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STUDY OF THE Bi_2Te_3–Tb_2Te_3 SYSTEM

Fuad Sadigov, Zivar Hasanova, Rahila Mirzayeva, Rahman Fatullazade, Samina Sultanova, Zakir Ismailov
Baku State University, Baku, Azerbaijan,

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The interaction in the Bi_2Te_3-Tb_2Te_3 system was investigated using differential thermal, X-ray phase, microstructure analysis and microhardness measurement methods, and the phase diagram of the system was constructed.

It was found that the Bi_2Te_3-Tb_2Te_3 system is quasibinary. As a result of the peritectic reaction in the system, the $BiTbTe_3$ compound is formed. The electrophysical properties of the $BiTbTe_3$ compound have been studied. It has become clear that this compound is an "n"-type semiconductor, with a band gap of ~0.21 eV. It has been established that in the Bi_2Te_3-Tb_2Te_3 system, a ternary compound containing $BiTbTe_3$ is formed. The $BiTbTe_3$ compound crystallizes in the orthorhombic syngony of the stibnite type: a=12.25, b=12.66, c=4.76 Å.

Keywords: liquidus system, quasi-binary, eutectic, temperature, sections, phase, diagram.

INTRODUCTION

The efficiency of the production of new technology devices is inextricably linked with the development of semiconductor materials science [1-3]. At present, to meet the demand for semiconductor electronics, radio electronics and automation using known elementary or binary semiconductors does not always satisfy the requirements of technology, therefore, an intensive search for complex materials with a favorable combination of properties is given [4-6].

Rare earth chalcogenides and their complex phases are semiconductor materials with complex functional properties such as photovoltaic [7,8], thermoelectric [9-12], magnetic [13-15] and luminescent [16,17]. New phases obtained through chemical interactions based on compounds with complex physicochemical and physical properties can also be useful materials for applications. Therefore, the study of the Bi_2Te_3–Tb_2Te_3 system is of scientific and practical interest [18–21].

EXPERIMENTAL

During the synthesis of samples included in the Bi_2Te_3–Tb_2Te_3 system, high-purity starting materials were used. Thus, terbium metal of the TbM-1 brand with a purity level of 99.9%, bismuth (Bi) of the B-4 category, and tellurium (Te) of the same purity class were used in the experiment. These components were prepared with considerable care before starting the synthesis, and the synthesis process was planned taking into account their individual physicochemical properties.

First, each element or primary compound (e.g., binary components) was crushed into a fine powder. These powders were then weighed to the nearest 0.001 gram on an analytical

E-mail address: zakir-51@mail.ru

balance for accurate weighing. The prepared mixtures were filled into quartz ampoules with special heat resistance.

The air inside each ampoule was evacuated to a level of 10^{-3} mm of mercury, that is, the air was rarefied. This was done in order to prevent unwanted reactions in the presence of oxygen during the synthesis and to obtain compounds of high purity. The mouths of the ampoules were tightly heated using an oxygen-fuel flame and hermetically sealed.

The synthesis process was carried out in several stages. First, the elemental components were completely melted inside the ampoule at a temperature of 1600 K for 6 hours. At this high temperature, direct chemical reactions occur between the components and a homogeneous alloy is obtained. After this stage, the furnace was turned off and the alloy was cooled very slowly. Slow cooling conditions are important to ensure the formation of the desired phases and crystal structures in the sample.

It is worth noting that at every stage of the process – powdering, drawing, preparation of ampoules and synthesis – high standards of accuracy and purity were strictly observed. This approach plays an important role in ensuring both the chemical homogeneity of the alloys and the accuracy of subsequent physicochemical analyses.

Samples with a content of 60 mol% Tb_2Te_3 and higher were obtained as sinters. They were crushed again and turned into tablets. Alloys with a content of less than 60 mol% are compact, dark gray in color with a metallic luster. After synthesis, in order to achieve homogeneity of the alloy, it was additionally annealed at a temperature of 50-100 K below the solidus for 250 g.

RESULTS AND DISCUSSION

The obtained samples were subjected to detailed physicochemical studies. Based on the results obtained by the above methods, a phase diagram of the Bi_2Te_3–Tb_2Te_3 system was constructed (Figure 1).

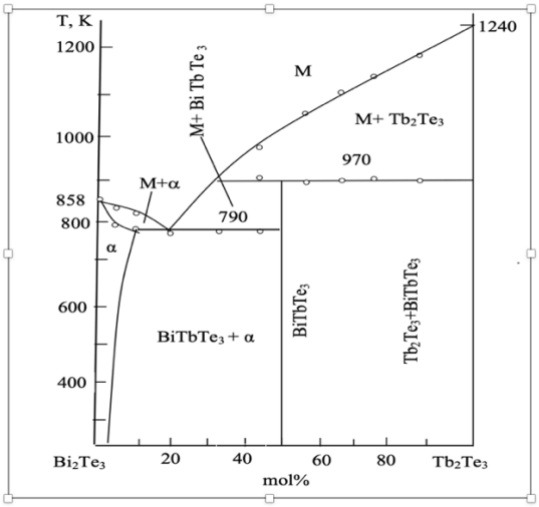

Figure 1. State diagram of the the Bi_2Te_3- Tb_2Te_3 system

As can be seen from the figure, the system is quasi-binary and eutectic. It is clear from the phase diagram of the Bi_2Te_3-Tb_2Te_3 system that the peritectic formation of the compound containing $BiTbTe_3$ in a 1:1 ratio occurs at a temperature of 970K.

$$M + Tb_2Te_3 \leftrightarrow BiTbTe_3$$

A solubility range of up to 3 mol.% has been found at 300K. $BiTbTe_3$ forms a eutectic with Bi_2Te_3 at 85 mol.%.

The compound $BiTbTe_3$, an α-solid solution based on Bi_2Te_3, forms a eutectic with 6 mol% Tb_2Te_3 which melts at 970 K. The solubility of Tb_2Te_3 in Bi_2Te_3 at 30K is 3mol%. X-ray diffraction patterns of $BiTbTe_3$, powders have been indexed to show that the compound

crystallizes in an orthorhombic syngony with a Sb_2S_3-type structure. The unit cell parameters are a=12.25, b=12.66, c=4.76 Å.

This process is important for studying the interactions of elements in materials and for more accurately determining their nature. (Table 1)

Table 1. Composition expression of Bi_2Te_3 –Tb_2Te_3 system alloys

	Composition mol %		Composition, mol %		
N	Tb2Te3	Bi2Te3	Tb	Bi	Te
1.	1	99	0,0041	0,51	0,478
2.	2	98	0,0083	0,512	0,479
3.	3	97	0,0125	0,50	0,479
4.	5	95	0,02	0,498	0,480
5.	10	90	0,04	0,474	0,483
6.	20	80	0,085	0,426	0,488
7.	25	75	0,107	0,401	0,490
8.	33,3	66,7	0,144	0,360	0,495
9.	40	60	0,17	0,326	0,498
10.	50	50	0,22	0,275	0,504
11.	60	40	0,26	0,222	0,509

During the conducted research, the alloys were tested for their resistance to various chemicals. It was found that these alloys remain stable when exposed to organic solvents, including benzene and toluene, as well as water and air, and no chemical changes occur. However, mineral acids and alkaline media affect them, causing structural damage and decomposition. This property is important in assessing the chemical stability of alloys.

In order to obtain a homogeneous structure, the samples were subjected to thermal annealing at a temperature range of 500–600 K for 200 hours. This thermal process creates conditions for possible crystallization and phase stabilization in the alloy structure. After thermal treatment, the samples were gradually cooled to room temperature and then subjected to extensive physicochemical analyses.

This approach is important in terms of studying the stability of the obtained materials and their behavioral characteristics under various conditions.

Differential thermal analysis (DTA) results showed that all thermal effects observed during heating are endothermic in nature and are accompanied by reversible processes. Two main heating effects were noted in the obtained thermograms. Based on the principle of compatibility, these effects were analyzed and it was found that a new compound containing $BiTbTe_3$ is formed as a result of the combination of components in the system in a 1:1 molar ratio. This new phase is formed as a result of a peritectic transformation reaction occurring at a temperature of 1050 K. Such a transformation reaction allows for a more accurate analysis of changes in the composition of the system and the sequence of phase formation.

The results of X-ray phase analysis (XRF) also confirmed this finding. Thus, the reflections obtained in the X-ray diffraction spectrum of the sample synthesized in a 1:1 ratio of components differed sharply from those of the initial components. This proves that a new crystalline phase was formed in that ratio.

At the same time, according to the results of microstructural analysis (MSA), all samples, except for those with 0–5 and 50 mol% content, were found to be two-phase. These observations support the results of both DTA and RFA analyses and indicate the presence of a multiphase structure in the system.

The comprehensive study of such multiphase systems allows for more extensive and reliable information on the structural properties and physical behavior of alloys. Such information serves as an important scientific basis for the analysis of future application areas and functional properties of the material.

The analyses conducted for the determination of microhardness showed that the samples were surface polished and polished according to the MQA methods. 8-10 marks were made on the samples using a diamond pyramid using the PMT-3 device and the diameter of

the obtained rhombic marks was measured and the microhardness was determined using the formula H_(μ)=(1.852•D)/d². The results showed that the hardness values obtained in the 1:1 ratio are significantly different. These findings confirm the results of DTA, RFA and MQA analyses. This once again proves the formation of a new phase containing $BiTbTe_3$ in the system. Such analyses provide more detailed information about the physical properties and structural changes of the alloys. An incongruent compound containing $BiTbTe_3$ is formed by a peritectic transformationreaction in a 1:1 ratio of the components in the system.

$$M + Tb_2Te_3 \rightleftarrows BiTbTe_3(970\ K)$$

In order to determine the solid solution limits, additional alloys were synthesized using 1 mol% Tb_2Te_3 and subjected to 350 h of heat treatment at appropriate temperatures. According to the results of microstructural analysis, the solubility limits for Tb_2Te_3 range from 3 mol% at 300K to 6 mol% at 830K.

The eutectic in the system is formed by a 3-phase nonvariant equilibrium reaction at 790K with a 5 mol % Tb_2Te_3 composition.

Electrophysical properties of the compound $BiTbTe_3$

It is already known from the literature that compounds of the $A_{2v}X_3$ and Ln_2X_3 (A_v–Sb, Bi; Ln–NTE; X–Se,Te) type are among the promising semiconductor materials and are widely used in the production of energy converters. The study of alloys obtained from solid solution domains formed on the basis of $A_{2v}Te_3$ compounds in the Tb-A_v-Te ternary system creates conditions for obtaining new materials with valuable physicochemical and electrophysical properties.

Since Bi_2Te_3 is a semiconductor material with a defect structure, it is necessary to study the temperature dependence of the electrical conductivity and thermoelectric coefficient of terbium and its ternary telluride alloys in the solid solution region based on it.

The temperature dependence of the specific electrical conductivity (σ) of the $BiTbTe_3$ compound is semiconducting up to about 450 K from room temperature (Figure 2). The ternary compound corresponds to impurity conductivity in this range, and above 500 K it exhibits intrinsic conductivity properties (Figure 2).

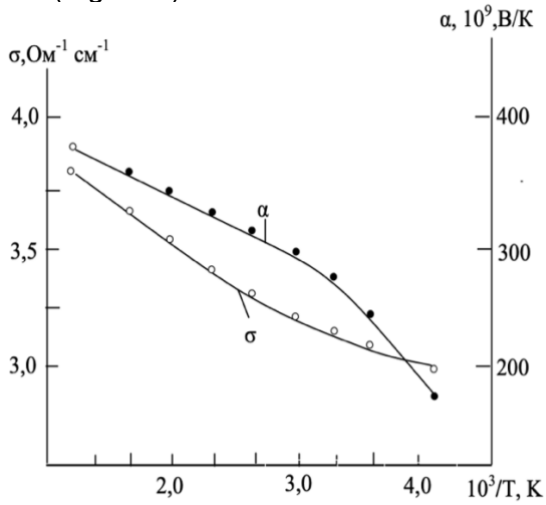

Figure 2. Temperature dependence of the electrical conductivity(σ) of the $BiTbTe_3$ compound

The calculated energy band gap (ΔE) for $BiTbTe_3$ is approximately 0.21 eV. At the same time, the variation of the thermoelectric coefficient (α) of the $BiTbTe_3$ compound with temperature is also demonstrated.

The figure shows that with increasing temperature, α increases. Later, its saturation is observed, and then a decrease occurs. While σ first decreases, then increases. Such an unusual feature suggests that the thermoelectric power variation is related to semiconductors with complex energy band structures. Based on this, it can be assumed that the newly formed

$BiTbTe_3$ compound also has a complex energy band structure and appears to be similar to the energy level structure of bismuth sesquitelluride [12-14]. Based on the thermoelectric power and Hall coefficients, the $BiTbTe_3$ compound was determined to be an "n"-type semiconductor.

CONCLUSION

1. The interaction in the Tb_2Te_3-Bi_2Te_3 system was investigated and a phase diagram of the system was constructed using differential thermal, X-ray phase, microstructure analyses, and microhardness measurement methods.
2. It has been found that the Tb_2Te_3-Bi_2Te_3 system is quasibinary. The $BiTbTe_3$ compound is formed as a result of a peritectic reaction in the system.
3. The electrophysical properties of the $BiTbTe_3$ compound have been studied. It has become clear that this compound is an "n" type semiconductor, with a band gap of ~0.21 eV.
4. It has been established that in the Bi_2Te_3-Tb_2Te_3 system, a ternary compound containing $BiTbTe_3$ is formed. The $BiTbTe_3$ compound crystallizes in the orthorhombic syngony of the stibnite type: a=12.25, b=12.66, c=4.76 Å.

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