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SYNTHESIS AND THERMOELECTRIC PROPERTIES of $TuSnSe_2$ COMPOUND

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In this research work, the interaction of the SnSe-TuSe system was studied, and as a result of complex physicochemical analyses, the solubility region of TuSe in SnSe (75-100%) was determined. It was also determined that the $TuSnSe_2$ compound was obtained in a 1:1 ratio of its components, and a phase diagram of the system was constructed. X-ray structure and differential thermal analysis of the sample showed that this compound crystallizes in a hexagonal syngony. Some kinetic parameters of the triple compound $TuSnSe_2$ were determined at room temperature. Electrical conductivity (σ), thermo electromotive force (e.m.f.) (α) and thermal conductivity (χ) were studied in the temperature range T=300÷800K. In order to determine the variation in the charge carrier scattering mechanism the temperature dependences of the Hall mobility and electrical conductivity of this compound were also investigated. Based on the sign of the thermo-electromotive force and the Hall coefficient, it was determined that the conductivity in this compound is n- type. Based on the obtained results, it was determined how the concentration of charge carriers and the Hall mobility changed. Anomaly changes are observed in the temperature dependence of the electrical conductivity, thermoelectric potential and total thermal conductivity in the temperature interval T=460÷500K.
Keywords: *Electrical conductivity; Triple compound; Hexagonal syngony; Hall mobility*
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1. INTRODUCTION

Interest in the study of semiconductor compounds of $A^{IV}B^{VI}$-type is driven by prospects for their use in semiconductor devices. For example, SnS and SnSe are used as the main materials for obtaining active elements operating in the infrared region of the optical spectrum in thermodynamic converters [1,2]. They are also used as absorber layers in thin-film solar energy converters [3,4], as photoconductors [5], as semiconductor sensors [6], and as microbatteries [7].

Thus, the fundamental properties of these compounds - small band gap, high conductivity, relatively high radiation resistance, and the predominance of ionic bonding expand their application possibilities [8]. In recent years, significant efforts have been devoted to developing photovoltaic devices using low-cost materials and simpler, more cost-effective fabrication technologies. SnSe, which has complex ionic-covalent chemical bonds, crystallizes in a deformed NaCl-type structure and has a high degree of defects and vacancies in both sublattices [9].

The high concentration of these defects, especially tin vacancies (~10^{17} cm^{-3}), results in the formation of positive-type conductivity in SnSe. On the other hand, rare earth metals are distinguished by their unique specific properties [10, 11]. It is known that the physical properties of compounds formed from defect-structured substances and lanthanide atoms vary depending on the nature of their constituent atoms.

This is due to the fact that the 4*f* level in the electronic structure of lanthanoid element atoms is not completely filled, the 4*f*- 5*d*- 6*s* transition easily occurs, and the formation of variable valence due to mobile electrons at the 4*f* level of atoms makes materials obtained with their participation an interesting object of research. For this reason, the study of the complex $TuSnSe_2$ compound with the participation of lanthanide elements, including the Tu element, is of particular interest.

Due to the presence of mobile electrons in the internal 4*f* levels in the electronic structure $f \rightarrow d \rightarrow s$ transitions easily occur, which leads to the formation of variable valence in them. Although rare earth metals are trivalent, intermediate valence arises due to transitions between electronic energy levels. This significantly affects the kinetic properties of materials obtained with their participation. The partial replacement of tin with rare-earth metals in SnSe leads to the emergence of certain physical properties. In this regard, the synthesis of new materials based on alloys and compounds involving rare earth metals demonstrates the importance of their investigation. The special importance of this research is the possibility of obtaining new promising materials with the required physical properties based on alloys and compounds with the participation of rare earth elements. [12, 13].

2. EXPERIMENTAL PROCEDURE

In this work, the SnSe-TuSe system was studied in the entire concentration range. However, since the melting temperature of the TuSe compound is very high, it was not possible to synthesize samples containing 75-100% TuSe.

A physicochemical analysis of the SnSe-TuSe system was conducted and a phase diagram of the system was constructed. At 10 mol% TuSe, a eutectic point is obtained and its melting point is 1053.2 K (780°C). The triple

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compound $TuSnSe_2$ decomposes at 1053.2 K before reaching its melting point 1093.2 K. Therefore, it cannot be synthesized by direct melting of its components and it is obtained by pressing [14].

The process is carried out in the following sequence: To ensure the homogeneity and mechanical strength of the material, the components are ground into a fine powder, mixed by mechanical vibration, and then pressed. Pressing was carried out in two sequential processes: cold and hot pressing. In cold pressing, the sample was kept under a pressure of P = 7.4 ton/cm^2 for 5 minutes. In hot pressing, the press mold was heated to t = 663.15 K and kept under pressure P = 5 ton/cm^2 for 5 minutes.

To create homogeneity in the obtained substance, the ampoule was placed horizontally in a heater at a temperature of 953.15 K and kept for 336 hours, during which the infusion was carried out.

To determine the stoichiometric composition and crystal structure of the compound, a physicochemical analysis was carried out. The results of the complex physicochemical analyses are given in Table 1.

Table 1. Physicochemical parameters of the $TuSnSe_2$ compound

Thermal heating efficiency	Density×10^3 g/m^3		Microhardness, *MPa*	Lattice parameters, Å		
	ρ_{pikno}	ρ_{rent}		*a*	*b*	*c*
716.86	7.22	7.34	263	4.77	-	11.58

The table notes show that the obtained $TuSnSe_2$ compound is a crystal with a stoichiometric composition, a defective and partially deformed hexagonal structure.

3. RESULTS AND DISCUSSION

The main kinetic parameters of the obtained $TuSnSe_2$ triple compound were determined at room temperature, the Hall coefficient (R), electrical conductivity (σ), thermo electromotive force (α) and thermal conductivity (λ) were studied in the temperature range T = 300÷800 K. The concentration of charge carriers (n) and the Hall mobility (μ) of the sample were calculated. The results obtained for the main kinetic parameters of the $TuSnSe_2$ triple compound at a temperature of 300 K are given in Table 2.

Table 2. Some kinetic parameters of the $TuSnSe_2$ compound (300 K)

Compound	R, cm^2/C	P(n)·10^{19}, cm^{-3}	σ, Ω^{-1}·cm^{-1}	μ, cm^2/V·sec	α, μV/K	λ, W/cmK
$TuSnSe_2$	-0.22	2.8	16.2	4	-155	14.67

Figure 1 shows a graph of the temperature dependence of the electrical conductivity in the $ln\,\sigma = f(10^3/T)$ coordinates of the triple compound $TuSnSe_2$ in the temperature range T=300÷750 K

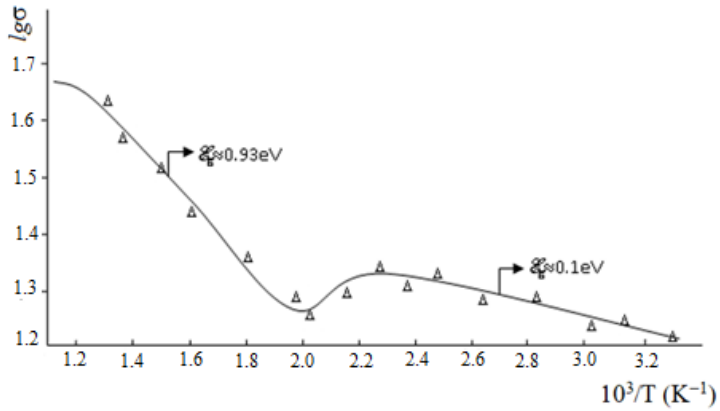

Figure 1. Temperature dependence of the electrical conductivity of the triple compound $TuSnSe_2$

The temperature dependence of the electrical conductivity can be analyzed as follows:

1. In the temperature range T=300÷440 K, the change in electrical conductivity varies according to the law $\sigma \sim T^{1.2}$, and the activation energy of charge carriers is $\Delta E_g \approx 0.1$eV.
2. In the temperature range T>510 K, this variation is according to the law of $\sigma \sim T^{1.7}$, and the width of the bandgap is $\Delta E_g \approx 0.93$eV [15].
3. In the temperature range T=440÷520 K, an anomalous change is observed. This change is most likely due to a sharp decrease in the mobility of charge carriers.

It should be noted that the main reason for the observed anomalous change is the region where the concentration of charge carriers does not change (n=const) and the region where the specific conductivity corresponds to a decrease. Thus, the concentration of charge carriers does not change with increasing temperature (n = const), that is, all free electrons in the conduction band participate in conduction.

To excite the donor (acceptor) levels, a certain amount of energy is required (the temperature should be increased). Analyses show that the decrease in σ due to the decrease in the Hall mobility of charge carriers is approximately 0.06%. The remaining part of the decrease in the value of σ is due to the anomalous change as shown above. This anomalous change is also confirmed by the properties observed in the temperature dependence of thermo-electromotive force (e.m.f.) and electrical conductivity (Fig. 2)

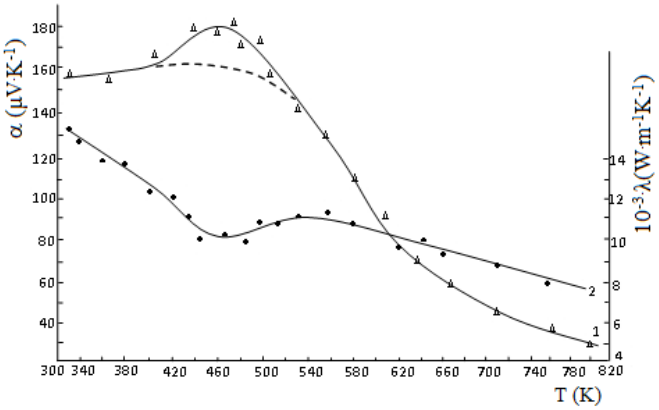

Figure 2. Temperature dependence of the thermo e.m.f. (1) and thermal conductivity (2) of the $TuSnSe_2$ compound

As can be seen from the figure, a gradual increase in the thermo e.m.f. is observed in the temperature range T = 300÷420 K. In the temperature range T = 440÷500 K α(T) changes anomalously; at temperatures T ≥ 500 K the magnitude of α(T) decreases monotonically with increasing temperature, and this rate of decrease follows the law $\alpha \sim T^{-1.38}$. The anomalous change in the temperature range T = 440÷500 K is likely to be due to a structural transformation, as in SnSe [3,4]. The anomaly in the SnSe crystal is explained by the transition of the orthorhombic structure to the cubic structure [5]. The physicochemical analysis of the obtained triple compound $TuSnSe_2$ shows that it crystallizes in a hexagonal syngony.

It is likely that a structural transformation occurs at T = 440÷500K. In order to determine the type of this structural transformation, its mechanism, and at the same time how the scattering mechanism of charge carriers changes, and to identify a general pattern, the temperature dependences of the Hall coefficient and electrical conductivity of this compound were also studied. The variations in the charge carrier concentration and Hall mobility were determined based on the obtained values.

4. CONCLUSIONS

Physicochemical analyses indicate that a eutectic is formed at the 10 mol% TuSe compound and its melting temperature is 1053.15 K. X-ray structure and differential thermal analysis showed that this compound crystallizes in a hexagonal syngony. Based on the sign of the thermo e.m.f. and the Hall coefficient, it was determined that this compound has n-type conductivity. In the temperature dependence of the electrical conductivity, thermo e.m.f., and coefficient of thermal conductivity anomaly changes are observed in the T = 460÷500 K temperature interval. Based on the values of electrical conductivity, carrier concentration and Hall conductivity, it was determined that this compound is a partially compensated semiconductor. From the temperature dependence of electrical conductivity, the activation energy of charge carriers ($E_g \approx 0.1$ eV) and the energies of the bandgap ($E_g \approx 0.93$ eV) were calculated.

Since the localized energy levels in the ground and excited states are close to the chemical potential, the effective potential created by the 4*f* scattering of Tu^{3+} ions affects the change in kinetic parameters. These energy levels are close to the Fermi energy level and affect the electronic spectrum and valence of the material. This causes changes in the values of physical parameters.

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СИНТЕЗ ТА ТЕРМОЕЛЕКТРИЧНІ ВЛАСТИВОСТІ СПОЛУКИ $TuSnSe_2$

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У цій дослідницькій роботі було вивчено взаємодію системи SnSe-TuSe, і в результаті комплексних фізико-хімічних аналізів було визначено область розчинності TuSe в SnSe (75-100%). Також було встановлено, що сполуку $TuSnSe_2$ отримано у співвідношенні її компонентів 1:1, і побудовано фазову діаграму системи. Рентгеноструктурний та диференціально-термічний аналіз зразка показали, що ця сполука кристалізується в гексагональній сингонії. Деякі кінетичні параметри потрійної сполуки $TuSnSe_2$ були визначені за кімнатної температури. Електропровідність (σ), термоелектрорушійна сила (ЕРС) (α) та теплопровідність (χ) були досліджені в діапазоні температур T = 300÷800 K. Для визначення зміни механізму розсіювання носіїв заряду також було досліджено температурні залежності рухливості Холла та електропровідності цієї сполуки. На основі знака термоелектрорушійної сили та коефіцієнта Холла було встановлено, що провідність у цій сполуці є n-типу. На основі отриманих результатів було визначено, як змінювалися концентрація носіїв заряду та рухливість Холла. Спостерігаються аномальні зміни в температурній залежності електропровідності, термоелектричного потенціалу та загальної теплопровідності в інтервалі температур T=460÷500K.

Ключові слова: *електропровідність; потрійна сполука; гексагональна сингонія; рухливість Холла*