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Full Length Research Paper

A new calculation method for thermal and electical characterization in CdTe and CdSe semiconductors

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A new calculation method has been developed and used to model electron transport properties in semiconductor devices under thermal and electrical applications. Using the relaxation-time approximation, the Boltzmann transport equation is solved using the currently established values of the material parameters. This method is used to carry out the thermal energy flux, electrical conductivity, seebeck coefficient and thermal conductivity. Using the driven equations, thermal and electrical properties in CdTe and CdSe materials were been calculated. The calculated results are in fair agreement with other recent calculations obtained by experimental methods.

Key words: Boltzmann equation, seebeck coefficient, thermal energy flux, relaxation-time.

INTRODUCTION

The II–VI semiconductor compounds, particularly CdSe and CdTe, are of great interest because they are potential candidates in many practical applications like solar cells, optical detectors, dosimeters of ionized radiation, field effect transistors, and optoelectronic devices. Its suitable band gap, optical properties, and very good stability, recommend cadmium sellenide as a very promising semiconducting material for optoelectronic applications, especially for solar cell structures. The performance of the devices based on CdSe thin films depends on the structural and electronic properties of the layers obtained under various experimental conditions (Bertazzi et al., 2007). The electronic and optical properties of semiconductors are strongly influenced by the doping process, which provides the basis for tailoring the desired carrier concentration and, consequently, the absorption, emission and transport properties. When the density of n-type or p-type doping becomes sufficiently high, the impurity band merges with the conduction or valence band and causes the formation of a band tail and band gap shrinkage (Özgür et al., 2005). In this work, we shall discuss theoretical data obtained for thermal and electrical properties of CdSe and CdTe. In order to analyze and improve the design of CdSe and CdTe-based devices, an understanding of the thermal and electron transport that occurs within these materials is necessary. While electron transport in bulk of these materials have been extensively examined (O'Leary et al., 2006), the sensitivity of these results to variations in the material parameters is yet to be considered. 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 (Jacoboni and Lugli, 1989). However, in more general cases the Boltzmann transport equation is often exceedingly difficult to solve directly (Moglestue, 1993). 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. 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.

Details of the model and the thermal and electrical calculations are presented subsequently, followed by the results of calculations carried out on CdSe and CdTe structures are interpreted.

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 dΩ= $\sin\theta d\theta d\phi$) will be dΩ/4π. A charge q (= -e for electrons and +e for holes) moving in the (θ,φ) direction within a solid angle dΩ causes 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,

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

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

With the relaxation-time approximation, the Boltzmann transport equation for electrons take the following form,

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

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 $\frac{\partial f}{\partial t} << \vec{v}.\nabla f$, 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, Equation 3 becomes

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

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 for example, 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 is somewhat inconvenient. However, both reference systems will yield the same result.

From Equation 5,

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

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

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

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

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

From Equation 12, we obtain

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

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, both 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 (for example, due to the gradient in carrier concentration) or the gradient in electrostatic potential (that is, 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, that is, $\Delta V = \Delta\Phi / q$. 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

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

and

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

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

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

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

Note that

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

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

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

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

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

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

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 ≠ 0 is

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

Equations 23 and 24 can be rearranged as

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

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

where

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

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

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

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

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

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

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, that is, $J_Z = 0$. 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 previously, 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

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

$$= -\frac{1}{qT}\left(\mu - \frac{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^2\tau dE}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}\right)$$

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

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

Combine Equations 35 and 37

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

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

$$\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}E^s dE = f_0E^s\,|_0^{\infty} - s\int_{E=0}^{\infty}f_0E^{s-1}dE = -s\int_{E=0}^{\infty}f_0E^{s-1}dE \tag{39}$$

Using Equation 38 to reduce Equation 39 to

$$S = -\frac{1}{qT}\left(\mu - \frac{(r+5/2)\int_{E=0}^{\infty}f_0E^{r+3/2}dE}{(r+3/2)\int_{E=0}^{\infty}f_0E^{r+1/2}dE}\right) \tag{40}$$

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

$$\int_{E=0}^{\infty}f_0(E,\mu)E^n dE = (k_BT)^{n+1}\int_0^{\infty}f_0(\zeta,\eta)\zeta^n d\zeta = (k_BT)^{n+1}F_n(\eta);\ \ \eta = \mu / k_BT \tag{41}$$

where the Fermi-Dirac integral is defined as

$$F_n(\eta) = \int_0^{\infty}f_0(\zeta,\eta)\zeta^n d\zeta \tag{42}$$

Use Equation 42 to reduce Equation 41 to

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

Seebeck coefficient for metals:

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

$$F_n(\eta)=\int_0^{\infty} f_0\zeta^n d\zeta=-\frac{1}{n+1}\int_0^{\infty}\frac{\partial f_0}{\partial \zeta}\zeta^{n+1}d\zeta$$
$$=-\frac{1}{n+1}\int_0^{\infty}\frac{\partial f_0}{\partial \zeta}\left(\eta^{n+1}+\sum_{m=1}^{\infty}\left.\frac{d^m\left(\zeta^{n+1}\right)}{d\zeta^m}\right|_{\zeta=\eta}\frac{(\zeta-\eta)^m}{m!}\right)d\zeta$$
$$=-\frac{1}{n+1}\int_0^{\infty}\frac{\partial f_0}{\partial \zeta}\left(\eta^{n+1}+(n+1)\eta^n(\zeta-\eta)+(n+1)n\eta^{n-1}\frac{(\zeta-\eta)^2}{2}+\ldots\right)d\zeta$$
$$=\frac{\eta^{n+1}}{n+1}+n\eta^{n-1}\frac{\pi^2}{6}+\ldots \tag{44}$$

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)

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

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.

Thermal conductivity of electrons

From Equation 21

$$-\frac{1}{q}\frac{d\Phi}{dZ}=-\frac{L_{12}}{L_{11}}\left(-\frac{dT}{dZ}\right)+\frac{1}{L_{11}}J_Z \tag{46}$$

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

$$J_{q_Z}=\frac{L_{21}}{L_{11}}J_Z+\left(L_{22}-\frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right)=\Pi J_Z+k_e\left(-\frac{dT}{dZ}\right) \tag{47}$$

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,

$$J_{q_Z}=\left(L_{22}-\frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right) \tag{48}$$

The thermal conductivity of electrons

$$k_e=-\frac{J_{q_Z}}{\frac{dT}{dZ}}=\left(L_{22}-\frac{L_{12}L_{21}}{L_{11}}\right)=\left(L_{22}-L_{21}S\right)$$
$$=\frac{2}{3mT}\left(\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}-\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)^2\tau dE\right) \tag{49}$$

Equation 45 can be reduced to the following by expanding the (E-μ) term in the two integrals,

$$k_e=\frac{2}{3mT}\left(\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E\tau dE}-\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E^3\tau dE\right) \tag{50}$$

For metals, S is usually very small so that from Equation 49

$$k_e=\left(L_{22}-L_{21}S\right)\approx L_{22}=-\frac{2}{3mT}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}D(E)E(E-\mu)^2\tau dE \tag{51}$$

Note that

$$\frac{\partial f_0}{\partial T}=\frac{df_0}{d\eta}\frac{\partial \eta}{\partial T}=-\frac{df_0}{d\eta}\frac{E-\mu}{k_BT^2} \tag{52}$$

Compare Equation 51 with Equation 5, we can obtain

$$\frac{\partial f_0}{\partial E}=-\frac{T}{E-\mu}\frac{\partial f_0}{\partial T} \tag{53}$$

Combine Equations 53 and 52,

$$k_e=\frac{2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial T}D(E)E(E-\mu)\tau dE \tag{54}$$

We can use E = $mv^2/2$ to rewrite Equation 54 as

$$k_e=\frac{1}{3}\int_{E=0}^{\infty}\frac{\partial f_0(E)}{\partial T}D(E)v^2(E-\mu)\tau dE \tag{55}$$

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 55 can be approximated by taking v = v_F and τ= τ_F, that is, the Fermi velocity and the scattering mean free time of Fermi electrons,

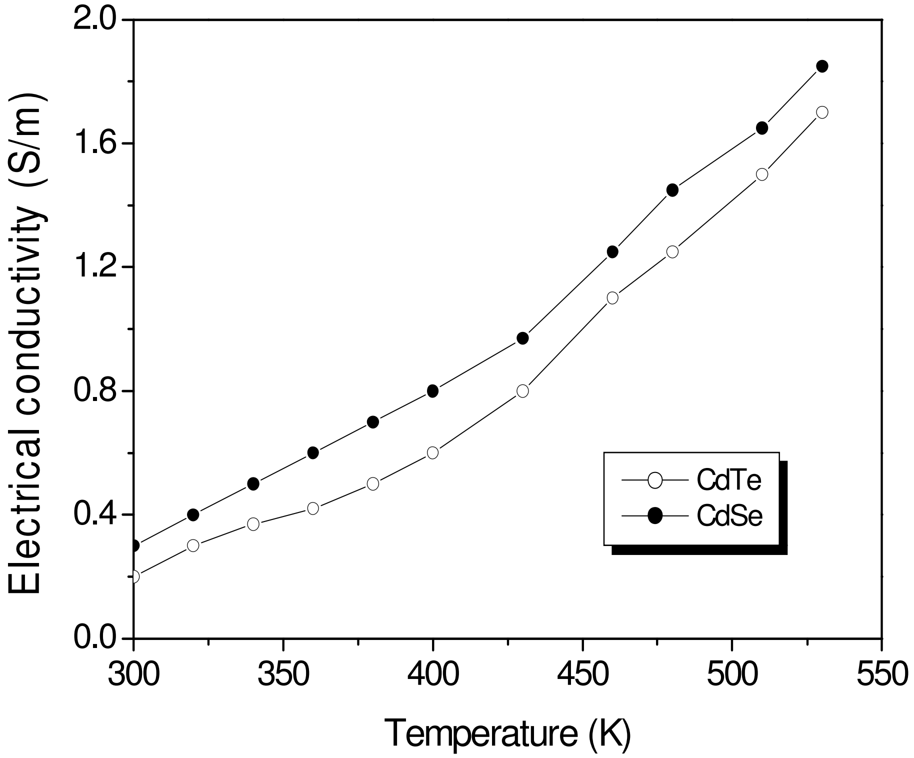

Figure 1. Calculated temperature dependence of electrical conductivity of CdTe and CdSe materials.

$$k_e = \frac{1}{3} v_F{}^2 \tau_F \int_{E=0}^{\infty} \frac{\partial f_0(E)}{\partial T} D(E)(E-\mu)dE = \frac{1}{3} v_F{}^2 \tau_F C_e = \frac{1}{3} C_e v_F l_F \qquad (56)$$

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

CALCULATION RESULTS

Electrical conductivity of CdTe and CdSe semiconductors are determined using our calculation method. The variation in electrical conductivity of CdTe and CdSe with temperature are shown in Figure 1.

It is observed that the conductivity increases non-linearly with the increase in temperature. This is explained in terms of structural changes occurring in these materials with temperature. In deposited CdTe and CdSe materials there are some lattice defects, geomerical and physical imperfections randomly distributed on the surface and the volume of the materials. The roughness of the surface, grain boundaries and inclusions in the volume are the main components of the geomerical imperfection. The importance factor, which is resposible for the physical properties of the material, is the structure. The materials are composed of randomly oriented grains with the appearance of the grain boundaries. An increase of temperature of the material affects the structure significantly causing a considerable increase in the mean size of the grain and a decrease in the drain boundary area. This decrease is due to the migration of the smaller crystallites and joining of those grains, which are similarly oriented, to form bigger crystallites. Because of these structural changes the inter grain boundary area decreases and so there is a decrease in the scattering of electrons. Consequenly, the carrier concentration also increases with the increase of temperature. This in turn increases the conductivity of given sample.

The thermal conductivity of undoped CdTe and CdSe materials have been calculated. The results are shown in Figure 2. These results show that the thermal conductivity of the CdTe is much less than that of the CdSe. In the 20 to 100 K range the thermal conductivity of the two materials is about 2% of the value imposed by boundary scattering at the walls of the crystal.

CONCLUSION

In conclusion, we have quantitatively obtained temperature-dependent of electrical and thermal conductivity of CdTe and CdSe semiconductors. The behaviour of two compounds are similar, although the CdSe material shows a better thermal and electrical

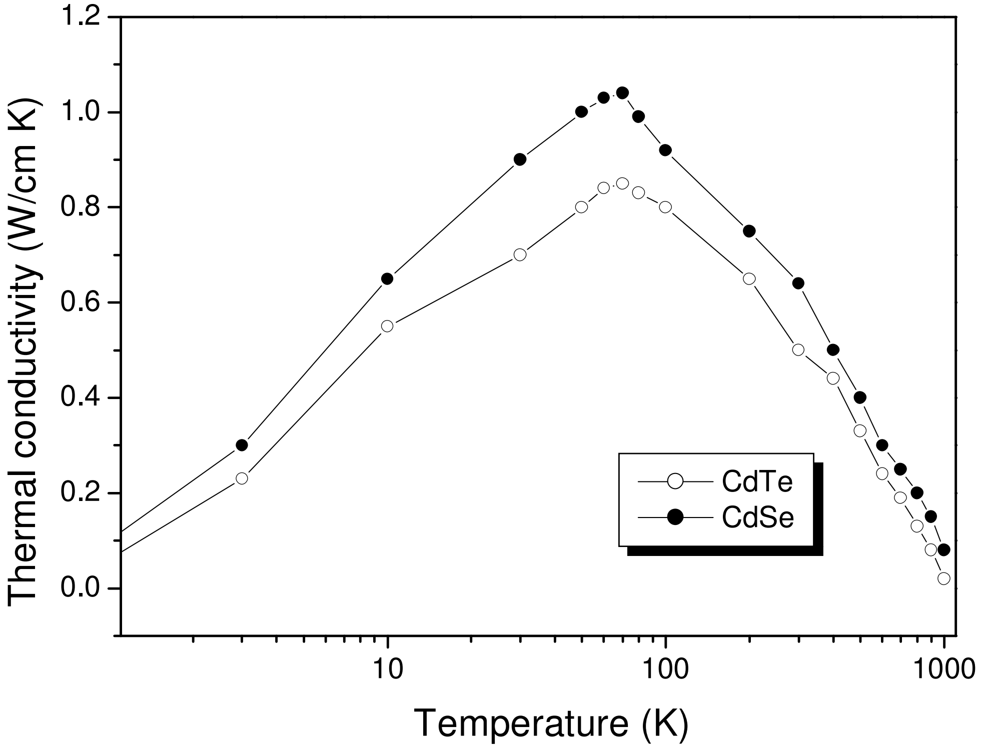

Figure 2. Calculated values for the thermal conductivity of CdTe and CdSe materials versus temperature.

conductivity in all temperature ranges.

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