THERMOELECTRIC PROPERTIES OF n-TYPE Bi$_2$Te$_3$ WIRES

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Abstract

We report here a theoretical model for the thermoelectric properties of cylindrical Bi$_2$Te$_3$ wires of a classical size. The thermoelectric figure of merit $ZT$ is calculated for the monopolar n-type Bi$_2$Te$_3$ wire under applied radial electric field. The radial variation of the local thermopower $S(\rho)$, reduced electron Fermi level $\eta(\rho)$, and electron concentration $n(\rho)$ are also investigated when the screening length is less than the wire diameter.

Introduction

Over the past few years there has been renewed interest in the field of thermoelectrics accompanied by the development of synthetic semiconductors that possess Seebeck coefficients of hundreds of microvolts and provided a useful amount of electrical power [1,2]. Shik [3], and Hicks and Dresselhaus [4] and Hicks et al. [5] proposed to use quantum superlattices in order to improve the thermoelectric performance.

A measure of thermoelectric quality of a material is the dimensionless figure of merit $ZT$ [6]

$$ZT = TS^2/\sigma k,$$

where $T$ is the temperature, $\sigma$ is the electroconductivity, $S$ is the Seebeck coefficient, and $\kappa$ is the thermal conductivity and the latter consists of electronic $\kappa_e$ and lattice $\kappa_L$ components at absolute temperature $T$(K). The product

$$P = \sigma S^2,$$

is known as the “power factor,” It carries the main contribution to $ZT$ [6]. A good thermoelectric material must have a large Seebeck coefficient, $S$, to produce the required voltage, high electrical conductivity, $\sigma$, to reduce the thermal noise (joule heating, $I^2R$), and a low thermal conductivity, $\kappa_e$ to decrease thermal losses from the thermocouple junctions. It is important to note that a low thermal conductivity in a good thermoelectric material means a low value of its lattice component $\kappa_L$ as a major contributor since its electronic component $\kappa_e$ as a minor contributor is proportional to the electrical conductivity.

Thermoelectric properties are explained by the figure of merit, for a material depends upon the carrier concentration. Metals are poor thermoelectric materials with a low Seebeck coefficient, because they have large electronic contribution to thermal conductivity, so $\sigma$ and $\kappa$ will cancel each other. Insulators have a high Seebeck coefficient, and a small electronic contribution to thermal conductivity, but their charge density and therefore electrical conductivity are low leading to a low thermoelectric effect. The best thermoelectric materials are those between metals and insulators; i.e. semiconductors with an electronic density of $10^{19}$ 1/cm$^3$.

Bismuth telluride Bi$_2$Te$_3$ and its alloys with Bi$_2$Se$_3$ have the highest $ZT\approx1$ at 300 K, and are extensively employed in terrestrial cooling. Bismuth Telluride system which is the
most commonly used semiconductor material for cooling applications, has a maximum performance at approximately 80° C with an effective operating range (EOR) of –100° C to +200° C.

Thermoelectric materials are solid-state devices with no moving parts, the combined cooling/heating ability makes them attractive for many electrical energy generation and cooling applications. Thermoelectric coolers are solid-state heat pumps used in applications where temperature stabilization, temperature cycling, or cooling below ambient temperatures are required. Thermoelectric coolers/refrigerators are ideally suited to a wide variety of applications due to their small size, high reliability, wide operating temperature range, low power requirements, and no gases refrigerant or liquid containing requirement. Furthermore, they can provide pinpoint cooling for heat sensitive electronic components such as infrared detectors, low noise amplifiers and computer chips. Compact cooling units are also used to stabilize the operating temperature of laser diodes, optics. Some CCD (charge-coupled device) detectors in digital cameras use the thermoelectric effect to help to cool them. Similar thermoelectric components can be found in portable beverage chillers, which are powered by automobile battery [7]. Thermoelectric materials are also used for niche applications where highly accurate temperature control is required.

Most present-day materials have values of ZT<1. Current development in the field of thermoelectrics concentrates on improvements of existing thermoelectric materials and on optimizing device design. The main goal is to find substances and/or structures with large ZT.

Cylindrical surrounding-gate MOSFETs are intensively studied at present. The length l, over which the source and drain perturb the channel, is 1/π of the device channel thickness in the double-gate case, and 1/4.8 of the effective diameter in the cylindrical case. The tighter confinement present in the cylindrical structure offers better control of short-channel effects.

**Figure of Merit of the Wire**

The formula for the effective figure of merit (EFM) of the inhomogeneous film under the electric field effect (EFE) has been stated in paper [8]. Using the same technique we can state analogous formula for the effective figure of merit of the inhomogeneous wire at the same conditions. The EFM of the wire is defined by

\[
ZT = \left( \frac{\sigma S}{\kappa} \right)^2 \frac{T}{\langle \sigma \rangle \kappa}
\]

where we average a function f over the wire radius

\[
\langle f \rangle = \frac{1}{\pi R^2} \int_0^R f(\rho)d(\pi \rho^2)
\]

The electroconductivity is given by

\[
\sigma(\rho) = e \mu n(\rho)
\]

For the sake of simplicity we take into account scattering of electrons only by acoustic phonons. In this case the local S assumes the form [9]

\[
S(\rho) = \frac{k}{e} \left[ \frac{\Phi}{\Phi_0} \left( \eta(\rho) \right) \right]
\]

where \(\eta(\rho)\) is the reduced Fermi level of the electrons
\[
\eta(\rho) = \frac{\mu_F - E_C + e\Phi(\rho)}{k_B T} \quad (5)
\]

The potential \( \phi(\rho) \) in a dimensionless form \( \varphi = \frac{e\Phi(\rho)}{k_B T} \) is found by the solution of the corresponding Poisson equation in the range \( 0 < \rho < R \). The latter in the terms of dimensionless radial cylindrical coordinate \( \tau = \rho/R \) has the form

\[
\frac{1}{\tau} \frac{d}{d \tau} \left( \tau \frac{d \varphi}{d \tau} \right) = \left( \frac{R}{R_c} \right)^2 n(\varphi, \eta_n) - n_o
\]

\( n(\varphi, \eta) = \frac{2}{\sqrt{\pi}} N_c \Phi_{1/2} (\eta_a + \varphi) \quad (6) \)

where \( N_c \) is the electron density of states

\[
N_c = 2N_r^{1/2} \left( \frac{m_c kT}{2\pi \hbar^2} \right)^{3/2}
\]

\( m_c \) are the electron effective masses, and \( N_r \) is the number of electron valleys, \( n_o \) is the homogeneous carrier concentration at \( \varphi = 0 \), and

\[
\Phi_q(\eta) = \int_{-\infty}^{\infty} \frac{x^q}{1 + \exp(x - \eta)} dx, \quad \eta_n = \frac{\mu_F - E_C}{k_B T} \quad (7)
\]

The first distinct feature of coaxial structure is the geometrical enhancement of the electrical field at the wire surface due to cylindrical configuration, which in term of displacement becomes

\[
D = \varepsilon E = \varepsilon_d E_d = \frac{\varepsilon}{\varepsilon_d} \frac{U_g}{R \ln (R_d/R)} \quad (8)
\]

Here \( \varepsilon \) and \( \varepsilon_d \) are the dielectric constants of semiconductor and glass respectively, \( E \) and \( E_d \) are the electric fields, \( U_g \) is the gate voltage, \( R \) and \( R_d \) are the semiconductor and glass radii, respectively.

From (9) the boundary conditions for Poisson Eq.(6) at the wire surface are

\[
\left. \frac{d \varphi}{d \tau} \right|_{\tau = 1} = -\text{sign}(U_g) \frac{eU_g \varepsilon_d}{\varepsilon kT \ln (R_d/R)} \quad (10),
\]

and at wire center \( \left. \frac{d \varphi}{d \tau} \right|_{\tau = 0} = 0 \) due to the vanishing value of the electrical field at this point of axial symmetry.

In our model we assume that: (a) quantum size effect is neglected, i.e. the system is purely classical, (b) thermoconductivity \( \kappa \) is independent on the carrier concentration, (c) scattering of electrons is due to only interaction with acoustic phonons, (d) semiconductor is of n type (monopolar), (e) the parabolic approximation is valid to calculate energy spectrum.

**Numerical results**

Table I presents the set of the characteristics for the uncharged intrinsic thermoelectric wire on the base of Bi_2Te_3.

Newton’s method \([11,12]\) is applied to solve numerically nonlinear differential equation (6).
Figure 1 shows dependence of the figure of merit ZT and Seebeck coefficient on the gate voltage overlapping the wire. The inflection point of S and maximum of ZT corresponds to transition nondegenerate semiconductor to degenerate semiconductor, when the Fermi level intersects the conduction band edge. In this case the reduced Fermi level changes its sign. Hence, the Seebeck coefficient undergoes inflection corresponding equation 4, because the character of electron-acoustical phonon interaction is changed.

### TABLE I. Characteristic properties of the uncharged Bi$_2$Te$_3$ wire

<table>
<thead>
<tr>
<th>Property</th>
<th>Temperature, K</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dielectric constant, $\varepsilon$</td>
<td>100</td>
<td>300</td>
</tr>
<tr>
<td>Number of electron valleys, N$_c$</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>Number of hole valleys, N$_v$</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>Electron mass (density of states), m$_c$</td>
<td>0.45m$_0$</td>
<td>150</td>
</tr>
<tr>
<td>Hole mass (density of states), m$_v$</td>
<td>0.69m$_0$</td>
<td>150</td>
</tr>
<tr>
<td>Electron mobility, $\mu$$_n$</td>
<td>1200</td>
<td>300</td>
</tr>
<tr>
<td>Hole mobility, $\mu$$_v$</td>
<td>510 cm$^2$/V·sec</td>
<td>300</td>
</tr>
<tr>
<td>Carrier (electron) concentration, n$_e$</td>
<td>$1.78\times10^{19}$ cm$^{-3}$</td>
<td>300</td>
</tr>
<tr>
<td>Electron Fermi level, E$_F$</td>
<td>-0.0206 eV</td>
<td>300</td>
</tr>
<tr>
<td>Screening length, $R_e$</td>
<td>30 nm</td>
<td>300</td>
</tr>
<tr>
<td>Thermal conductivity, $\kappa$</td>
<td>1.45</td>
<td>300</td>
</tr>
</tbody>
</table>

The maximum value of ZT≈2 occurs at the gate voltage 50 V. This value of ZT is higher than predicted for the metal gate-dielectric layer- PbTe thermoelectric film structure [8]. The large positive (negative) value of the gate voltage corresponds to small (large) concentration of electrons. It looks like the closed (opened) stage of a transistor. We see that the Seebeck coefficient decreases when the concentration of electrons increases.
Figures 2(a) and 2(b) show the variation and the values of the reduced Fermi level $\eta(\rho)$ and the electron concentration $n(\rho)$ inside the wire, calculated with the corresponding value gate potential $U_g=50\,\text{V}$.

![Figure 2](image1)

Figure 2. (a) Space variation of the reduced Fermi level $\eta$ (eV) with respect to the conduction band edge. The wire diameter is $R=180\,\text{nm}$. Gate voltage $U_g=50\,\text{V}$. (b) space variation of the electron concentration $n_e$ (cm$^{-3}$)

![Figure 3](image2)

Figure 3. Space variation of the wire thermopower $S_n$ ($\mu\text{V/K}$). The average of the thermopower over the wire diameter $196\,\mu\text{V/K}$. The temperature is $T=300\,\text{K}$.

Figures 4(a) and 4(b) present the local dependence of the effective figure of merit $M_n(\rho)$ at $U_g=50\,\text{V}$ and $100\,\text{V}$ correspondingly. $M_n(\rho)$ changes only by about a factor 1.5 along the radius of the wire. Dependence $M_n(\rho)$ exhibits maximum when $U_g>50\,\text{V}$ (see Fig. 4(b)). This is the result of the interplay between the change of the carrier concentration, i.e. conductivity and thermopower along the wire diameter. The extreme point corresponds to the case when the rate of electroconductivity increasing is totally compensated by the rate of thermopower decreasing.

![Figure 4](image3)
Conclusions

The results presented above should be considered as a general qualitative description of the influence of EFE doping on the thermoelectric properties of the Bi₂Te₃ wire, rather than as a stringent quantitative characterization. A much more elaborate calculation is required. The dispersion has to be considered in the nonparabolic approximation. The effect of electric field on the thermoconductivity and mobility should be taken into account.

The thermoelectric figure of merit ZT is investigated for n-type Bi₂Te₃ wire of diameter of 360 nm under the applied radial electric field at temperature T=300 K. It is shown that maximum ZT=2.01 at gate voltage $U_g=50$ V corresponds to transition nondegenerate semiconductor to degenerate semiconductor, when the Fermi level intersects the conduction band edge. If the gate voltage is more than 50 V then the local dependence of the figure of merit exhibits non-monotonic behavior corresponding to the degenerate semiconductor. This is the result of the interplay between the change of the carrier concentration and thermopower along the wire diameter. The extreme point corresponds to the case when the rate of electroconductivity increasing is totally compensated by the rate of thermopower decreasing.

References