ELECTRONIC TRANSPORT PROPERTIES OF THE $Bi_{0.5}As_{1.5}Te_{2.98}Se_{0.02}$ SINGLE CRYSTAL: PART I

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Abstract

Bismuth telluride thermoelectric material with the composition of $Bi_{0.5}As_{1.5}Te_{2.98}Se_{0.02}$ was studied in this work. During the experiment, the values of conductivity (σ), resistivity (ρ), Hall coefficient (R_H), magnetic resistance (ΔR) and vertical/horizontal resistance ratio (α) were examined using a Hall Effect system based on the Van der Pauw method. The Hall Effect was measured at temperature of liquid nitrogen with silver contacts with an applied magnetic field strength of 0.37 T at different current intensities. Measurements of the Hall effect and thermoelectric properties at currents of 0.05 and 0.1 mA indicate that bulk sample was p-type conduction, suggesting that major conductivity carriers were holes. At current of 0.5 mA Hall coefficient was negative.

Keywords: *electronic transport properties, Hall and Van der Pauw method, single crystal*

1 INTRODUCTION

Thermoelectric materials play a role in the primary power generation and energy conservation. The Seebeck and Peltier effects are used to achieve the thermoelectric power generation and thermoelectric cooling, respectively. Thermoelectric effect is a reversible cross-coupling effect between the electrical and thermal transport.

The main goal of thermoelectric materials usage is an energy conversion. There are thermoelectric materials that are used for direct energy conversion. As early as 1963, the scientists discovered that the most favorable semiconductor thermoelectric materials for direct energy conversion are materials with a relatively large energy gap, ranging from about 0.6 to ~ 2.5 eV [1]. There are two types of materials for converting the sun energy into heat energy. The first group includes materials that operate at temperatures below 100°C. And in the second group are materials whose operating temperature is above 300°C. The number of semiconductor materials is very large.

In order to evaluate the thermoelectric materials performance, the energy conversion efficiency of thermoelectric devices is evaluated by a figure of merit, ZT *[K^{-1}]*.

The figure of merit (ZT) is defined as:

$$ZT = \frac{\sigma\, S^2}{\kappa} * T \quad (1)$$

where T is the temperature, S is the Seebeck coefficient, σ is the electronic conductivity and k is the total thermal conductivity which is the sum of electronic (k_e) and lattice thermal (k_L) conductivities [2]. The performance of thermoelectric materials is quantified by a dimensionless thermoelectric figure of merit, ZT, which is defined by the

Seebeck coefficient, electric conductivity, and thermal conductivity. The challenge to create the high ZT thermoelectric materials lies in achieving simultaneously high σ, high S, and low κ. There is a strong correlation of these three parameters.

Great efforts have been devoted to the research of thermoelectric materials.

Thermoelectric (TE) materials can play an important role in reducing the carbon emission by converting waste heat into electricity [3]. Bismuth telluride and its alloys are the best-known TE materials for the ambient temperature applications [4-7].

This work is focused on the electronic transport properties of $Bi_{0.5}As_{1.5}Te_{2.98}Se_{0.02}$ single crystal. Herein, the As-doping effects on electronic transport properties of single crystal bulk are reported.

2 EXPERIMENTAL

Single crystal ingot of the $Bi_{0.5}As_{1.5}Te_{2.98}Se_{0.02}$ was synthesized using the Bridgman method at the maximum temperature of about 600ºC by spontaneous nucleation. High purity elements (5 N) were used as the source material. Bismuth (Sigma – Aldrich, 99.999%), arsenic (Koch-Light Laboratories Ltd Colnbrook Bucks England, 99.999%), Tellurium (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.

The Hall effect measurements were conducted using the Hall Effect Measurement System Ecopia HMS-3000 at the Faculty of Technical Sciences, University of Novi Sad in Serbia.

Software for the Hall Effect measurement system (Ecopia, HMS-3000) automatically calculated conductivity, resistivity, A-C cross Hall coefficient, B-CD cross Hall coefficient, magnetic resistance and vertical/horizontal resistance ratio. Calculations were done on the basis of voltage, obtained by the Van der Pauw laws, and input data was entered into the software (sample thickness *D*, current intensity *I*, the magnetic induction of permanent magnet *B*). The measured samples were cleaned in acetone before they are used for measurements.

3 RESULTS AND DISCUSSION

Samples used for the Hall effect measurements were prepared to be in the form of thin disc cut perpendicular to the long axis of a single crystal ingot. All samples were carefully inspected for cavities and scratches and polished if necessary. All measurements were carried out at temperature of liquid nitrogen with silver contacts. The source of magnetic field, applied perpendicular to the Hall element, was a permanent magnet of 0.37 T. The Hall effect measurements were done to obtain the electronic transport properties.

Table 1 *Results of the Hall and Van der Pauw method for sample 5/6 (⊥) at temperature of liquid nitrogen with silver contacts*

Current intensity *I* [mA]	Conductivity σ [1/Ωcm]	Resistivity ρ [Ωcm]	A-C Cross Hall coefficient R_{H1} [cm^3/C]	B-D Cross Hall coefficient R_{H2} [cm^3/C]	Magnetic resistance ΔR [Ω]	Vertical/ Horizontal resistance ratio α
0.05	$1.175x10^2$	$8.507x10^{-3}$	$3.079x10^1$	$1.662x10^0$	$3.885x10^{-2}$	$-5.527x10^{-1}$
0.1	$5.670x10^2$	$1.764x10^{-3}$	$5.045x10^0$	$1.207x10^0$	$8.538x10^{-3}$	$-1.614x10^{-1}$
0.5	$7.516x10^2$	$1.330x10^{-3}$	$-4.399x10^{-1}$	$-2.052x10^0$	$1.628x10^{-3}$	$2.744x10^{-1}$

The electronic transport properties of the $Bi_{0.5}As_{1.5}Te_{2.98}Se_{0.02}$ single crystal were measured. The results of electronic transport properties i.e. conductivity, resistivity, A-C cross Hall coefficient, B-CD cross Hall coefficient, magnetic resistance and vertical/horizontal resistance ratio for the studied sample 5/6 (⊥) are given in Table 1.

Sample, tested by the Hall and Van der Pauw method, was cut from a part of ingot normally to the crystallization direction (⊥). In the following, this sample will be referred to as 5/6 (⊥). Sample 5/6 (⊥) of circular cross-section is 1.55 mm thick.

Measurements were made at currents of: 0.05; 0.1 and 0.5 mA. The conductivity of sample is ranged from 1.175×10^2 to 7.516×10^2 1/Ωcm. The resistivity decreased with increasing current intensity. The values of the Hall coefficient at current intensity of 0.05 and 0.1 mA are positive, indicating that sample is of a p-type and that the majority of charge carriers are holes. For the current intensity of 0.5 mA, the value of the Hall coefficient is negative, indicating that the sample is n-type and that the majority of charge carriers are electrons.

4 CONCLUSION

This work is the result of testing the properties of an arsenic-doped bismuth telluride semiconductor monocrystalline compound. The Hall and Van der Pauw methods were used for material characterization. The electrical properties of this crystal were measured and the conductivity, resistivity, A-C cross Hall coefficient, B-CD cross Hall coefficient, magnetic resistance and vertical/horizontal resistance ratio were observed. The arsenic-doped bismuth and tellurium bulk monocrystal was successfully synthesized by the Bridgman method.

After added a small amount of As-doping on Bi sites, the electronic transport properties could not be enhanced. This investigation has paved a way for further development and characterization of thermoelectric materials science.

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