EXPERIMENTAL AND THEORETICAL TEMPERATURE DEPENDENCES OF THE KINETIC COEFFICIENTS OF Bi_2Te_3

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Abstract

Using the previously determined experimental temperature dependences of electrical conductivity and thermopower, theoretical calculations of temperature dependences of electrical conductivity, thermopower, mobility, and chemical potential of both a bulk bismuth telluride crystal and a Bi_2Te_3 microwire have been conducted.

Keywords: thermoelectric materials, microwire, bismuth telluride, electrical conductivity, thermopower, chemical potential.

Rezumat

În baza datelor experimentale ale dependenței conductivității electrice și forței termoelectromotoare de temperatură, obținute anterior, se efectuează calcule teoretice ale dependenței de temperatură a conductivității electrice, forței termoelectromotoare, mobilității și potențialului chimic atât a cristalului masiv de telurură de bismut, cât și a microfirului din Bi_2Te_3.

Cuvinte cheie: materiale termoelectrice, microfir, telurură de bismut, conductivitate electrică, forță termoelectromotoare, potențial chimic.

1. Introduction

Most of high-quality thermoelectric materials are narrow-gap semiconductors characterized by a combination of a high electrical conductivity, a high thermopower, and a low thermal conductivity. The Bi_2Te_3 semiconductor compound and solid solutions based on it are among the best low-temperature thermoelectric materials; they are commonly used in thermoelectric energy converters, refrigerators, and thermostats. Considerable interest in studying the properties of narrow-gap semiconductors, particularly bismuth telluride single crystals, is attributed to the wide possibilities of their practical use as thermoelectric materials and promising topological insulators. The search for methods to increase the thermoelectric efficiency of these substances is not only of a fundamental scientific value, but also of practical importance [1–3].

2. Results and Discussion

Calculations of the temperature dependences of the kinetic coefficients of a bulk bismuth telluride crystal and a Bi_2Te_3 microwire were conducted using the previous experimental data described in [4–6].

Figure 1 shows the temperature dependences of the electrical conductivity of *n*- and *p*- type Bi_2Te_3 current carriers [6]. Figure 2 shows the temperature dependences of the mobility calculated from the electrical conductivity (μ_1, μ_2) and the μc_1 and μc_2 values calculated by the formula

$$\mu = AT^r \tag{1}$$

where *r* is the effective scattering parameter and *A* is a constant.

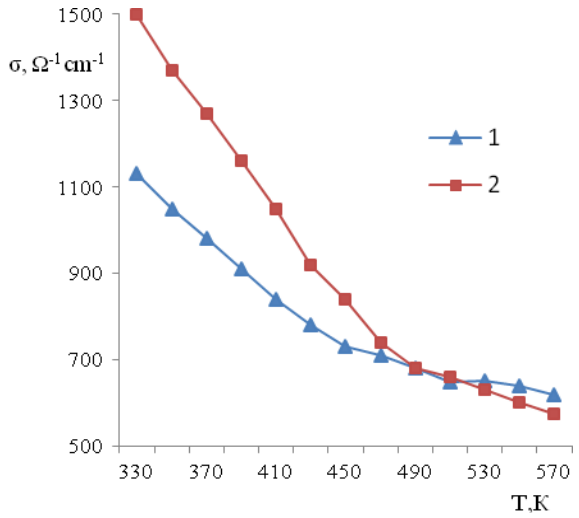

Fig. 1. Temperature dependences of the electrical conductivity of (*1*) *n*-type and (*2*) *p*-type Bi_2Te_3 current carriers [6].

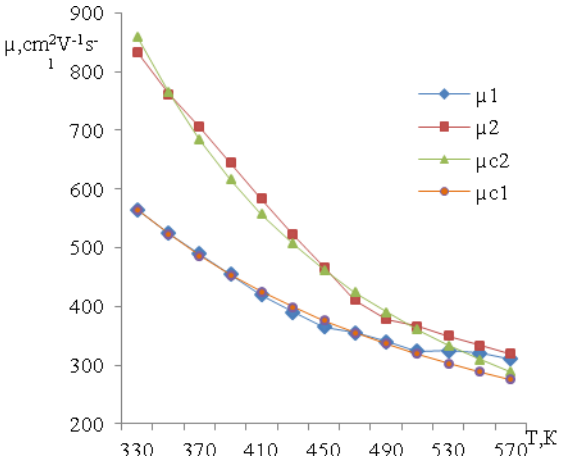

Fig. 2. Temperature dependences of mobility μ_1 and μ_2, which is calculated from electrical conductivity, and mobility μc_1 and μc_2, which is calculated by formula (1).

The *r* and *A* parameters were calculated from the temperature dependence of mobility μ_1 and μ_2; they are listed in Table 1.

Table 1. Parameters *r* and *A* for *n*-type and *p*-type Bi_2Te_3 crystals

Crystal	*r*	*A*, $cm^2 V^{-1} s^{-1}$
n-type Bi_2Te_3	–1.3	1.15×10^6
p-type Bi_2Te_3	–2	9.01×10^7

In the case of purely acoustic scattering of charge carriers, in terms of classical statistics, the mobility is $\mu \sim T^{-1.5}$ [7]. An increase in the exponent of the temperature dependence of the charge carrier mobility can be attributed to the presence of additional scattering mechanisms. It is evident from Table 1 that, for *n*-type and *p*-type Bi_2Te_3, $r = -1.3$ and -2, respectively. This fact suggests that, for *n*-type Bi_2Te_3, charge carrier scattering occurs on acoustic phonons, while p-type Bi_2Te_3 is characterized by mixed scattering: both on acoustic and optical phonons and on impurities.

Figure 3 shows the temperature dependences of the electrical conductivity of current carriers of a Bi_2Te_3 microwire. Figure 4 shows the temperature dependences of the mobility calculated from the electrical conductivity by formula (1).

The *r* and *A* parameters were calculated from the temperature dependence of mobility μ; they are listed in Table 2.

Table 2. Parameters *r* and *A* for a Bi_2Te_3 microwire

T, K	*r*	*A*, $cm^2 V^{-1} s^{-1}$
20–80	–0.28	5.39×10^4
100–200	–0.91	9.14×10^5
220–300	–1.48	1.9×10^7

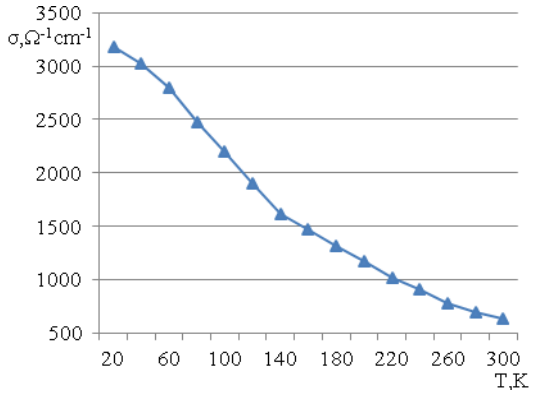

Fig. 3. Temperature dependence of the electrical conductivity of a *p*-type Bi_2Te_3 microwire.

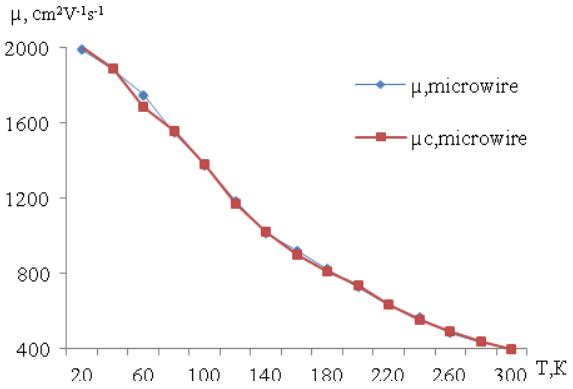

Fig. 4. Temperature dependences of mobility μ calculated from the electrical conductivity and mobility μc calculated by formula (1) for a *p*-type Bi_2Te_3 microwire.

It is evident from Table 1 that the effective scattering parameter *r* significantly depends on temperature. Vibrations of the crystal lattice decrease with a decrease in temperature; however, at room temperature, the effective scattering parameter *r* of a *p*-type Bi_2Te_3 microwire is 1.35 times lower than that in a bulk crystal.

Figure 5 shows the temperature dependences of the thermopower of (*1*) *n*-type and (*2*) *p*-type Bi_2Te_3 [6].

Using the experimental temperature dependence of the thermopower (α) of Bi_2Te_3, the temperature dependence of the chemical potential (η) of Bi_2Te_3 was calculated by the following formula [8]:

$$\eta = \frac{k_0}{e}\frac{\pi^2}{3}\frac{k_0}{\alpha}T(r+1), \tag{2}$$

where k_0 is the Boltzmann constant, e is the elementary electric charge, r is the effective scattering parameter, T is the temperature, and α is the thermopower.

Figure 6 shows the calculated temperature dependences of the chemical potential of (*1*) *n*-type and (*2*) *p*-type Bi_2Te_3.

Figure 7 shows the temperature dependences of the thermopower of a *p*-type Bi_2Te_3 microwire, which were used to calculate the temperature dependences of the chemical potential by formula (2).

Figure 8 shows the temperature dependences of the chemical potential (η) of a *p*-type Bi_2Te_3 microwire.

It is evident from Figs. 6 and 8 that, in a temperature range of 300–500 K, the chemical potential for bulk Bi_2Te_3 semiconductors is in the valence band, while the chemical potential of a Bi_2Te_3 microwire is in the valence band in a temperature range above 120 K and in the band gap in a temperature range of 40–120 K.

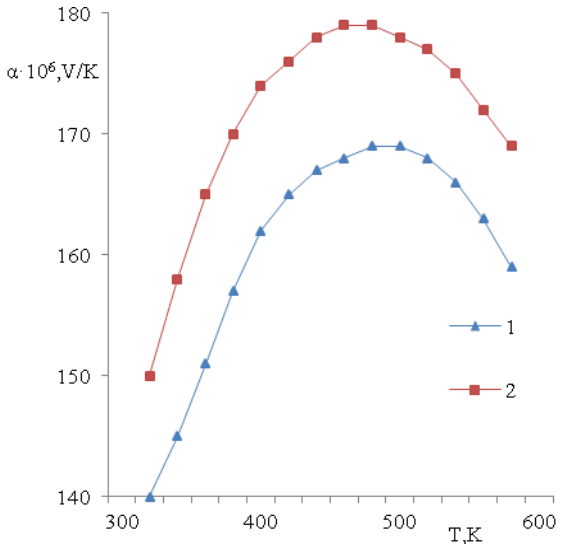

Fig. 5. Temperature dependences of the thermopower of (*1*) *n*-type and (*2*) *p*-type Bi_2Te_3 [6].

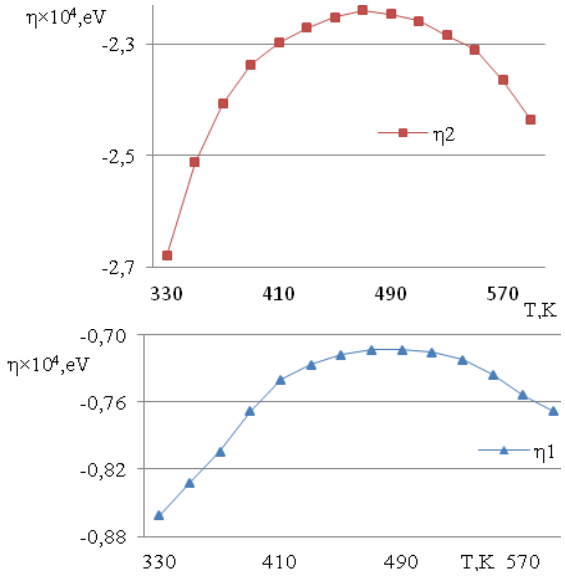

Fig. 6. Temperature dependences of the chemical potential (η) of (*1*) *n*-type and (*2*) *p*-type Bi_2Te_3.

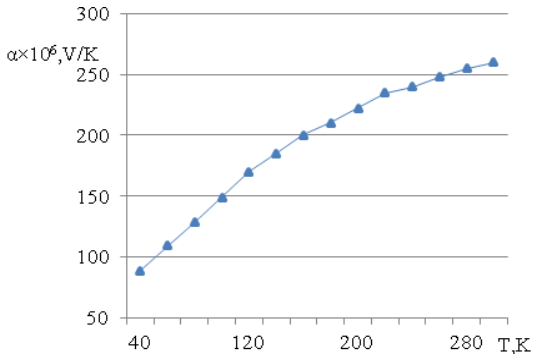

Fig. 7. Temperature dependence of the thermopower of a *p*-type Bi_2Te_3 microwire [4].

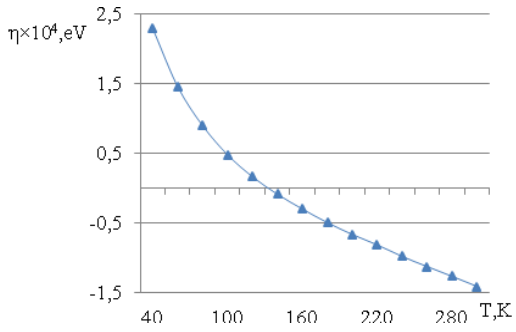

Fig. 8. Temperature dependence of the chemical potential (η) of a *p*-type Bi_2Te_3 microwire.

3. Conclusions

The effective scattering parameter has been calculated from the temperature dependence of the mobility of *n*- and *p*-type Bi_2Te_3 crystals and a *p*-type Bi_2Te_3 microwire. It has been shown that the effective scattering parameter *r* of a *p*-type Bi_2Te_3 microwire is 1.35 times lower than that of a bulk crystal. The temperature dependences of the chemical potential of *n*- and *p*-type Bi_2Te_3 crystals and *p*-type Bi_2Te_3 microwires have been calculated. It has been shown that, in bulk Bi_2Te_3 semiconductors, in a temperature range of 300–500 K, the chemical potential is in the valence band, while the chemical potential of the microwires is in the band gap in a temperature range of 40–120 K and in the valence band at temperatures above 120 K.

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