fact, as well as the absence for the same 2C-$TlGaSe_2$ sample in the temperature range T = 100-300 K of a fourfold increase in the unit cell parameter c indicates that in the 2C-$TlGaSe_2$ polytype, as well as in 2C-$TlInS_2$ crystals [3], the order parameter of the ferroelectric *PT* is spontaneous polarization. As for the existence of an incommensurately modulated structure in 2C-$TlGaSe_2$ crystals, it is possible that it arises as a result of a phase transition occurring at a temperature of T ~ 245 K, the existence of which was repeatedly reported earlier [4, 5].

Thus, the data obtained indicate a significant effect of polytype on the physical mechanism and temperature position of structural phase transformations occurring in $TlGaSe_2$ crystals

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THERMO-FIELD PULA-FRENKEL EFFECT IN $TlFeS_2$ CRYSTALS

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Abstract. *Based on the study of the dependence $\sigma \sim (E^{1/2})$, it was shown that the current in the nonlinear region (taking into account the thermal-field effect of Poole-Frenkel) is due to a weak field effect, both when measured in parallel and perpendicular to the crystallographic axis crystal $TlFeS_2$. The calculated values of the concentration of ionized centers N_t, the mean free path λ, and the values of the Frenkel coefficient in the shape of a potential well in $TlFeS_2$ crystals have been determined.*

Keywords: *electrical conductivity, crystal, electric field, ionization, capture centers*

The one-dimensional (1D) character of the structure of $TlFeS_2$ crystals is one of the attractive features of crystals of this family. The compound crystallizes in the monoclinic space group C_2/t with unit cell parameters a = 11.64 Å, b = 5.31 Å, c = 10.51 Å, and γ = 144.6°. In non-standard notation (I 11 2 / m), the lattice parameters are written as a = 6.83 Å, b = 10.51 Å Å, c = 5.31 Å and γ = 98.6° while the chains are FeS_4 tetrahedra with common faces located along the c axis [1, 2, 3, 4]. The magnetic properties of the $TlFeS_2$ crystal were studied in detail; in these works, the presence of one-dimensional antiferromagnetic ordering was established, and the presence of hopping conductivity was also established [5, 6, 7, 8, 9].

The aim of this work is to establish the conduction mechanism in the ohmic region of the I – V characteristic and the features of the Poole – Frenkel thermal field effect in the nonlinear region of the I – V characteristic of $TlFeS_2$ crystals.

The I – V characteristics were measured in a forward run, with an increase in the applied dc voltage along the c axis. The measurements were carried out at fixed temperatures in the range 80 - 300K.

In fig. 1 shows the current-voltage characteristics of $TlFeS_2$ crystals at different temperatures of the experiment, parallel along the *c* axis. The I - V characteristic reveals two sections are revealed: an ohmic one ($J \alpha U$) and a region of a sharper increase in voltage ($J \alpha U^n$, $n > 1$). The linear section expands with increasing temperature, and the transition voltage increases. As the voltage increases, the quadratic region of the dependence ($J \alpha U$) shifts to large values, and as the temperature rises, the threshold voltage, from which the quadratic region begins, shifts towards low voltages and n decreases. This shows that the sharp increase in the current is mainly due to the ionization of local levels in the field.

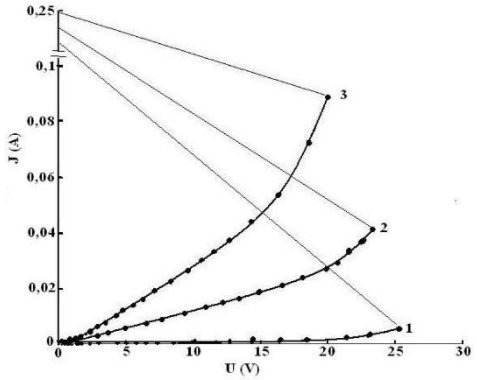

Fig. 1. The I - V characteristic of a $TlFeS_2$ crystal is measured parallel to the c axis at temperatures: 1-90, 2 - 200, 3 - 300 K

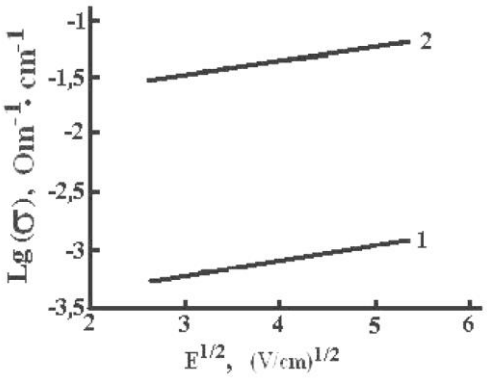

Fig. 2. Dependence of the electrical conductivity of $TlFeS_2$ single crystals on the field strength E at temperatures T, K: 1-90, 2-300

In a strong electric field, when the difference in the potential energy of an electron $\varepsilon ER(T)$ over the length of a characteristic jump $R(T)$ is equal to the width of the energy band around the Fermi level $\Delta\varepsilon(T)$, in which the jumps occur, the electron can move in the direction of the field, emitting phonons at each jump. According to Mott [10], the current in this case does not depend on temperature and grows with increasing field according to the law.

$$I(E) \sim exp\left\{-\left(\frac{E_0}{E}\right)\right\}^{1/2} \quad (1)$$

In fig. 2 shows the dependences of the electrical conductivity on the electric field at temperatures of 90 K and 300 K for the region of a sharp increase in the current in the coordinates $ln\sigma \sim \sqrt{E}$. As is known, the theory of exponential growth of electrical conductivity was first put forward by Frenkel [11] $\sigma = \sigma_0 \exp(\beta\sqrt{E})$ where β is the Frenkel coefficient:

$$\beta = \frac{\sqrt{a^3}}{k\beta T\sqrt{\pi\varepsilon\varepsilon_0}} \quad (2)$$

where *e* - is the electron charge, ε - is the dielectric constant of the vacuum, *k* - is the Boltzmann constant, *T* - is the absolute temperature.

The values of β are determined from the slope of straight lines (Fig. 2). The temperature dependence of β determined from the dependence $\sigma \sim f\left(E^{1/2}\right)$ at different temperatures is shown in Fig. 3.

As can be seen from Fig. 3, β increases with temperature displacement, while the $\beta \sim f(10^3/T)$ dependence is well satisfied. The temperature dependence of β is consistent with Frenkel's theory and

the extrapolation of the straight line $\beta \sim f(10^3/\mathrm{T})$, according to formula (3), leads to the origin. It was shown in [11] that the minimum value of the electric field corresponding to the nonlinear dependence $\sigma \sim f(E)$ contains information on the concentration of defects responsible for the thermal field ionization and conductivity of the $TlFeS_2$ crystal.

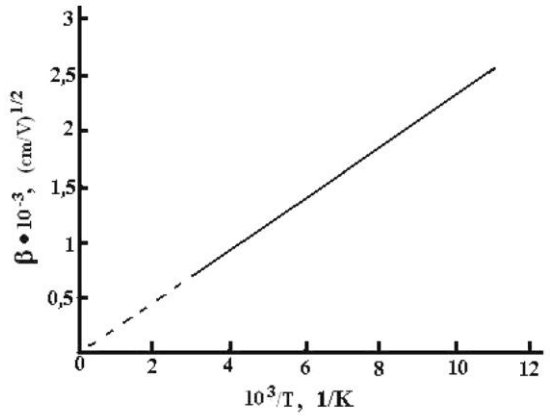

Fig. 3. Temperature dependence of the Frenkel coefficient β.

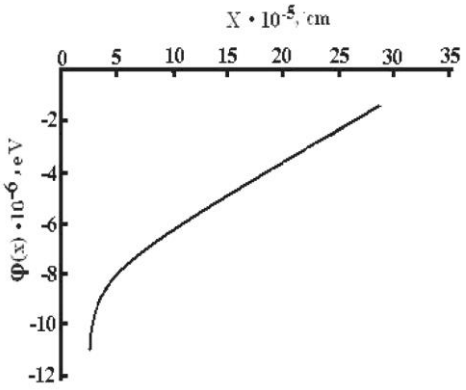

Fig. 4. The shape of the potential well of the crystal $TlFeS_2$.

According to the expression $N_f = \left(\frac{2e}{kT\beta}\sqrt{E_e}\right)^3$, having the values of the minimum electric field E_c, at which the nonlinear dependence of σ on E begins, the concentration of ionized centers N_f was estimated, which turned out to be equal to N_t = 1,4 x 10^{13} cm^3.

Determining the shape of the potential pit is of great importance. The function *cp(x)* is the potential energy, which depends on the distance to the impurity center or trap (*x* - is the distance along the direction of the applied field); it changes under the action of an electric field [12]. It follows from [12, 13] that

$$\varphi(x) = -\frac{kT\beta}{2}\sqrt{E} = eEx \; ; \; x = \frac{kT\beta}{2e\sqrt{E}} \quad (3)$$

Using the experimental data, the shape of the potential well in $TlFeS_2$ was determined, which is shown in Fig. 4. If the shape of the potential energy curve for interaction with a specific center is known, then information about the structure of the trapping centers can be obtained. As shown in [4], for the electron to leave the center, the condition $\varepsilon_e > E_0 - \Delta U_0$ must be satisfied. It is necessary that the electron retains energy until the moment when it passes the saddle point, and, at the same time, does not lose it during thermal collisions. This takes place only in those cases when the electron mean free path is greater than the effective dimensions of the potential well. The mean free path of an electron in $TlFeS_2$ crystals turned out to be $\lambda \sim 41 \cdot 10^{-6}$ cm.

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HETERO TRANSITIONS BASED ON *p* - $TlGaSe_2$ - *n* - $CuInSe_2$

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Abstract. *The current-voltage and lux-ampere characteristics, as well as the photovoltage spectra and the lux dependence of the photovoltage in the gate and photodiode modes of the p-$TlGaSe_2$ - p-$CuInSe_2$ heterojunction obtained for the first time are studied. It was found that this heterostructure has a pronounced diode character. The I – V characteristic of the structure under study is characterized by the fact that at low voltages it obeys well the law $I \sim exp\ (eU / \beta kT)$. The photovoltage spectrum covers a wide range of wavelengths (0.55 - 1.85 μm). In this case, pronounced maxima are observed at $\lambda = 0.59$ and $\lambda = 0.95$ μm. The relaxation time τ determined from the kinetics of the photovoltage in the valve mode is ~ 20 μs.*

Keywords: *heterostructure, current-voltage characteristic, photovoltage, spectrum, single crystal.*

The study of this system was primarily stimulated by the fact that *n* - $CuInSe_2$ single crystals are characterized by the presence of a direct transition near 1.2 μm [1] and, therefore, are of great interest for creating solar energy converters. The physical properties of *p* -$TlGaSe_2$ single crystals are considered in [6-9].

To create *p*-$TlGaSe_2$ - *n*-$CuInSe_2$ heterojunctions, *p*-$TlGaSe_2$ single crystals with a carrier concentration of ~ $10 \cdot ^{13}$ cm^{-3} (at $T = 300$ *K*) and *n*-$CuInSe_2$ single crystals with a carrier concentration of ~ $10 \cdot ^{16}$ cm^{-3} (at $T = 300$ *K*) grown by the Bridgman-Stockbarger method. Before preparing heterojunctions, the surface of $CuInSe_2$ samples was etched with a solution of potassium dichromate in sulfuric acid and then washed with distilled water and pure alcohol. The surface of the *p*-$TlGaSe_2$ samples was not chemically treated. Ohmic contacts were obtained by applying a silver paste to the structures under study. The ohmicity of the contacts was preliminary checked by studying the structures Ag - $TlGaSe_2$ - Ag and Ag - $CuInSe_2$ - Ag. It turned out that the current-voltage characteristics (*I – V* characteristics) of these systems are symmetric and obey a linear law up to ~ 15 *V*. At higher voltages, the symmetry of the *I – V* characteristics of Ag - $TlGaSe_2$ - Ag is somewhat violated.