## 03,13,01

# **Temperature dependence of the Hall coefficient and the specific electrical conductivity of a single crystal Bi0***.***6Sb1***.***4Te<sup>3</sup>**

© N.P. Stepanov<sup>1,4</sup>, M.S. Ivanov<sup>2</sup>, P.P. Konstantinov<sup>3</sup>, O.N. Uryupin<sup>3</sup>

<sup>1</sup> Transbaikal State University, Chita, Russia  $2$  Trans-Baikal Institute of Railway Transport, Chita, Russia <sup>3</sup> loffe Institute, St. Petersburg, Russia <sup>4</sup> Baikal State University, Irkutsk, Russia E-mail: np-stepanov@mail.ru

Received May 25, 2024 Revised May 25, 2024 Accepted June 7, 2024

> The results of a study of the temperature dependences of the Hall coefficient and the specific electrical conductivity of a single crystal  $Bi_{0.6}Sb_{1.4}Te_3$  obtained in the temperature range from 80 to 600 K. It is established that there are features in the change in the value of the specific electrical conductivity in the temperature range in which the maximum rate of decrease in diamagnetic susceptibility and deformation of the plasma edge due to convergence of energies are fixed for this crystal plasmon and electronic transition between nonequivalent extremes of the valence band.

**Keywords:** bismuth and antimony tellurides, temperature dependences, Hall coefficient, electrical conductivity.

DOI: 10.61011/PSS.2024.07.58989.137

### **1. Introduction**

Materials based on solid solutions of bismuth telluride and antimony continue to be the most required in industrial production of thermoelectric converters. Thanks to their practical importance they are rather well studied [1–3], but in thermoelectric material science the studies are ongoing to optimize their properties [4–7]. Results of in-deep studies ensure use of the accumulated knowledge to detail the processes occurred in their electronic system, without this further progress in thermoelectric characteristics improvement is impossible.

One of such processes, according to the study results in paper [8], determines the features of behaviour of temperature dependence of magnetic susceptibility of crystal Bi0*.*6Sb1*.*4Te3, presumably affecting the light holes concentration. As change in state of the electronic system determines the temperature course of the conductivity and the Hall coefficient, it is of interest to study their temperature dependencies in the crystal  $\text{Bi}_{0.6}\text{Sb}_{1.4}\text{Te}_{3.}$  Due to this paper objective is study of temperature dependences of conductivity and Hall coefficient of crystal Bi0*.*6Sb1*.*4Te<sup>3</sup> at temperatures of features observation in behaviour of the magnetic susceptibility.

# **2. Crystals, samples, experimental procedure**

We studied a single-crystal  $Bi_{0.6}Sb_{1.4}Te_3$  grown by the Czochralski method at A.A. Bajkov Institute of Metallurgy and Materials Science of the Russian Academy of Sciences. The Hall coefficient and conductivity were measured by two-frequency method with variable magnetic field with amplitude  $0.15$  T (50 Hz) and alternating current (72 Hz), in temperature range from 80 to 600 K, in laboratory of thermoelectric studies of Ioffe FTI [9].

### **3. Description of the experimental results**

Temperature dependence of Hall coefficient *R*(*T*) of crystal  $Bi_{0.6}Sb_{1.4}Te_3$  is shown in Figure 1. It is obvious that Hall coefficient increases with temperature rise to 350 K, than quickly decreases. We focus attention on what is seen in Figure 1, in range from 80 to 200 K the Hall coefficient increases practically linearly.

Temperature dependence of conductivity  $\delta(T)$  of singlecrystal  $Bi_{0.6}Sb_{1.4}Te_3$  is presented in Figure 2, where decrease in  $\delta$  is observed with temperature increasing. Also we can see that feature in behaviour of conductivity is observed, which is decrease in inclination of curve  $\delta(T)$ to axis of temperatures in range 120−145 K. At that in direct vicinity to it the inclination, on the contrary, increases. The experimental set-up to measure conductivity ensures tracking the trends of its temperature change with relative error 1−2 percent. This excludes ignoring said feature in temperature dependence of conductivity and its consideration as experiment error. More so that it is observed in the same temperature range in which for crystal  $Bi_{0.6}Sb_{1.4}Te_3$  abrupt decrease in diamagnetic susceptibility was registered [8].

Due to this, from data in Figure 2, the temperature dependence of first derivative of conductivity with respect to temperature, shown in Figure 3.

It is obvious from Figure 3, that in behaviour  $\left| d\delta/dT \right|$ the clearly expressed feature is observed, it means that upon decrease in temperature from 200 to 145 K |*dδ/dT*| increases and reaches first maximum, then decreases to minimum at temperature 130 K, and then again increases in range from 130 to 120 K, reaching absolute maximum at 120 K.

# **4. Discussion of experimental results**

First of all note that Figure 1 shows that temperature increasing from 350 to 600 K is accompanied by decrease in Hall coefficient by about three times, which is due to transition to own conductivity. Nevertheless, as can be seen from Figure 2, the conductivity of the crystal in this temperature range decreases by approximately two times, indicating substantial decrease in charge carrier mobility, which may be due not only to scattering on acoustic phonons but also probably near other processes characteristic of semiconductors having complex band structure [10–12].

From data Figure 1 it follows that in range 80−350 K increase in Hall coefficient is observed, it in crystals (Bi2−*x*Sb*<sup>x</sup>* )Te<sup>3</sup> is most adequately explained by transition of charge carriers from subzone pf heavy holes into subzone of light holes, intensity increases with temperature rise to values sufficient to start transition to own conductivity [13,14]. Paper [15] shows data of optical studies of crystal Bi0*.*6Sb1*.*4Te<sup>3</sup> in spectral region of monitoring the fundamental absorption edge in crystals  $(Bi_{2-x}Sb_x)Te_3$ .



**Figure 1.** Temperature dependence of Hall coefficient of singlecrystal Bi<sub>0.6</sub>Sb<sub>1.4</sub>Te<sub>3</sub>. Measurement was performed in direction perpendicular  $C_3$ .



**Figure 2.** Temperature dependence of conductivity of singlecrystal Bi<sub>0.6</sub>Sb<sub>1.4</sub>Te<sub>3</sub>. Measurement was performed in direction perpendicular C3.



**Figure 3.** Temperature dependence of modulus of the first derivative of the conductivity with respect to temperature of crystal Bi0*.*6Sb1*.*4Te3.

A decrease in the transition energy defining the magnitude of the optical band gap with temperature rise was observed, which can only be due to shift of the chemical potential level towards the valence band top. Hence, with temperature rise the electrons actually transit from the heavy hole subzone to the light holes subzone. As a result the concentration of heavy holes increases, and concentration of light movable holes making main contribution to the electrical conductivity decreases, this is characteristic of all crystals  $(Bi_{2-x}Sb_x)Te_3$ , of *p*-type of conductivity.

Thus, Figure 2 shows that in range 80−200 K, where Hall coefficient of crystal  $Bi<sub>0.6</sub>Sb<sub>1.4</sub>Te<sub>3</sub>$  increases in direct proportion to temperature, the electric conductivity decreases by 2.6 times. As at temperatures over 100 K in crystals (Bi2−*x*Sb*<sup>x</sup>* )Te<sup>3</sup> the lattice scattering prevails, and electronic system up to temperature 150−200 K is in state of heavy degeneracy, then according to theoretical description of the acoustic mechanism of scattering of degenerated charge carriers the relaxation time on temperature range from 80 to 200 K can change by approximately 2.5 times. Consequently, the decrease in the electrical conductivity in this temperature range can be partially attributed to the decrease in the concentration of light holes, which is reflected in the change in the Hall coefficient.

So, the observed in range 120−145 K change in increase rate of electrical conductivity, shown in Figure 3, is probably associated with effect of some process on the thermal crossflow of holes between non-equivalent extremums of the valence band, which, due to some reasons, occurs exactly in crystal  $Bi_{0.6}Sb_{1.4}Te_3$ , and only in narrow temperature range. Study results in paper [8] show that specific nature of crystal  $Bi_{0.6}Sb_{1.4}Te_3$  is that at temperatures close to 100 K, the plasmon energy  $- E_p$  in it is, firstly, comparable to the energy of thermal oscillations of the lattice, and, secondly, with energy of electronic transition —  $\Delta E$  via the energy gap between the top of heavy hole subzone and level of chemical potential located in light hole subzone.

The supposition about effect of converging the energies  $E_p$  and  $\Delta E$  on physical properties of the crystal Bi<sub>0.6</sub>Sb<sub>1.4</sub>Te<sub>3</sub> is currently confirmed by data obtained during experimental study of the plasma response of free charge carriers of this crystal to infrared radiation [16]. It is identified that upon decrease in temperature an additional kink appears on the reflectance spectrum curve in the interval of plasma edge observation frequencies. Study of the spectral dependencies of the real, imaginary parts of the dielectric permittivity function and the energy loss function show that the plasma edge deformation is due to the influence of the electronic transition. Thus, the data of the optical experiment confirm the assumption expressed in the paper [8] that the features in the temperature dependence behavior of the magnetic susceptibility of the crystal  $\text{Bi}_{0.6}\text{Sb}_{1.4}\text{Te}_3$  are due to the convergence of the energies of plasmon and the electron transition affecting the light holes.

# **5. Conclusion**

As conclusion note that during executed study we identified the features in change of electrical conductivity of the crystal  $Bi_{0.6}Sb_{1.4}Te_3$ , observed in the temperature range where we register maximum rate of decreasing of diamagnetic susceptibility and deformation of plasma edge due to converging of energies of plasmon and electronic transition between nonequivalent extremums of the valence band.

#### **Conflict of interest**

The authors declare that they have no conflict of interest.

#### **References**

- [1] B.M. Gol'tsman, V.A. Kudinov, I.A. Smirnov. Poluprovodnikovye termoelektricheskie materialy na osnove Bi<sub>2</sub>Te<sub>3</sub>. Nauka, M. (1972). (in Russian).
- [2] V.A. Kulbachinskij, H. Ozaki, I. Miahara, K. Funagaj. ZhETF **124**, *6*, 1358 (2003). (in Russian).
- [3] M.K. Zhitinskaya, S.A. Nemov, V.R. Mukhtarov, T.E. Svechnikova. FTP **45**, *8*, 1021 (2011). (in Russian).
- [4] S.J. Jung, S.K. Kim, H.H. Park, D.B. Hyun, S.H. Baek, J.S. Kim. J. Electron. Mater. **43**, 1726 (2014).
- [5] O. Meroz, N. Elkabets, Y. Gelbstein. ACS Appl. Energy Mater. **3**, 2090 (2020).
- [6] A.A. Shabaldin, P.P. Konstantinov, D.A. Kurdyukov, L.N. Lukyanova, A.Yu. Samunin, E.Yu. Stovpiaga, A.T. Burkov. FTP **53**, *6*, 751 (2019). (in Russian).
- [7] L. Chen, Q. Zhang, Z. Guo, Z. Yan, K. Song, G. Wu, X. Wang, X. Tan, H. Hu, P. Sun, G.-Q. Liu, J. Jiang. Mater. Today Phys. **21**, 100544 (2021).
- [8] N.P. Stepanov, M.S. Ivanov. FTP **56**, *12*, 1103 (2022). (in Russian).
- [9] M.V. Vedernikov, P.P. Konstantinov, A.T. Burkov. Development of Automated Techniques of Measuring the Temperature Dependences of the Transport Properties of Thermoelectric Materials. VIII Int. Conf. on Thermoelectric Energy Conversion. Nancy, France (1989). P. 45.
- [10] G.A. Ivanov. FTT **5**, *11*, 3173 (1963). (in Russian).
- [11] V.M. Grabov. Materialy dlya termoelektrich. preobrazovatelej. Tez. dokl. III Mezhgos. seminara. SPb, Rossiya (1993). S. 42. (in Russian)
- [12] V.M. Grabov, A.S. Parakhin, L.S. Bagulin, O.N. Uryupin, Izv. RGPU im. A.I. Gertsena, **6**, *15*, 86 (2006). (in Russian).
- [13] V.A. Kulbachinskii, V.G. Kytin, P.M. Tarasov, N.A. Yuzeeva. FTT **52**, *9*, 1707 (2010). (in Russian).
- [14] S.A. Nemov, N.M. Blagih, M.B. Dzhafarov. FTP **48**, *8*, 1027 (2014). (in Russian).
- [15] N.P. Stepanov, A.A. Kalashnikov, O.N. Uryupin. FTP **55**, *7*, 586 (2021). (in Russian).
- [16] N.P. Stepanov. Optika i spektroskopiya **131**, *9*, 1219 (2023). (in Russian).

*Translated by I.Mazurov*