

Synthesis and Properties of the Compound TbSbTe₃

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Abstract

Chemical interaction in the $\mathrm{Sb}_2\mathrm{Te}_3$ - $\mathrm{Tb}_2\mathrm{Te}_3$ system was studied using physicochemical analysis methods (differential thermal analysis, X-ray phase analysis, microstructural analysis, microhardness measurement and density determination). Based on the analysis results, a phase diagram of the $\mathrm{Sb}_2\mathrm{Te}_3$ - $\mathrm{Tb}_2\mathrm{Te}_3$ system was constructed. It was found that the $\mathrm{Sb}_2\mathrm{Te}_3$ - $\mathrm{Tb}_2\mathrm{Te}_3$ section is a quasi-binary section of the Tb-Sb-Te ternary system and belongs to the eutectic type. It is evident from the phase diagrams that in the $\mathrm{Sb}_2\mathrm{Te}_3$ - $\mathrm{Tb}_2\mathrm{Te}_3$ section, a new ternary incongruently melting compound of the TbSbTe $_3$ composition is formed by a peritectic reaction at a temperature of 980K with a component ratio of 1:1. According to the results of X-ray phase analysis, it was established that the TbSbTe $_3$ compound crystallizes in orthorhombic syngony with the lattice parameters: a =2.35, b=12.76, c=4.86 Å. The solubility of $\mathrm{Tb}_2\mathrm{Te}_3$ in $\mathrm{Sb}_2\mathrm{Te}_3$ is 3.0 mol.% at 300K, respectively. The electrophysical properties of the TbSbTe $_3$ compound have been studied. It has been shown that this compound is an «n»-type semiconductor, with a band gap of ~0.21eV.

Keywords: System; Analysis; Crystallization; Phase; Diagram; Temperature

Introduction

Modern scientific and technical progress is inextricably linked with the development of semiconductor technology [1-3]. The rapid development of the latter was the main stimulus for the search for complex semiconductor materials [4-6]. However, the growing need for semiconductor technology in materials is not yet fully satisfied due to the lack of materials with different combinations of optical, magnetic and electrophysical properties.

Chalcogenides of antimony of the composition $\mathrm{Sb}_2\mathrm{X}_3(\mathrm{X}\text{-Se},\ \mathrm{Te})$ and solid solutions based on them are used as a thermoelectric material in the manufacture of n-branches of thermoelectric devices [7,8]. Chalcogenides of rare earth elements and alloys based on them are promising compounds for the development of thermal materials [9-11]. Therefore, obtaining new materials based on them is an urgent task [12-15].

Experimental Part

The TbSbTe $_3$ compound is obtained by synthesizing the Sb $_2$ Te $_3$ - Tb $_2$ Te $_3$ compounds. Synthesis of the Sb $_2$ Te $_3$ - Tb $_2$ Te $_3$ - system. Terbium TbM-1 purity 99.9%, antibium grade (B-4) and Te, purity 99.999% were used for the synthesis of the samples.

The synthesis mode was selected based on the physicochemical properties of the elemental components and binary compounds. The ligatures were first crushed and finely ground, weighed on an analytical balance with an accuracy of one part per thousand, and filled into quartz ampoules.

The ampoules were evacuated to a pressure of 10^{-3} mm.cv.st using a vacuum apparatus and their mouths were sealed by soldering using an oxygen gas flame. This was achieved by direct melting of the components in evacuated quartz ampoules at 1600K for 6 hours, followed by slow cooling when the furnace was turned off.

The ligatures were first crushed and ground into fine powder, weighed on an analytical balance to the nearest thousandth, and filled into quartz ampoules. The ampoules were evacuated to a pressure of 10^{-3} mm.cv.st using a vacuum apparatus, and the mouths were sealed by soldering using an oxygen gas flame.

Samples with a content of 60 mol% ${\rm Tb_2Te_3}$ 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, 250g were additionally annealed at a temperature 50-100K below the solidus. The obtained samples were subjected to detailed physicochemical studies.

To achieve homogeneity of the alloy after synthesis, it was additionally annealed at temperatures 50-100K below the solidus for 250g. The obtained samples were subjected to detailed physicochemical study. The heating and cooling curves of the alloys were recorded on a Termoksan, X-ray diffraction was performed on an X-ray diffractometer.

Differential thermal analysis alloys of the system were carried out on a TERMOSKAN-2 device with an accuracy of 3-5 °C, a chromel-alumel thermocouple, and calcined ${\rm Al_2O_3}$ served as the standard. Heating rate of 9 degrees/min. High-temperature differential thermal analysis was carried out on a device (HTDA) - 8m2 in an inert atmosphere using a B-B/Re thermal suspension, degreasing speed of 5rev/min.

X-ray phase analysis was performed on an X-ray instrument of the D2 PHASER model through the use of $\text{CuK}\alpha$ radiation with a Ni filter. The micro-structural analysis of alloys was carried out using an MIM-8 microscope. In the study of alloy microstructure, an etchant of composition 1 N HNO3 + HF = 2:1 was used, the etching time was 20s. The microhardness of the phases was measured on a PMT-3 instrument with an accuracy of 5%, and the density of the samples was determined by the pycnometric method.

Results and Discussion

Based on the results obtained by the above methods, a phase diagram of the Sb_2Te_3 - Tb_2Te_3 system was constructed (Figure 1).

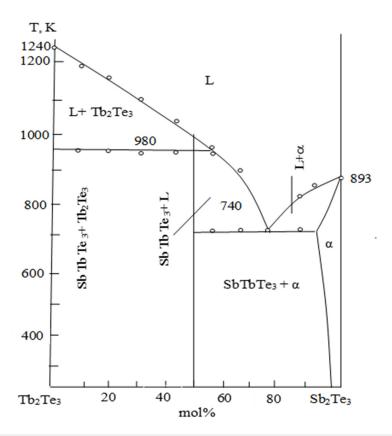


Figure 1: State diagram of the Sb₂Te₃- Tb₂Te₃ system.

As can be seen from the figure, the system is quasi-binary and eutectic. It is clear from the phase diagram of the $\mathrm{Sb_2Te_3}$ - $\mathrm{Tb_2Te_3}$ system that the peritectic formation of the compound containing $\mathrm{TbSbTe_3}$ in a 1:1 ratio occurs at a temperature of 980K.

$$L + Tb_2Te_3 \leftrightarrow TbSbTe_3$$

A solubility range of up to 3mol.% has been found at 300K. TbSbTe $_3$ forms a eutectic with Sb $_2$ Te $_3$ at 82mol.%. The solubility of Tb $_2$ Te $_3$ in Sb $_2$ Te $_3$ at 300K is 3mol%.

X-ray diffraction patterns of TbSbTe₃ powders have been indexed to show that the compound crystallizes in an orthorhombic

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syngony with a Sb_2S_3 -type structure. The lattice parameters are a=12.35, b=12.76, c=4.86Å.

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

Table 1: Expression of the compositions of Sb2Te3 -Tb2Te3 system alloys.

	Composition, mol%		Composition, mol%		
N	Tb ₂ Te ₃	Sb ₂ Te ₃	Tb	Sb	Те
1.	1	99	0,0042	0,517	0,478
2.	2	98	0,0083	0,512	0,479
3.	3	97	0,012	0,507	0,470
4.	5	95	0,021	0,498	0,480
5.	10	90	0,042	0,474	0,483
6.	20	80	0,08	0,426	0,488
7.	25	75	0,11	0,401	0,491
8.	33,3	66,7	0,14	0,360	0,495
9.	40	60	0,17	0,326	0,499
10.	50	50	0,22	0,275	0,504
11.	60	40	0,27	0,223	0,510

The effect of various reagents on the alloys was studied. It was found that they are not affected by "organic solvents" - benzene, toluene, as well as water and air, but are decomposed by the action of mineral acids and alkalis. To achieve homogeneity of the samples, they were annealed at a temperature of 500-600K for 200 hours.

The thermally treated samples were cooled to room temperature

and then subjected to complex physicochemical studies. This process is important for studying the stability of the alloy and its behavior in various conditions, as well as for more accurately determining the structure and properties of the substance.

According to the DTA (differential thermal analysis) results of the alloys, all effects observed in the heating curves are endothermic and reversible.

The results of the X-ray diffraction analysis showed that the X-ray reflections of the alloy obtained in a 1:1 ratio of the components differ sharply from those of the original components. This indicates the formation of a new phase in the system in a 1:1 ratio. This finding confirms the DTA results. According to the MQA results, all samples, except for the samples with a content of 0-5 and 50 mol%, are two-phase. This also supports the DTA and X-ray diffraction results. The study of such multiphase systems provides deeper information about the structural and physical properties of the alloy.

Electrophysical properties of the compound TbSbTe,

Since $\mathrm{Sb_2Te_3}$ 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 TbSbTe₃ compound is semiconducting up to about 450K above room temperature (Figure 2). The ternary compound corresponds to impurity conductivity in this range, while above 500K it exhibits intrinsic conductivity properties.

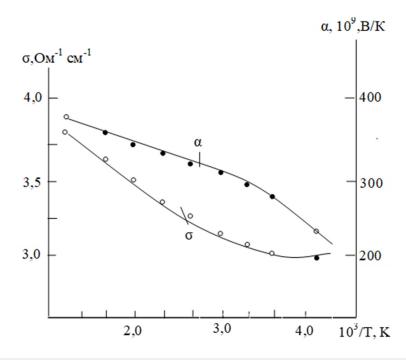


Figure 2: Temperature dependence of the electrical conductivity (a) of the TbSbTe, compound.

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The figure shows that α increases with increasing temperature. Later, its saturation is observed, and then a decrease occurs. While σ first decreases, then increases.

This 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 ${\rm TbSbTe}_3$ compound also has a complex energy band structure and appears to be similar to the energy level structure of bismuth sesquitelluride [16-18].

The calculated energy band gap (ΔE) for TbSbTe $_3$ is approximately 0.21eV. At the same time, the variation of the thermoelectric coefficient (α) of the TbSbTe $_3$ compound with temperature is also demonstrated. Based on the thermoelectric power and Hall coefficients, the TbSbTe $_3$ compound was determined to be an «n»-type semiconductor.

Conclusion

- The interaction in the Tb₂Te₃-Sb₂Te₃ system was investigated and a phase diagram of the system was constructed using differential thermal, X-ray phase, microstructural analyses, and microhardness measurement methods.
- It has been found that the Tb₂Te₃-Sb₂Te₃ system is quasi-binary.
 As a result of a peritectic reaction in the system, the TbSbTe3 compound is formed.
- 3. The electrophysical properties of the $TbSbTe_3$ compound have been studied. It has been shown that this compound is an «n»-type semiconductor, with a band gap of $\sim 0.21eV$.

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