \\ &= \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E (E-\mu) \tau \left(\frac{d\mu}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ} - qE_z\right) dE + \frac{\mu J_Z}{q} \\ &= \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E (E-\mu) \tau \left(\frac{d\Phi}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ}\right) dE + \frac{\mu J_Z}{q} \end{aligned} \tag{22}$$

where J_Z is the current density or charge flux given by equation 22. At temperature T = 0 K, the first term in the right hand side of equation 21 is zero, so that the energy flux at T = 0 K is

$$J_{E_Z}(T = 0K) = \frac{\mu J_Z}{q} \tag{23}$$

Because electrons do not carry any thermal energy at T = 0 K, the thermal energy flux or heat flux carried by the electrons at $T \neq 0$ is

$$\begin{aligned} J_{q_Z}(T) &= J_{E_Z}(T) - J_{E_Z}(T = 0) \\ &= \frac{2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E (E-\mu) \tau \left(\frac{d\Phi}{dZ} + \frac{E-\mu}{T}\frac{dT}{dZ}\right) dE \end{aligned} \tag{24}$$

Equations 23 and 24 can be rearranged as

$$J_z = L_{11}\left(-\frac{1}{q}\frac{d\Phi}{dZ}\right) + L_{12}\left(-\frac{dT}{dZ}\right) \tag{25}$$

$$J_{q_z} = L_{21}\left(-\frac{1}{q}\frac{d\Phi}{dZ}\right) + L_{22}\left(-\frac{dT}{dZ}\right) \tag{26}$$

Where

$$L_{11} = -\frac{2q^2}{3m} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E \tau dE \tag{27}$$

$$L_{12} = -\frac{2q}{3mT} \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E (E-\mu) \tau dE \tag{28}$$

$$L_{21} = -\frac{2q}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)\tau dE = TL_{12} \tag{29}$$

$$L_{22} = -\frac{2}{3mT}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)^2\tau dE \tag{30}$$

ELECTRICAL CONDUCTIVITY

In the case of zero temperature gradient and zero carrier concentration gradient, $\frac{dT}{dZ} = 0$ and $\frac{d\mu}{dZ} = 0$, equation 24 becomes

$$J_z = L_{11}(-\frac{1}{q}\frac{d\Phi}{dZ}) = L_{11}(-\frac{1}{q}\frac{d\mu}{dZ} + E_z) = L_{11}E_z \tag{31}$$

The electrical conductivity is defined as

$$\sigma \equiv \frac{J_z}{E_z} = L_{11} = -\frac{2q^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE \tag{32}$$

SEEBECK COEFFICIENT

In the case of non-zero temperature gradient along the Z direction, a thermoelectric voltage can be measured between the two ends of the solid with an open loop electrometer, i.e. $J_Z = 0$. Hence from equation 30 we obtain

$$J_z = L_{11}(-\frac{1}{q}\frac{d\Phi}{dZ}) + L_{12}(-\frac{dT}{dZ}) = 0 \tag{33}$$

Therefore

$$\frac{\left(\frac{d\Phi}{dZ}\right)}{\left(\frac{dT}{dZ}\right)} = -\frac{qL_{12}}{L_{11}} \tag{34}$$

As discussed above, the voltage that the electrometer measure between the two ends of the solid is $\Delta V = \Delta\Phi / q$. Similarly, $dV = d\Phi / q$. The Seebeck coefficient is defined as the ratio between the voltage gradient and the temperature gradient for an open loop configuration with zero net current flow

$$\begin{aligned} S &= -\frac{\left(\frac{dV}{dZ}\right)}{\left(\frac{dT}{dZ}\right)} = -\frac{1}{q}\frac{\left(\frac{d\Phi}{dZ}\right)}{\left(\frac{dT}{dZ}\right)} = \frac{L_{12}}{L_{11}} = \frac{1}{qT}\left(\frac{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)\tau dE}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}\right) \\ &= -\frac{1}{qT}\left(\mu - \frac{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^2\tau dE}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}\right) \end{aligned} \tag{35}$$

Combine equations 33, 34, and 35, we can write $J_z = \sigma(-\frac{1}{q}\frac{d\Phi}{dZ}) + \sigma S(-\frac{dT}{dZ})$ The scattering mean free time depends on the energy, and we can assume

$$\tau = \tau_0 E^r \tag{36}$$

where τ_0 is a constant independent of E. When E is measured from the band edge for either electrons or holes, the density of states

$$D(E) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3} E^{1/2} \qquad (37)$$

Combine equations 35 and 37

$$S = -\frac{1}{qT}\left(\mu - \frac{\int\limits_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E^2 \tau dE}{\int\limits_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E) E \tau dE} \right) = -\frac{1}{qT}\left(\mu - \frac{\int\limits_{E=0}^{\infty} \frac{\partial f_0}{\partial E} E^{2+r+1/2} dE}{\int\limits_{E=0}^{\infty} \frac{\partial f_0}{\partial E} E^{1+r+1/2} dE} \right) \qquad (38)$$

The integrals in equation 38 can be simplified using the product rule

$$\int\limits_{E=0}^{\infty} \frac{\partial f_0}{\partial E} E^s dE = f_0 E^s \Big|_0^{\infty} - s\int\limits_{E=0}^{\infty} f_0 E^{s-1} dE = -s\int\limits_{E=0}^{\infty} f_0 E^{s-1} dE \qquad (39)$$

Using equation 38 to reduce equation 39 to

$$S = -\frac{1}{qT}\left(\mu - \frac{(r+5/2)\int\limits_{E=0}^{\infty} f_0 E^{r+3/2} dE}{(r+3/2)\int\limits_{E=0}^{\infty} f_0 E^{r+1/2} dE} \right) \qquad (40)$$

The two integrals in equation 40 can be simplified with the reduced energy $\zeta = E / k_{BT}$

$$\int\limits_{E=0}^{\infty} f_0(E,\mu) E^n dE = (k_B T)^{n+1} \int\limits_{0}^{\infty} f_0(\zeta,\eta)\zeta^n d\zeta = (k_B T)^{n+1} F_n(\eta); \quad \eta = \mu / k_B T \qquad (41)$$

where the Fermi-Dirac integral is defined as

$$F_n(\eta) = \int\limits_{0}^{\infty} f_0(\zeta,\eta)\zeta^n d\zeta \qquad (42)$$

Use equation 42 to reduce equation 41 to

$$S = -\frac{1}{qT}\left(\mu - k_B T \frac{\left(r+\frac{5}{2}\right) F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right) F_{r+1/2}(\eta)} \right) = -\frac{k_B}{q}\left(\eta - \frac{\left(r+\frac{5}{2}\right) F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right) F_{r+1/2}(\eta)} \right) \qquad (43)$$

Seebeck coefficient for metals:

For metals with $\eta = \mu / k_B T >> 0$, the Fermi-Dirac integral can be expressed in the form of a apidly converging series

$$\begin{aligned}
F_n(\eta) &= \int\limits_{0}^{\infty} f_0 \zeta^n d\zeta = -\frac{1}{n+1}\int\limits_{0}^{\infty} \frac{\partial f_0}{\partial \zeta}\zeta^{n+1} d\zeta \\
&= -\frac{1}{n+1}\int\limits_{0}^{\infty} \frac{\partial f_0}{\partial \zeta}\left(\eta^{n+1} + \sum_{m=1}^{\infty} \frac{d^m\left(\zeta^{n+1}\right)}{d\zeta^m}\Bigg|_{\zeta=\eta} \frac{(\zeta-\eta)^m}{m!} \right) d\zeta \\
&= -\frac{1}{n+1}\int\limits_{0}^{\infty} \frac{\partial f_0}{\partial \zeta}\left(\eta^{n+1} + (n+1)\eta^n(\zeta-\eta) + (n+1)n\eta^{n-1}\frac{(\zeta-\eta)^2}{2} + \ldots \right) d\zeta \\
&= \frac{\eta^{n+1}}{n+1} + n\eta^{n-1}\frac{\pi^2}{6} + \ldots
\end{aligned} \qquad (44)$$

If we use only the first two terms of equation 44 to express the two Fermi-Dirac integrals in equation 43, we obtain the following (q = -e for electrons in metals)

$$S=-\frac{k_B}{q}\left(\eta-\frac{\left(r+\frac{5}{2}\right)F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)}\right)=\frac{k_B}{e}\left(\frac{\eta\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)-\left(r+\frac{5}{2}\right)F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)}\right)$$

$$=\frac{k_B}{e}\left(\frac{\eta\left(r+\frac{3}{2}\right)\left(\frac{\eta^{r+3/2}}{r+\frac{3}{2}}+\left(r+\frac{1}{2}\right)\eta^{r-1/2}\frac{\pi^2}{6}\right)-\left(r+\frac{5}{2}\right)\left(\frac{\eta^{r+5/2}}{r+\frac{5}{2}}+\left(r+\frac{3}{2}\right)\eta^{r+1/2}\frac{\pi^2}{6}\right)}{\left(r+\frac{3}{2}\right)\frac{\eta^{r+3/2}}{r+\frac{3}{2}}}\right) \tag{45}$$

$$=-\frac{\pi^2 k_B}{3e}\left(\frac{k_B T}{\mu}\right)\left(\frac{3}{2}+r\right)$$

This value can be either positive or negative depending on r, or how the scattering rate depends on electron energy. We can ignore the weak temperature dependence of μ and assume μ= E_F, the Fermi level that is the highest energy occupied by electrons at 0 K in a metal.

SEEBECK COEFFICIENT FOR NONDEGENERATE SEMICONDUCTORS

In non-degenerate semiconductors, μ is located within the bandgap with a distance from the conduction or valence band edges larger than 3kBT so that $\frac{E-\mu}{k_B T}=\zeta-\eta>3$. This is true for both electrons in the conduction band and holes in valence band. For holes in valence band, the energy is higher at a position further down below the valence band edge. When $\frac{E-\mu}{k_B T}=\zeta-\eta>3$, the Fermi-Dirac integrals become

$$F_n(\eta)=\int_0^\infty f_0(\zeta,\eta)\zeta^n d\zeta=\int_0^\infty\frac{1}{\exp(\zeta-\eta)+1}\zeta^n d\zeta\approx\int_0^\infty\frac{1}{\exp(\zeta-\eta)}\zeta^n d\zeta$$
$$=\exp(\eta)\int_0^\infty\exp(-\zeta)\zeta^n d\zeta=\exp(\eta)\Gamma(n+1) \tag{46}$$

where the gamma function has the property

$$\Gamma(n+1)=\int_0^\infty\exp(-\zeta)\zeta^n d\zeta=n\Gamma(n) \tag{47}$$

We can use equation 47 to reduce equation 42 to obtain

$$S=-\frac{k_B}{q}\left(\eta-\frac{\left(r+\frac{5}{2}\right)\exp(\eta)\Gamma\left(r+\frac{5}{2}\right)}{\left(r+\frac{3}{2}\right)\exp(\eta)\Gamma\left(r+\frac{3}{2}\right)}\right)$$
$$=-\frac{k_B}{q}\left(\eta-\left(r+\frac{5}{2}\right)\right)=-\frac{1}{qT}\left(\mu-k_B T\left(r+\frac{5}{2}\right)\right) \tag{48}$$

In this equation, μ is measured from the conduction band edge EC for electrons and from the valence band edge E_v for holes. Located within the bandgap, μ is negative for electrons, and is also negative for holes because the hole energy is higher when the energy level is moved further down. Also q = -e for electrons and +e for holes, so that the Seebeck coefficient is negative for electrons in the conduction band and positive for holes in the valence band.

If μ is measured from a global reference instead of the band edge as the zero energy point, we can express equation 48 for electrons and holes separately

$$S_e = -\frac{1}{eT}(E_c - \mu + (r + 5/2)k_B T) < 0, \qquad \text{for electrons} \tag{49}$$

$$S_h = \frac{1}{eT}(\mu - E_v + (r + 5/2)k_B T) > 0, \qquad \text{for holes} \tag{50}$$

The effective Seebeck coefficient in a nondegenerate semiconductors have contribution from both electrons and holes, i.e.

$$S = \frac{n\mu_e S_e + p\mu_h S_h}{n\mu_e + p\mu_h} \tag{51}$$

where n and p are electron and hole concentrations, respectively, and μ_e and μ_h the mobility of electrons and holes, respectively. The mobility is defined in the following section on Wiedemann-Franx law.

THERMAL CONDUCTIVITY OF ELECTRONS

From equation 21

$$-\frac{1}{q}\frac{d\Phi}{dZ} = -\frac{L_{12}}{L_{11}}\left(-\frac{dT}{dZ}\right) + \frac{1}{L_{11}} J_Z \tag{52}$$

Use equation 52 to eliminate $\frac{d\Phi}{dZ}$ from equation 21 b to obtain

$$J_{q_Z} = \frac{L_{21}}{L_{11}} J_Z + \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right) = \Pi J_Z + k_e\left(-\frac{dT}{dZ}\right) \tag{53}$$

The Peltier coefficient Π and thermal conductivity k_e are defined in the following.

In the case of zero current $J_Z = 0$ and non-zero temperature gradient along the Z direction,

$$J_{q_Z} = \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right) \tag{54}$$

The thermal conductivity of electrons

$$k_e = -\frac{J_{q_Z}}{\frac{dT}{dZ}} = \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right) = \left(L_{22} - L_{21}S\right)$$

$$= \frac{2}{3mT}\left(\frac{\left(\int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E(E-\mu)\tau dE\right)^2}{\int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E\tau dE} - \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E(E-\mu)^2 \tau dE\right) \tag{55}$$

Equation 55 can be reduced to the following by expanding the (E-μ) term in the two integrals,

$$k_e = \frac{2}{3mT}\left(\frac{\left(\int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E\tau dE} - \int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E^3 \tau dE\right) \tag{56}$$

For metals, S is usually very small so that from equation 56

$$k_e = \left(L_{22} - L_{21}S\right) \approx L_{22} = -\frac{2}{3mT}\int_{E=0}^{\infty} \frac{\partial f_0}{\partial E} D(E)E(E-\mu)^2 \tau dE \tag{57}$$

Note that

$$\frac{\partial f_0}{\partial T}=\frac{df_0}{d\eta}\frac{\partial \eta}{\partial T}=-\frac{df_0}{d\eta}\frac{E-\mu}{k_B T^2} \tag{58}$$

Compare equation 57 with equation 5, we can obtain

$$\frac{\partial f_0}{\partial E}=-\frac{T}{E-\mu}\frac{\partial f_0}{\partial T} \tag{59}$$

Combine equations. 59 and 56,

$$k_e=\frac{2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial T}D(E)E(E-\mu)\tau dE \tag{60}$$

We can use E = $mv^2/2$ to rewriteequation 60 as

$$k_e=\frac{1}{3}\int_{E=0}^{\infty}\frac{\partial f_0(E)}{\partial T}D(E)v^2(E-\mu)\tau dE \tag{61}$$

When E is far away from μ, $f_0(E)$ remains to be either 0 or 1 as the temperature changes, so that $\frac{\partial f_0(E)}{\partial T}$ is non-zero only when E is close to μ. Therefore, equation 61 can be approximated by taking v = v_F and $\tau = \tau_F$, i.e. the Fermi velocity and the scattering mean free time of Fermi electrons,

$$k_e=\frac{1}{3}{v_F}^2\tau_F\int_{E=0}^{\infty}\frac{\partial f_0(E)}{\partial T}D(E)(E-\mu)dE=\frac{1}{3}{v_F}^2\tau_F C_e=\frac{1}{3}C_e v_F l_F \tag{62}$$

This is essentially the Kinetic theory expression of the thermal conductivity.

WIEDEMANN-FRANZ LAW

From equation 24, the electrical conductivity is

$$\sigma\equiv\frac{J_z}{E_z}=-\frac{2e^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE \tag{63}$$

$\frac{\partial f_0(E)}{\partial E}$ is non-zero only when E is close to μ, and can be approximated to as a delta function

$$\frac{\partial f_0(E)}{\partial E}\approx-\delta(E-\mu) \tag{64}$$

Combine equations 64 and 63,

$$\sigma\equiv\frac{J_z}{E_z}=\frac{2e^2}{3m}\int_{E=0}^{\infty}\delta(E-\mu)D(E)E\tau dE=\frac{2e^2}{3m}D_{E=\mu}\mu\tau_{E=\mu}=\frac{2e^2}{3m}D_F\mu\tau_F \tag{65}$$

We can use $\mu\approx E_F=m{v_F}^2/2$ to reduce equation 65 to

$$\sigma=\frac{e^2}{3}D_F{v_F}^2\tau_F \tag{66}$$

Note that the electron concentration can be calculated as

$$\begin{aligned}n&=\int_{E=0}^{\infty}f_0(E)D(E)dE=\int_{E=0}^{\infty}f_0(E,T=0)D(E)dE=\int_{E=0}^{E_F}D(E)dE\\&=\int_{E=0}^{E_F}\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{2/3}E^{1/2}dE=\frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{2/3}{E_F}^{3/2}=\frac{2}{3}D_F E_F\approx\frac{2}{3}D_F\mu\end{aligned} \tag{67}$$

Combine equations 67 and 65, we obtain

$$\sigma=\frac{e^2}{m}n\tau_F \tag{68}$$

If we use the following definition of electron mobility

$$\mu_e = \frac{e}{m}\tau_F \tag{69}$$

we obtain from equation 68

$$\sigma = ne\mu_e \tag{70}$$

Note that μ_e is electron mobility and is different from μ that is chemical potential.

We can use equations 68 and 62 to calculate the ratio between the electron thermal conductivity and electrical conductivity

$$\frac{k_e}{\sigma} = \frac{\frac{1}{3}{v_F}^2\tau_F C_e}{\frac{e^2}{m}n\tau_F} = \frac{mC_e{v_F}^2}{3ne^2} \tag{71}$$

Here we have assumed that the τ_F is the same in the thermal conductivity and electrical conductivity expressions. As discussed in Chen, these two τ_F terms can be different.

Note that the electron specific heat of metals has been derived previously as

$$C_e = \frac{1}{2}\pi^2 nk_B T / T_F = \frac{\frac{1}{2}\pi^2 nk_B T}{\frac{m{v_F}^2}{2k_B}} = \frac{\pi^2 n{k_B}^2 T}{m{v_F}^2} \tag{72}$$

Combine equations 71 and 72, we obtain

$$\frac{k_e}{\sigma} = \frac{m{v_F}^2}{3ne^2}\frac{\pi^2 n{k_B}^2 T}{m{v_F}^2} = \frac{\pi^2{k_B}^2 T}{3e^2} \tag{73}$$

We define the Lorentz number

$$L = \frac{\pi^2{k_B}^2}{3e^2} = 2.45 \times 10^{-8} (\mathrm{W\Omega/K^2}) \tag{74}$$

So that we obtain the Wiedemann-Franz law

$$\frac{k_e}{\sigma} = LT \tag{75}$$

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