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PROPERTIES OF Se DOPED Bi_2Te_3 BASED MATERIAL

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Abstract

The possibility of producing high quality Bi_2Te_{3-x} single crystal doped with Se using the Bridgman method was examined. Single crystal was successfully prepared. The $Bi_2Te_{2.7}Se_{0.3}$ single crystal in 11 mm × 80 mm size was grown. Measurements of the thermoelectric properties indicate that bulk sample was of n-type conductivity, suggesting that major conductivity carriers were electrons. The resistivity (ρ), conductivity (k) and Seebeck coefficient (S) were measured simultaneously in temperature range from 40°C to 320°C. The obtained result of Seebeck coefficient (S) and resistivity (ρ) were presented in our investigation earlier. The obtained empirical formula does not deviate from the given compound formula.

***Keywords**: single crystal, semiconductor, Bridgman method, doping, thermoelectric*

1. INTRODUCTION

Thermoelectric materials are attracting attention because of their ability to directly convert heat into electricity. Bismuth tellurides (Bi_2Te_3) are important thermoelectric materials used to convert heat into electricity and vice versa. The application of thermoelectric devices requires materials that exhibit superior thermoelectric performance [1]. Single crystals of bismuth–tellurium semiconductor compounds represent one of the most important classes of thermoelectric materials due to their excellent electrical and thermal properties. Among them, compounds belonging to the Bi–Te system, such as Bi_2Te_3 and its selenium-containing solid solutions, occupy a prominent position because of their high thermoelectric figure of merit (ZT) in the temperature range around room temperature. In addition to their application in thermoelectric coolers and power generators, these materials have attracted considerable attention in recent years as topological insulators, exhibiting conductive surface states while maintaining an insulating bulk [2-5]. Selenium is commonly introduced into the crystal lattice as an isovalent dopant substituting tellurium atoms. Such substitution influences the electronic band structure, suppresses the formation of antisite defects, and allows more precise control of the electrical conductivity. At appropriate selenium concentrations, an increase in the bulk electrical resistivity and an improvement in carrier mobility can be achieved, which are particularly important for thermoelectric and

electronic applications [2,4]. The growth of high-quality Bi–Te single crystals is most commonly performed using the Bridgman (Bridgman–Stockbarger) crystal growth technique. This method is based on the controlled directional solidification of a melt through a well-defined temperature gradient, enabling the formation of crystals with a preferred crystallographic orientation and a low density of structural defects. Crystal growth may be performed either using a seed crystal or by spontaneous nucleation. In the spontaneous nucleation approach, crystallization begins with the spontaneous formation of one or several nuclei at the bottom of the ampoule. Under suitable thermal conditions, one nucleus gradually becomes dominant and develops into a single crystal. Although spontaneous nucleation generally provides less control than seeded growth, careful optimization of the pulling rate and temperature gradient makes it possible to obtain high-quality single crystals suitable for scientific investigations [6,7]. The quality of the obtained single crystal is strongly influenced by several processing parameters, including the crystallization rate, temperature gradient, purity of the starting elements, and vacuum conditions during synthesis. Improper growth conditions may result in impurity segregation, crack formation, secondary-phase inclusions, and an increased density of dislocations. In selenium-doped Bi–Te crystals, particular attention must be paid to the distribution of selenium along the crystal because the segregation coefficient may lead to compositional variations during solidification. Consequently, the Bridgman technique remains one of the most reliable and widely used methods for producing large, high-quality single crystals intended for detailed structural, electrical, and thermoelectric characterization [5-9]. The subject of this study is the synthesis of selenium-doped Bi–Te single crystals by spontaneous nucleation using the Bridgman crystal growth technique. Following crystal growth, characterization was carried out to evaluate the influence of selenium doping and growth conditions on the crystal quality, microstructure, and the potential application of the material in thermoelectric and electronic devices.

2. EXPERIMENTAL

Single crystal ingot of Bi_2Te_3 doped with selenium was synthesized using the Bridgman method at the maximum temperature of about 700ºC. High purity elements (5 N) were used as the source material. Tellurium (Sigma – Aldrich, 99.999%), bismuth (Sigma – Aldrich, 99.999%) and selenium (Alfa Aesar, 99.999%) were taken in a certain proportion. The temperature gradient was 2ºC/mm in the zone of heating and 5ºC/mm in the zone of cooling. The ingot was grown at the speed of 2.2 mm/h. Measurements of thermoelectric properties of single crystal was carried out by home-made impedance meter based on the ″Lagre ΔT method″ [10] with temperature range from 40 to 320°C. Home-made impedance meter simultaneously measured all three thermoelectric parameters, Seebeck coefficient, conductivity and resistivity. The measurement process was performed in vacuum of 10^{-2} to 10^{-3} Pa on sample with a height of about 11 mm and a diameter of 80 mm and took at least 15 hours. The measurement principle is such that the sample in a vacuum is heated on the hot side to a temperature determined by the measurement program. Once this temperature is reached, the heater is turned off, and the measurements begin. These measurements are taken during the cooling process of the sample at one-minute intervals until the sample cools down below 40°C. The entire process is automated, and the measurement results are recorded on a computer. It is

essential that the upper and lower surfaces of the sample are plane-parallel to ensure optimal contact between the sample and the hot and cold sides of the system.

3. RESULTS AND DISCUSSION

Bismuth, tellurium and selenium are merged in a stoichiometric ratio of 2:3, namely with given compound formula of $Bi_2Te_{2.7}Se_3$. The results of conductivity (k) in the temperature range from 40 to 320°C for a bulk n-type single crystal is given in Figure 1.

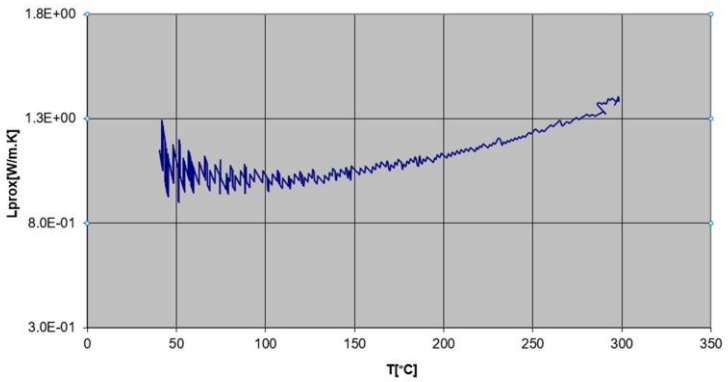


Figure 1. *Temperature dependence of conductivity for sample $Bi_2Te_{2.7}Se_3$*

The measured average thermal conductivity of the $Bi_2Te_{2.7}Se_{0.3}$ single crystal, grown by the Bridgman method with spontaneous nucleation, is 1.069 $Wm^{-1}K^{-1}$ over the temperature range of 40–320 °C (313–593 K). This value is consistent with those reported in the literature for high-quality n-type $Bi_2(Te,Se)_3$ thermoelectric materials, where the total thermal conductivity typically ranges from approximately 0.9 to 1.4 $Wm^{-1}K^{-1}$, depending on the chemical composition, carrier concentration, crystal orientation, and crystalline quality [11].

4. CONCLUSION

Possibility of producing high quality $Bi_2Te_{2.7}Se_3$ single crystal using the Bridgman method was examined. As part of research on the influence of selenium as dopant on bismuth telluride, a successful synthesis of single crystal was carried out. Bulk sample was characterized by Seebeck coefficient (S), thermal conductivity (κ) and electrical resistivity (ρ) measurements, as a function of temperature in the range of 40 - 320°C by a home made impedance meter. Figure of merit was calculated using measured values for electrical resistivity, Seebeck coefficient and thermal conductivity. The prepared single crystal has a figure of merit (Z) of 4.86 x 10^{-3} K^{-1} at 40°C. Values of ZT are about 1.0 at 27°C for commercialized p and n type of bismuth telluride ingots. T is absolute temperature. Conventional Bi_2Te_3 based materials have a peak ZT of about 0.25 at

250°C [12]. The obtained empirical formula does not deviate from the given compound formula.

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REFERENCES

[1] E. Požega, S. Bernik, D. Božić, S. Magdalinović, M. Đukić, J. Gligorijević Sokolović, R. Rajković, Proceedings of 56th International october confeernce on Mining and Metallurgy, 22-25 October Bor Lake, Serbia, 2025, 502-505.
[2] S.K. Kushwaha, Q.D. Gibson, J. Xiong, I. Pletikosić, A.P. Weber, A.V. Fedorov, N.P. Ong, T. Valla, R.J. Cava, J. Appl. Phys., 115 143708 (2014) 1-9.
[3] Y. Pan, D. Wul, J.R. Angevaare, H. Luigjes, E. Frantzeskakis, N. de Jong, E. van Heumen, T.V. Bay, B. Zwartsenberg, Y.K. Huang, M. Snelder, A. Brinkman, M.S. Golden, A. de Visser, New J. Phys. 16 123035 (2014) 1-16.
[4] D. Perrin, M. Chitroub, S. Scherrer, H. Scherrer, J. Phys. Chem. Solids, 61 (2000) 1687–1691.
[5] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys., 82 (4) (2010) 1-25.
[6] J. P. Garandet, Prog. Cryst. Growth Charact. Mater., 38 (1999) 133–159.
[7] E. Požega, S. Bernik, S. Marjanović, A. Petrović, I. Svrkota, A. Stojić, D. Simonović, Sci. Sintering, 56(2024) 395-403.
[8] E. Požega, N. Vuković, L. Gomidželović, M. Janošević, M. Jovanović, S. Marjanović, M. Mitrović, Sci. Sintering, 55 (1) (2023) 57-70.
[9] E. Požega, S. Marjanović, N. Vuković, L. Gomidželović, M. Mitrović, M. Janošević, D. Adamović, Sci. Sintering, 55 (3) (2023) 331-338.
[10] S. Bernik, M. Pribošek, Proceedings of the 49th International conference on Microelectronics, Devices and Materials, 25-27 September, Kranjska Gora, Slovenia, 2013, 121–126.
[11] X. Yan, B. Poudel, Y. Ma, W.S. Liu, G. Joshi, H. Wang, Y. Lan, D. Wang, G. Chen, Z.F. Ren, Nano Lett., 10 (9) (2010) 3373–3378.
[12] H. Mun, K.H. Lee, S.J. Kim, J.Y. Kim, J.H. Lee, J.H. Lim, H.J. Park, J.W. Roh, S.W. Kim, Mater., 8 (2015) 959-965.