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Research Article

Synthesis and Study of Physical Properties of New Single Crystals of $(Bi_2Te_3)_{1-x}La_x$ Solid Solution

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Abstract

In the present study, bismuth telluride (Bi_2Te_3) was selected as the base material due to its well-known thermoelectric characteristics. This semiconductor compound plays a crucial role in applications such as energy conversion, cooling technologies, and waste heat recovery systems. Lanthanum is a rare-earth element. To enhance its functional properties, lanthanum (La) was introduced into the Bi_2Te_3 matrix, forming $(Bi_2Te_3)_{1-x}La_x$ solid solutions. It is an interesting and promising area of research in the field of obtaining single-crystal thermoelectric materials. The investigation of such doped single crystals represents a promising direction for improving thermoelectric efficiency. Lanthanum (La) has been widely employed as a dopant to optimize carrier concentration, modify the crystal lattice, and improve the thermoelectric performance of Bi_2Te_3-based materials. A detailed analysis of the $(Bi_2Te_3)_{1-x}La_x$ system was carried out, including the construction of phase diagrams. It was established that within the composition range $x = 0.01–0.05$, a solid solution region based on Bi_2Te_3 exists at room temperature. Additionally, a eutectic interaction between Bi_2Te_3 and La was identified at approximately 15 at.% La with a temperature close to 440 °C. Lanthanum doping resulted in measurable changes in the physical properties of Bi_2Te_3 single crystals. The results demonstrate that lanthanum incorporation yields single crystals with enhanced thermoelectric and galvanomagnetic properties, making them attractive for advanced material applications.

Keywords: microsolidity, solid solution, density, single crystal, thermoelectric, photovoltaic, optics, electrical converter

1. Introduction

The rapid progress of modern technologies has significantly increased the demand for novel single-crystal materials. Such materials are widely utilized in semiconductor devices, optoelectronics, photovoltaics, and various branches of applied science.

However, the fabrication of high-quality single crystals remains a complex and resource-intensive process. High synthesis temperatures are generally required for crystal growth. It requires elevated temperatures, strict control of growth conditions, extended processing time, and a high degree of purity. Single crystals are often sensitive to crystal defects and mechanical stresses during fabrication. They are susceptible to structural defects and external mechanical stresses during crystal growth. Monocrystals take a very long time to grow, which increases the production costs of the resulting product. Even minor structural imperfections can adversely affect the performance of the final material.

Bismuth telluride (Bi_2Te_3) is considered one of the most efficient thermoelectric materials currently available. It is formed by combining bismuth and tellurium in a stoichiometric ratio and possesses a rhombohedral crystal structure. Bismuth telluride is commonly used in thermal power converters, cooling systems, and energy recovery. At the same time, it is more widely used in thermoelectric conductors [1], [2], [3]. This structural feature enables its modification through doping with rare-earth elements, which has been reported to improve the thermoelectric performance of Bi_2Te_3-based materials. Previous studies have demonstrated that rare-earth doping can effectively modify the crystal structure and improve the thermoelectric performance of Bi_2Te_3-based materials [4], [5], [6], [7], [8]. The chemical composition of bismuth telluride is as follows: it is a stoichiometric compound consisting of two bismuth atoms and three tellurium atoms. The crystal structure of this material belongs to the rhombohedral class. This structure helps it to obtain promising thermoelectric materials from rare-earth elements, as well as multicomponent phases obtained on their basis. One of the key advantages of Bi_2Te_3 is its ability to exhibit both p-type and n-type conductivity [3]. It combines relatively high electrical conductivity with low thermal conductivity, which is essential for efficient thermoelectric conversion [9]. Taking advantage of these properties, it is used in thermoelectric generators and thermoelectric cooling systems.

In addition, the fact that this crystal has a thermoelectric effect makes its application in the field of electronics indispensable. Due to the Seebeck effect, Bi_2Te_3 can directly convert thermal energy into electrical energy [3]. Its high Seebeck coefficient and figure of merit (ZT) make it a leading material for thermoelectric applications [9]. The Bi_2Te_3 crystal has a high Seebeck coefficient, meaning that a strong electric field is generated when a temperature difference is applied from one side to the other.

2. Materials and Methods

To synthesize alloys of the $(Bi_2Te_3)_{1-x}La_x$ system, the Bi_2Te_3 compound was first synthesized. The alloys in the system were synthesized from elements with the following purities: Bi - 99.999%, Te - 99.999%, La - 99.98%. To conduct a comparative analysis of the obtained single crystal, 1%, 2%, 3%, and 5% La were used. At this time, the mass of the single crystal, Bi_2Te_3 = 417.96 + 382.8 = 800.76 g mol^{-1}, and the mass of the lanthanum, La = 138.91 g, were used.

The mass ratios of the newly purchased monocrystals were as follows:

- 99% Bi_2Te_3 + 1% La = 792.7524 + 1.3891 = 794.1415 g

Bi_2Te_3 = 1.9965 g
La = 0.0035 g

- 97% Bi_2Te_3 + 3% La = 776.7372 + 4.1673 = 780.9045 g

Bi_2Te_3 = 1.9819 g
La = 0.0181 g

- 95% Bi_2Te_3 + 5% La = 760.722 + 6.9455 = 767.6675 g

Bi_2Te_3 = 1.9819 g
La = 0.0181 g

The alloy of the $(Bi_2Te_3)_{1-x}La_x$ system was synthesized from the Bi_2Te_3 compound and the La element in quartz ampoules with air sucked in to a pressure of 0.133 Pa at a temperature range of (700−1000) ^{0}C. The synthesized sample was thermally treated at 500 ^{0}C for 200 hours to bring it to equilibrium. Equilibrium $(Bi_2Te_3)_{1-x}La_x$ solid solution alloys were studied using physicochemical analysis methods.

X-ray diffraction analysis of the obtained alloys was performed on a D2 PHASER X-ray diffractometer. In this case, CuKα radiation and a Ni filter were used as the anode. Microstructural analysis was performed using a MIM-8 microscope. Density was determined by the pycnometric method. Toluene was used as the filling solvent.

3. Results and Discussion

Figure 1 shows the phase diagram of the $(Bi_2Te_3)_{1-x}La_x$ system. The α phase corresponds to a Bi_2Te_3-based solid solution, which remains stable up to approximately 5 at.% La. At higher La concentrations, a two-phase region (α + M) is observed, indicating that the solubility limit of La has been exceeded and a La-rich secondary phase forms. A eutectic reaction occurs at approximately 15 at.% La and 440 °C.

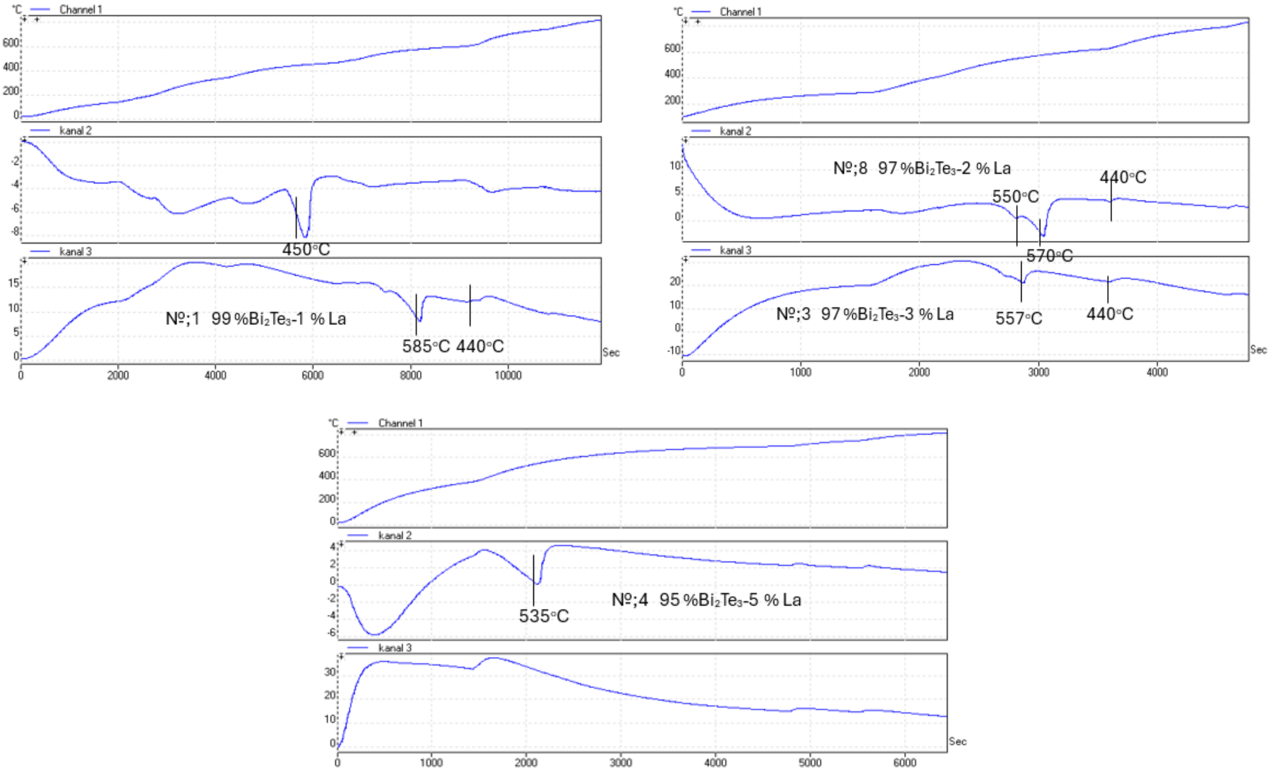

Figure 1. Diagrams of phase equilibria in the $(Bi_2Te_3)_{1-x}La_x$ systems.

The interpretation of the obtained diagrams can be explained as follows. The solvus line (solubility limit) indicates the maximum amount of a rare-earth element that can dissolve in Bi_2Te_3 at room temperature [5], [6], [10].

This interval depends on the radius and electronic structure of the La atom. The eutectic point indicates the lowest melting temperature (between 425–450°C) and the composition corresponding to this temperature (12–15 at.% La). This dependence shows that this temperature and composition depend on the strength of the interaction between the rare-earth element and Bi_2Te_3. The liquidus and solidus curves define the crystallization interval of the system.

The difference between these lines indicates the crystallization interval of the system. As the amount of rare-earth element increases, the melting temperature decreases (to the eutectic point).

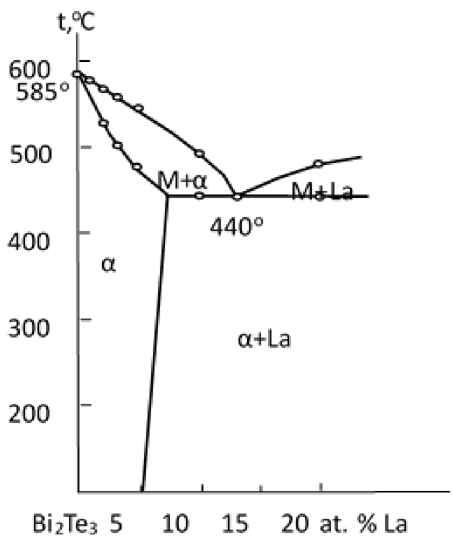

Figure 2. Graphical representation of selected physicochemical properties of the $(Bi_2Te_3)_{1-x}La_x$ (x = 0.01, 0.02, 0.03, and 0.05) alloy system.

X-ray diffraction analysis confirmed the formation of the Bi_2Te_3-based solid solution. The observed shift of diffraction peaks toward lower diffraction angles suggests a slight lattice expansion resulting from the incorporation of La into the Bi_2Te_3 crystal structure. Similar structural changes have been reported for other rare-earth-doped Bi_2Te_3 systems [4], [5], [7], [11], supporting the formation of a substitutional solid solution.

Table 1. Dependence of alloys in the $(Bi_2Te_3)_{1-x}La_x$ systems on composition, DTA, density, and microhardness.

Composition of phases, % $(Bi_2Te_3)_{1-x}(La)_x$ $(Bi_2Te_3)_{1-x}(La)_x$	Melting temperature, °C	Density, g/cm³	Microhardness, MPa
97% Bi_2Te_3-3% La	510.580	8.85	960
95% Bi_2Te_3-5% La	460.575	8.87	970
90% Bi_2Te_3-10% La	440.590	8.88	975
87% Bi_2Te_3-13% La	440	8.90	Eutectic
20% Bi_2Te_3-20% La	440.520	8.91	980

As shown in Table 1, the density increased slightly from 8.85 to 8.91 g cm^{-3} with increasing La concentration, while the microhardness increased from 960 to 980 MPa. These trends suggest that lanthanum incorporation modifies the crystal lattice and improves resistance to localized plastic deformation.

4. Conclusion

In the presented work, a new single crystal was obtained based on the combination of Bi_2Te_3 (bismuth telluride) and La (lanthanum). The modification of its structure through lanthanum doping successfully modified the crystal structure and physical properties.

The conducted study shows that the addition of lanthanum results in limited solubility within the Bi_2Te_3 matrix and leads to the formation of a eutectic-type system. Furthermore, a slight increase in density and microhardness is observed with increasing lanthanum content.

These observations are consistent with structural modifications induced by lanthanum incorporation into the Bi_2Te_3 lattice. The obtained materials demonstrate improved characteristics, indicating their suitability for applications in energy systems, cooling technologies, and advanced electronic devices.

Overall, the Bi_2Te_3–La system represents a promising direction for the development of high-performance thermoelectric materials and functional single crystals.

The Bi_2Te_3 + La compound has great potential in the field of thermoelectric materials development. The research allows optimizing electrical and thermal properties by modifying the nanostructure and crystal structure of the material. This research could lead to more effective applications in the fields of renewable energy, cooling systems, and energy recovery in the future. At the same time, it is possible to produce high-quality sensors, lasers, and other precision research instruments from monocrystals obtained in the fields of chemistry and medicine.

Author Contributions

All authors reviewed, edited, and approved the manuscript.

Conflict of Interest

The authors declare no conflicts of interest.

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Abbreviations

Bismuth Telluride (Bi_2Te_3), Lanthanum (La), X-ray Diffraction (XRD).

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