INFLUENCE OF TEMPERATURE, FREQUENCY AND COMPOSITION OF $TlIn_{1-x}Er_xSe_2$ SOLID SOLUTIONS ON THEIR DIELECTRIC PERMITTIVITY AND CONDUCTIVITY

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$TlIn_{1-x}Er_xSe_2$ (x=0; 0,001; 0,005; 0,01) solid solutions have been obtained by direct synthesis method from initial elements. By X-ray method there have been determined crystallographic parameters of $TlIn_{1-x}Er_xSe_2$ crystals. It is shown that with the increase of Eb concentration in the crystals the unit cell parameters *a* and *c* decrease. There have been measured dielectric characteristics of Er-doped $TlInSe_2$ crystals. It is found that doping of $TlInSe_2$ crystals by erbium leads to decrease in the values of the dielectric permittivity and the electrical conductivity, not having a substantial effect on the behavior of temperature dependences of given characteristics and phase transitions temperatures. The density of states at the Fermi level; the average time of charge carrier hopping between localized states, average hopping distance, scattering of trap states near the Fermi level have been evaluated for crystals of $TlIn_{1-x}Er_xSe_2$ solid solutions.

Keywords: chalcogenides, semiconductors, solid solutions, unit cell parameters, dielectric permittivity, specific electric conductivity, phase transition
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$TlInSe_2$ ternary compound belongs to the great group of $TlA^{III}B_2^{IV}$ (A=In, Ga, B= S, Se, Te)-typed semiconductors-segnetoelectrics has the interesting set of physical properties both scientifically and practically. Most of this group crystals are layered that leads to the strong anisotropy of their physical characteristics. Layered packets can be shifted easily with respect to each other that brings about to the advent of polytype modifications and as a result the substantial influence of production method and external effects on their properties [1,2]. For some of this family with the temperature change the sequence of structural phase transitions due to the presence of long–period commensurate and incommensurate modulated superstructures have been observed [3,4]. There have been a number of works in which the investigation results of various physical properties of given crystals owing to the temperature and anomalies on the curves of these dependences are revealed that are indicative of phase transitions in $TlA^{III}B^{IV}$-typed compounds [5-7]. While investigating thermal capacity and crystallographic parameters of $TlInSe_2$ crystals the authors [6-7] found out phase transitions at T_1=135K and T_2=185K and suppose that these transitions are due to the modulated structure. Although in [8] by investigating $TlInSe_2$ crystal thermal capacity within temperatures 42÷300K no anomalies on the curve C_0= f(T) are found out. This family crystals are of significant practical interest for optoelectronics as they are optically active and have high photosensitivity within wide spectral range.

It is known that composition change by various element doping and creating solid solutions has a significant influence on physical properties [9-12]. In [9,10] there have been presented the results of influence of Eb-doping on the physical properties of $TlGaS_2$ and $TlGaSe_2$ crystals. It is shown that partial substitution of Ga by Er leads to the decrease of dielectric permittivity, specific conductivity and to the increase of charge carrier concentration in forbidden band.

It is of great interest to establish how $TlInSe_2$ compound doping affects on its physical properties. Therefore, the aim of the given work is to investigate structural and dielectric characteristics of $TlIn_{1-x}Er_xSe_2$ system due to the temperature, frequency and composition.

$TlIn_{1-x}Er_xSe_2$ solid solutions have been obtained by direct synthesis method from initial elements taken in stoichiometric relations by their immediate alloying in vacuum up to 10^{-3}Pa. From $TlInSe_2$-based obtained samples $TlIn_{1-x}Er_xSe_2$ single crystals are growth by using Bridgman method. X-ray diffraction study of $TlIn_{1-x}Er_xSe_2$ crystals was carried out on X-ray diffractometr DRON-3 with using CuK_α monochromatic radiation. Registration of diffraction spectra was made out automatically in step-by-step regime with 0,03° along 2θ. The calculations of unit cell parameters are conducted on the base of recorded diffraction patterns using the method of Rietveld analysis with Fullprof program packet. Measurements of dielectric constant (ε) and electric conductivity (σ) were carried out by method of plane condensator by digital meter E-7-20 at frequencies 10^3-10^6 Hz within temperature range 85-300 K. The temperature was controlled by differential chromel-copel thermocouple and multipurpose digital voltmeter. There has been used the method of continuous quazi-static heating at a rate of ~ 0.5 K/min for measurements. Measurement accuracy of temperature is 0.1-0.2 K. Error of dielectric characteristics measurements is ~ 0.5%.

From diffraction patterns of mono-and polycrystalline samples of $TlIn_{1-x}Er_xSe_2$ it was found that the obtained $TlIn_{1-x}Er_xSe_2$ crystals (x=0;0.001; 0.005; 0.01) are homogenous. It was shown that $TlIn_{1-x}Er_xSe_2$ doped by Er crystallizes into the structure with space group D_{4h}^{18}-*I*4/mcm. On the base of obtained roentgenograms there have been calculated unit cell parameters *a* and *c* of crystals under investigation depending on the composition. Calculation results are shown in Fig.1. It is seen that the partial substitution of In by Er brings about the decrease of unit cell parameters. In Fig.2 there have been presented temperature dependences of dielectric permittivity of $TlIn_{1-x}Er_xSe_2$ crystals at the frequency of 1 MHz. The dependences within the phase transitions for the first and fourth compositions ($TlInSe_2$ and $TlIn_{0.99}Er_{0.01}Se_2$) have been shown in the upper left corner of Figure 2.

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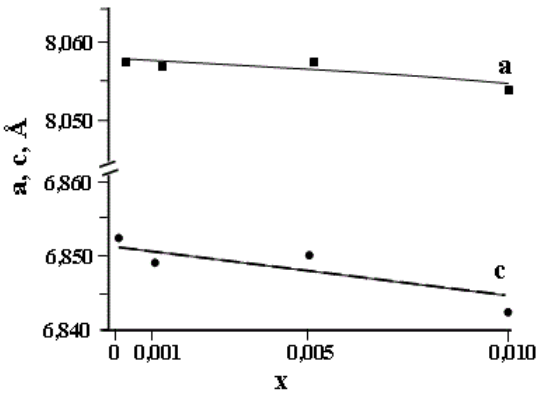

Fig.1 Concentration dependences of $TlIn_{1-x}Er_xSe_2$ unit cell parameters

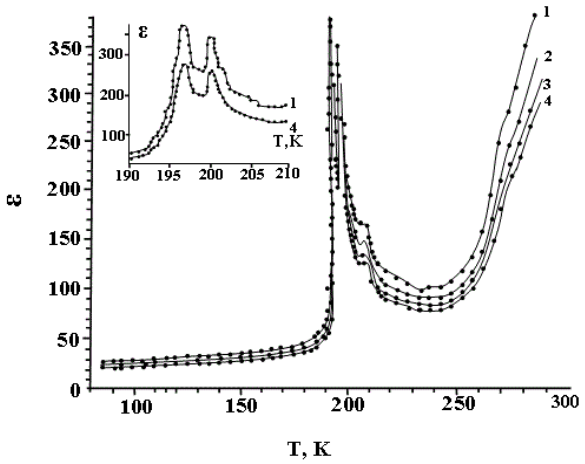

Fig.2 Temperature dependences of dielectric permittivity of $TlIn_{1-x}Er_xSe_2$ crystals: 1 - x = 0; 2 - x = 0.001; 3 – x = 0.005; 4 – x = 0.01.

It is seen that the partial substitution of In by Er leads to the slight decrease of magnitude ε and does not affect on the view of temperature dependence and anomaly positions related to the phase transitions of the second kind of "commensurate- noncommesurate phase" that are characteristic of given compound [5].

At all studied frequencies the *ac* - conductivity of the Er–doped $TlInSe_2$ crystals (Figure 3) varies according the law $\sigma_{ac} \sim f^{0.8}$, characteristic of hopping conduction through localized states near the Fermi level [13]. In terms of Mott theory, we calculated the density of states at the Fermi level from the measured experimental values of the conductivity $\sigma_{ac}(f)$. Calculated values of N_F for $TlIn_{1-x}Er_xSe_2$ (x = 0.005 and 0.01) single crystals were equal to $8 \cdot 10^{17}$ and $1.2 \cdot 10^{18}$ $eV^{-1} \cdot cm^{-3}$, correspondingly. The theory of ac hopping conductivity provides an opportunity to determine the average distance R and time τ of charge carrier hopping from one localized state to another. Calculated values of τ and R for both $TlIn_{1-x}Er_xSe_2$ (x = 0.005 and 0.01) single crystals were equal to $5{,}7 \cdot 10^{-2}$ μs and 320 Å, correspondingly. We estimate also energetic scattering of trap states near the Fermi level: ΔE = 0.018 eV for $TlIn_{1-x}Er_xSe_2$ crystals with $_x$ = 0.005 and 0.012 eV for x = 0.01.

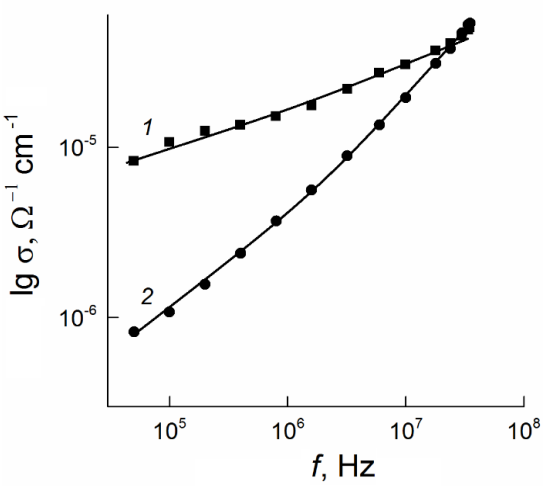

Fig. 3. AC-conductivity of $TlInSe_2$ (curve 1) and $TlInSe_2$:Er (1 mol % Er) (curve 2) vs frequency at *T* = 300 K.

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