Electronic transport in one-dimensional systems

* M P Singh & C M Bhandari

Department of Physics, University of Allahabad 211 002

Indian Institute of Information Technology, Allahabad 211 002

Email: cmbhandari@yahoo.com; singhmps74@rediffmail.com

Received 9 April 2003; revised 20 May 2003; accepted 8 October 2003

Electronic thermal transport and electrical transport in quasi one-dimensional structures is the subject matter of present communication. Expressions have been obtained for electronic thermal conductivity, electrical conductivity and Lorenz factor. Results of calculation for polycrystalline bismuth telluride have been presented at 300 K for different carrier densities and wire diameters. It is concluded that, cross-sectional size of the wire influences the Lorenz factor in carrier density range $10^{15}$-$10^{17}$ m$^{-3}$. Effect of cross-sectional size on electrical conductivity and electronic thermal conductivity is appreciable at carrier densities above $10^{15}$ m$^{-2}$.

[Keywords: Electronic thermal conductivity, Electrical conductivity, Lorenz factor, Polycrystalline bismuth telluride, Bismuth telluride]

1 Introduction

An understanding of electronic behaviour in thermoelectric semiconductors is of importance in the context of developing efficient materials for specific applications$^{[1-7]}$. One of the objects in this effort is to develop materials with large electrical to thermal conductivity ratio$^{[8-10]}$. This short communication deals with electronic contribution to electrical as well as thermal conductivity. Results of calculation have been presented for one-dimensional system of polycrystalline bismuth telluride. An understanding of the variation in electronic properties with the carrier density and wire diameter is useful for materials research$^{[8-10]}$.

2 Procedure and Theory

A brief outline of theory and procedure adopted is being indicated in this communication. A detailed account of work including electrical conductivity, thermal conductivity, thermo power and figure-of-merit will form subject matter of a future communication.

The system under consideration is in the form of wire of length $L$ along the $z$-axis having rectangular cross-section with transverse dimensions $a$ and $b$. The energy eigenvalues are given by$^{[11-15]}$:

$$E_{nlz} = n^2 E_0^l + l^2 E_0^0 + E_k$$

$n, l = 1, 2, 3, ..., ...

(1)

where

$$E_0^l = \frac{\pi^2 \hbar^2}{2 m^* a^2}, \quad E_0^0 = \frac{\pi^2 \hbar^2}{2 m b^2}, \quad E_k = \frac{\hbar^2 k^2}{2 m}$$

(2)

Here, $k$ is the wave vector, and the energy along $z$-direction varies quasi continuously. Also, $m^*$ is electron effective mass. This picture is valid for a spherical energy band. The system under consideration having a multi-valleyed energy band structure, the total density of states effective mass is expected to take care of the $N_e$ equivalent valley.

$$m^* = N_e^{\frac{1}{3}} (m_1 m_2 m_3)^{\frac{1}{3}}$$

(3)

Here, $m_1, m_2, m_3$ are components of the effective mass tensor along principal axes.

Electrical and thermal currents are linear functions of the gradient of electric field and temperature$^{[6]}$.

$$J_z = L_{EE} E + L_{ET} \nabla T$$

$$w = L_{TE} E + L_{TT} \nabla T$$

(4)
The electrical and thermal conductivities of the electronic system can be related to the coefficients $L_{ii}$. The electrical conductivity ($\sigma$) is defined as:

$$\sigma = L_{xx} \quad \ldots (5)$$

and electronic contribution to thermal conductivity ($k_e$) is given by:

$$k_e = \left( \frac{L_{xx} L_{yy}}{L_{xx}} \right) \quad \ldots (6)$$

The electrical conductivity ($\sigma$) is defined as:

$$\sigma = \frac{e}{abL} \sum f_i \nu_i \quad \ldots (7)$$

$$w = \frac{1}{abL} \sum f_i E_{ik} \nu_i \quad \ldots (8)$$

Here, $f_i$ is electron distribution function and $\nu_i$ is electron drift velocity.

The electric and thermal currents can be calculated by solving the Boltzmann transport equation in relaxation-time approximation. The electron distribution function is given by:

$$f_k = f_k^0 + \tau_{int}(k) \int_{E_k}^{E_k^0} \frac{1}{h} \frac{dE_k}{dk}$$

$$e \left( E - \frac{1}{e} \frac{\partial E_F}{\partial z} \right) \left( \frac{E_{ik} - E_k}{T} \right) \frac{\partial T}{\partial z} \left( - \frac{\partial f^0}{\partial E_{ik}} \right) \quad \ldots (9)$$

The carrier relaxation time should be known for the evaluation of the integral. The authors consider scattering of electrons by acoustic phonons. The relaxation time for acoustic phonons scattering in one-dimensional systems is given by:

$$\tau_{ac}(k) = \frac{4}{9} \frac{\hbar^2 c_{11} ab}{2 \varepsilon_1 (k_T \xi)} \quad \ldots (10)$$

Here, $c_{11}$ is the longitudinal elastic constant and $\varepsilon_1$ is the deformation potential. After solving above equation one can obtain:

$$J_x = \frac{-e}{a \eta^2} \sum_{i,j} \int \frac{1}{m^*} \frac{dE_k}{dk} \tau_{int}(k)$$

$$w = \frac{1}{a \eta^2} \sum_{i,j} \int \frac{1}{m^*} \frac{dE_k}{dk} \tau_{int}(k)$$

$$- \frac{\partial f}{\partial E_{ik}} \left( E - \frac{1}{e} \frac{\partial E_F}{\partial z} \right) \left( \frac{E_{ik} - E_k}{T} \right) \frac{\partial T}{\partial z} \left( - \frac{\partial f^0}{\partial E_{ik}} \right) \quad \ldots (11)$$

$$w = \frac{1}{a \eta^2} \sum_{i,j} \int \frac{1}{m^*} \frac{dE_k}{dk} \tau_{int}(k)$$

$$- \frac{\partial f}{\partial E_{ik}} \left( E - \frac{1}{e} \frac{\partial E_F}{\partial z} \right) \left( \frac{E_{ik} - E_k}{T} \right) \frac{\partial T}{\partial z} \left( - \frac{\partial f^0}{\partial E_{ik}} \right) \quad \ldots (12)$$

Here, the size quantum limit (SQL) is considered and all electrons are assumed to be in the
ground state \( n = l = 1 \). Considering a square cross-section \( (a=b) \). The generalized expressions are obtained as:

\[ L_{EE} = \frac{e^2}{\pi a^2} \left( \frac{h}{m^*} \right)^2 I_0 \]  \hspace{1cm} \text{(13)}

\[ L_{EF} = \frac{e^2}{\pi a^2} \left( \frac{h}{m^*} \right)^2 \left[ 2E_n^0 - E_F \right] I_0 + I_1 \]  \hspace{1cm} \text{(14)}

\[ L_{TE} = \frac{e^2}{\pi a^2} \left( \frac{h}{m^*} \right)^2 \left[ 2E_n^0 I_0 + I_1 \right] \]  \hspace{1cm} \text{(15)}

\[ I_{1T} = \frac{1}{T} \left[ 4(E_n^0)^2 - 2E_n^0 E_F \right] I_0 + \left( 4E_n^0 - E_F \right) I_1 + I_2 \]  \hspace{1cm} \text{(16)}

where \( I_n = \int dk k^2 \tau_{nf}(k) \left( \frac{\partial f}{\partial E_{nk}} \right) E_n^0 \) \hspace{1cm} \text{(17)}

The multi-valley structure of energy bands with \( N_v \) equivalent valleys has been taken into consideration. A number of equivalent valleys can accommodate more carriers, thereby increasing electrical conductivity without having adverse effect on thermo-power. The effect of non-parabolicity of energy bands has not been considered in the present work. The effect of non-parabolicity of energy bands and effect of inter-valley scattering of carriers is presently under investigation. With the help of these equations, one obtains the following expressions for the electrical and electronic thermal conductivity in terms of reduced Fermi energy

\[ \xi_{SD} = \frac{E_F}{k_B T} \]

\[ \sigma = \frac{2}{9\pi m^* E_F^2} e^2 N_v \frac{F_0(\xi_{SD})}{\xi_{SD}^2} \]  \hspace{1cm} \text{(19)}

\[ k_c = \frac{2}{9\pi m^* E_F^2} N_v \frac{k_B T}{\xi_{SD}} \left( \frac{4F_0^2(\xi_{SD})}{F_0(\xi_{SD})} \right) \]  \hspace{1cm} \text{(20)}

The Lorenz number is defined as

\[ L = \frac{\sigma}{\sigma T} \left( \frac{k_B}{e} \right) L_j, \text{ where } L_j \text{ is so-called dimensionless Lorenz factor:} \]

\[ L_j = \left( \frac{3F_0(\xi_{SD})}{F_0(\xi_{SD})} \right) \]

\[ F_0(\xi_{SD}) = \int_0^\infty dx \frac{x^n}{\exp(x - \xi_{SD}) + 1} \]  \hspace{1cm} \text{(22)}

The Fermi level can be related to carrier concentration with the following expression:

\[ \xi_{SD} = \ln \left( \frac{\sqrt{2\pi m_h a b}}{\gamma \delta \sqrt{m^* k_B T}} \right) \]  \hspace{1cm} \text{(23)}

where

\[ \gamma = \sum_a \exp \left( - \frac{n^2 E_a^0}{k_B T} \right) \text{ and } \delta = \sum_j \exp \left( - \frac{J^2 E_j^0}{k_B T} \right) \]

---

**Table 1** — Physical parameters of polycrystalline bismuth telluride used in the calculations

<table>
<thead>
<tr>
<th>( c_{ij} )</th>
<th>10^11 Nm^{-2}</th>
<th>( m^* m_0 )</th>
<th>( N_v )</th>
<th>( e ) /eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.19</td>
<td>0.15</td>
<td>6</td>
<td>6.3</td>
<td></td>
</tr>
</tbody>
</table>

---

**3 Results and Discussion**

Physical parameters required in the calculation are presented\(^7\) in Table 1. Theoretically all electronic transport parameters are expressed in
terms of reduced Fermi energy, which itself depends upon carrier density and temperature. Treating carrier density as a variable in theoretical calculations has become customary; such plots scan the whole range of doped semiconducting material. From an experimental point of view, this amounts to studying different samples with different doping levels. The formalism developed above has been applied to polycrystalline bismuth telluride at 300 K. Electrical and electronic thermal transport properties are of primary concern in the present study. Calculations refer to room temperature (300 K) with acoustic phonon scattering being the only mechanism to limit phonon mean free path.

Fig. 1 shows electrical conductivity of polycrystalline bismuth telluride at 300 K against carrier density for different wire diameters. As expected, electrical conductivity rises with carrier density. The effect of reduction in wire diameter is to reduce $\sigma$. A change in $a$ from 300 to 130 A results in about 65% reduction in $\sigma$ at $n = 10^{22} \text{m}^{-3}$. At $n = 10^{20} \text{m}^{-3}$, corresponding change in $\sigma$ is about 10%. Similar pattern of change is visible in electronic thermal conductivity displayed in Fig. 2. Fig. 3 gives dimensionless Lorenz factor $L_4$ against carrier density for different wire diameters. The variation in $L_4$ shows some interesting features. The dispersion between $L_4$ values for various wire diameters is observable only in the carrier density range $10^{13}-10^{20} \text{m}^{-3}$. In both non-degenerate and degenerate regions, curves seem to converge. Starting from around 2 in the non-degenerate limit, $L_4$ converges to the usual metallic value at high carrier densities. At $n = 10^{21} \text{m}^{-3}$, values for $a = 130$ A and 300 A are 2.2 and 2.4, respectively, whereas at $10^{20} \text{m}^{-3}$, the corresponding values are 2.85 and 3.00, respectively. These values can be compared with observed values of Lorenz factor only after lattice thermal conductivity is accounted for.

Acknowledgement

One of the authors (MPS) thankfully acknowledges financial assistance from the CSIR, New Delhi. The authors thank Prof G K Pandey and Dr M D Tiwari for their interest and support.

References