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ELECTRICAL PROPERTIES OF TlInSe₂ CRYSTAL

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Abstract. The temperature and frequency dependences of the dielectric permittivity of TlInSe₂ crystals are studied at AC. The dielectric constant values were determined. It is assumed that the increase in ϵ' is associated with an increase in the concentration of defects with increasing temperature. It has been established that in the temperature range 290 - 380K at frequencies 10^2 - 10^6 Hz for electrical conductivity the law $\sigma \sim f^S$ ($0.1 \leq S \leq 1.0$) is satisfied. In a TlInSe₂ crystal, the change in electrical conductivity depending on frequency can be explained as follows: in crystals, there are clusters containing localized states with close energies, and electron hopping occurs between them. In the TlInSe₂ compound, conductivity is characterized by band-hopping mechanisms.

Keywords: crystal, dielectric constant, concentration, capacitor, dielectric losses, crystal structure

TlInSe₂ KRİSTALININ ELEKTRİK XASSƏLƏRİ

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Xülasə. Dəyişən elektrik sahəsində TlInSe₂ kristallarda dielektrik nüfuzluğun temperatur və tezlikdən asılılıqları tədqiq edilmişdir. Dielektrik nüfuzluğunun qiyməti müəyyən edilmişdir. Təyin olunmuşdur ki, temperaturun artması ilə ϵ' -in qiymətinin artması defektlərin konsentrasiyasının artması ilə əlaqədardır. Müəyyən edilmişdir ki, 290 - 380 K temperatur intervalında 10^2 - 10^6 Hz tezliklərdə elektrik keçiriciliyi üçün $\sigma \sim f^S$ ($0.1 \leq S \leq 1.0$) qanunu ödənilir. TlInSe₂ kristalında elektrik keçiriciliyinin tezlikdən asılılığının dəyişməsi belə izah oluna bilər: Kristallarda oxşar enerjilərə malik lokallaşdırılmış vəziyyətləri ehtiva edən klasterlər var və onların arasında elektron sıcrayışı baş verir. TlInSe₂ birləşməsində keçiricilik zona-sıcrayış mexanizmləri ilə xarakterizə olunur.

Açar sözlər: kristal, dielektrik sabiti, konsentrasiya, kondensator, dielektrik itkisi, elektrik keçiriciliyi, kristal quruluşu

Introduction. A³B³C₂⁶-type compounds have been widely studied by researchers because these compounds have unique properties under the influence of various external influences [1-9]. TlInSe₂ compounds are materials in which, under certain conditions, the features of low-dimensional (1D) systems appear [10], and therefore these compounds are widely studied. The temperature dependence of the heat capacity, lattice parameters and photoconductivity of TlInSe₂ was studied [11, 12].

The experiments were carried out in the temperature range of 5-300K, the thermodynamic parameters of the crystal were calculated, and the presence of a phase transition in the temperature range of 135-184K was shown. The authors of [10] studied the band structure of the TlInSe₂ crystal using the method of linear combinations of atomic orbitals.

In TlInSe₂ crystals [13], the effect of negative differential resistance was discovered, which, according to the authors of these articles, has a purely thermal mechanism, and voltage oscillations were also discovered in the region of negative differential resistance.

Methods. TlInSe₂ samples by direct alloying of high purity elements (99.999%) in stoichiometric quantities were obtained. To measure the electrical properties, 0.5 mm thick plates were prepared from samples of TlInSe₂ crystals, onto which plates of silver paste were applied. The capacitors were placed in a cryostat, controlled in the temperature range from 290 to 380K. The temperature measurement accuracy was ± 0.5 K.

The temperature measurement accuracy was ± 0.5 K. Measurements of capacitance, dielectric loss tangent and resistance were carried out using digital impedance meters E7-25 (frequencies 25 - 10⁶ Hz). A measuring voltage of 1V was applied to the sample. From formulas

$$\varepsilon' = \frac{Cd}{\varepsilon_0 S} \text{ и } \varepsilon'' = \operatorname{tg} \delta \varepsilon'$$

the real and imaginary parts of the dielectric constant were calculated accordingly.

In Fig. Figure 1 shows the temperature dependences of the real part of the dielectric constant (ε') of TlInSe₂ compounds at various frequencies (f).

It follows from the figure that in the studied materials, a thermally activated increase in ε' is mainly observed. This can be explained as follows. It is known that in the case of parallel connection C_R and R , the real part of the dielectric constant is described by the relation [14]

$$\varepsilon' = \frac{\sigma}{\varepsilon_0 \omega \operatorname{tg} \delta} \quad (1)$$

where σ is the electrical conductivity, $\operatorname{tg} \delta$ is the dielectric loss tangent, $\omega = 2\pi f$ is the frequency, ε_0 is the electrical constant. In semiconductors, with increasing temperature, electrical conductivity increases mainly due to the concentration of carriers.

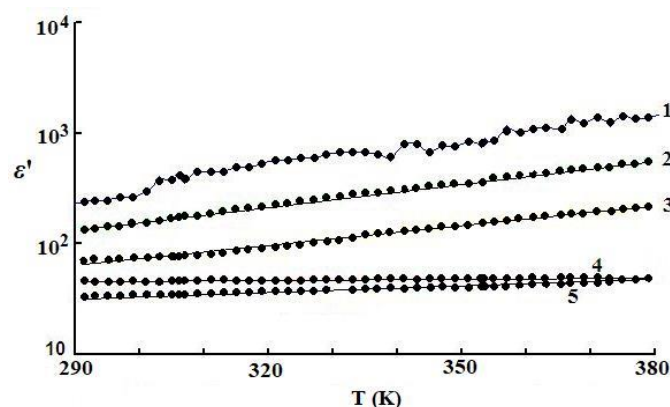


Fig. 1. Temperature dependences of the real part of the dielectric constant of TlInSe₂ crystals for measurement frequencies: 1 - 100, 2 - 1000, 3 - 10000, 4-100000 and 5-1000000 Hz [9]

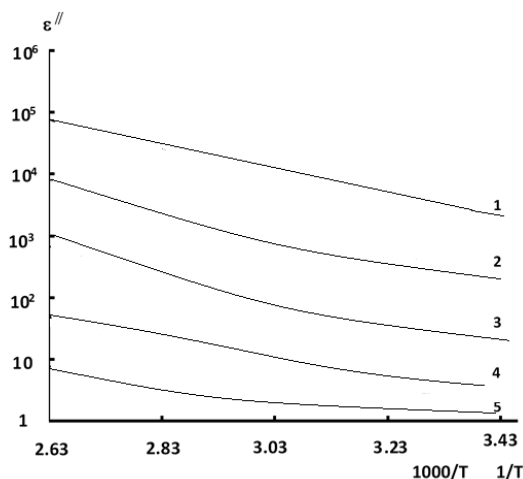


Fig. 2. Temperature dependences of the imaginary part of the dielectric constant of TlInSe₂ crystals for measurement frequencies: 1–10², 2–10³, 3–10⁴, 4–10⁵, 5–10⁶ Hz [9]

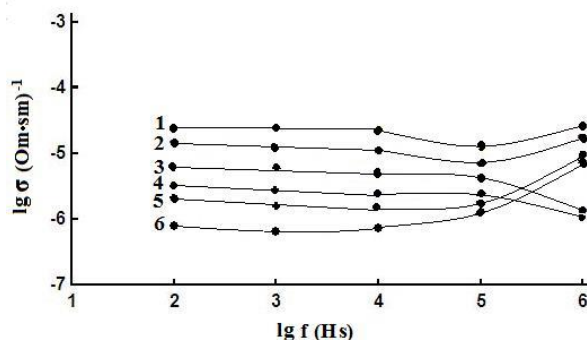


Fig. 3. Dependences of electrical conductivity on measurement frequency at different temperatures, K: 1 - 377, 2 - 359, 3 - 339, 4 - 321, 5 - 309, 6 – 294 [9]

From (1) it is clear that the real part of the dielectric constant is directly proportional to the electrical conductivity and $\text{tg } \delta$ weakly depends on temperature.

Therefore, with increasing temperature, σ increases and ϵ' increases accordingly. In the temperature range 290 - 380 K at frequencies 10² - 10⁶ Hz, the value of the real part of the dielectric constant varies within the range of 33 - 1390. With increasing frequency, ϵ' decreases. In Fig. 2 shows the temperature dependences of the imaginary part of the dielectric constant (ϵ'') of TlInSe₂ crystals.

It can be seen that at 10² - 10⁶ Hz frequencies, the dependence $\text{lg } \epsilon'' \sim 10^3/T$ is dominated by straight lines with different slopes. In the temperature range, with increasing frequency, the values of the activation energy ($\Delta E^{\epsilon''}$) decrease. It can be seen that the activation energy is a function of frequency.

In Fig. 3 shows the dependence of electrical conductivity on frequency at various temperatures in TlInSe₂. At first, with increasing frequency (10² - 10⁴ Hz), the electrical conductivity increases, then in the frequency range 10⁴ - 10⁶ Hz the dependence is complex. Electrical conductivity values strongly depend on the frequency of the electric field. Thus, the value of σ increases with increasing frequency. This behavior of the electrical conductivity of TlInSe₂ is apparently due to the peculiarities of the crystal structure. For TlInSe₂ crystals in the frequency range 10² - 10⁴ Hz, with increasing frequency, the electrical conductivity increases according to the law

$$\sigma \sim f^S \quad (0,1 \leq S \leq 1,0) \tag{2}$$

At a temperature of 294K in the frequency range $10^2 - 10^4$ Hz, S receives a value of 0.077 - 1.00, and at a temperature of 377K and the same frequency, S changes in the region of 0.1. It can be seen that at low temperatures of the studied frequencies the value of S changes more than at high temperatures. In TlInSe₂ compounds, the mechanism of the dependence of the increase in electrical conductivity on frequency can be explained as follows: it is known that if in crystals and amorphous semiconductors the dependence of the change in electrical conductivity on frequency obeys the pattern $\sigma(\omega) \sim \omega^S$ ($0.1 \leq S \leq 1.0$), then it can be assumed that there is a hopping mechanism in conductivity [11].

Based on the Debye analysis of the frequency dependence of conductivity, the frequency and temperature dependences of conductivity were theoretically studied [15], where the frequency dependence of conductivity is established as

$$\sigma(\omega)_T \propto \omega \left[\ln \left(\frac{\nu_f}{\omega} \right) \right]^4 \alpha \omega^s, \quad S \leq 1 \quad (3)$$

and the temperature dependence of conductivity is determined

$$\sigma(T)_\omega \propto T^{-1} \exp \left(\frac{T}{T_0} \right) \quad (4)$$

where ν_f is the phonon frequency, T_0 is the characteristic temperature. According to (4), with the above mechanism of conductivity at temperatures above $T > T_0$, the temperature dependence of electrical conductivity on the scale $\ln(\sigma \cdot T) \sim f(T)$ should give a straight line. In Fig. 4 shows the experimental dependence $\ln(\sigma \cdot T) \sim f(T)$ at 10^5 Hz. It can be seen that the dependence is linear. This corresponds to the hopping mechanism of conduction. Note that a compound of the $A^3B^3C_2^6$ type has some properties (for example, the switching effect, instability currents, etc.) that are characteristic of amorphous bodies [16]. These systems can be viewed as disordered systems.

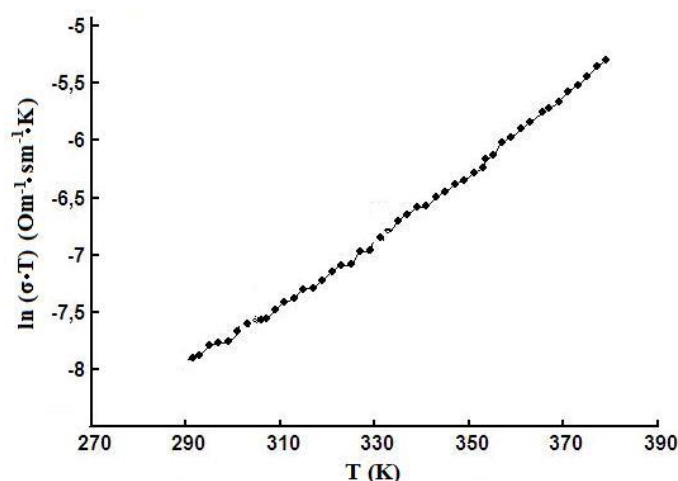


Fig. 4. Dependence $\ln(\sigma \cdot T) \sim f(T)$ for TlInSe₂ crystals at 10^5 Hz [9]

Therefore, in the TlInSe₂ crystal, the adoption of the conductivity of the hopping mechanism is natural. In compounds of type $A^3B^3C_2^6$, based on the formation of local levels, the following may occur:

- 1) the formation of antistructural defects based on the mutual substitution of cations;
- 2) violation of the periodic arrangement of stoichiometric voids;
- 3) violation of long-range order;
- 4) content of uncontrolled impurities.

The probability of the formation of antistructural defects based on the mutual substitution of cations in TlInSe₂ compounds is low, because the ionic radii of Tl and In differ from each other ($R_{\text{Tl}} = 0,164\text{\AA}$; $R_{\text{In}} = 0,92\text{\AA}$). We believe that the creation of defects in TlInSe₂ occurs due to the disruption of the periodic arrangement of stoichiometric voids. In [17], the problems of hopping conduction in disordered systems are considered from the point of view of the cluster approximation.

In a TlInSe₂ crystal, the change in electrical conductivity depending on frequency can be explained using the multiplet model [18], since in crystals there are clusters containing localized states with close energies, and electron hopping occurs between them. As the frequency increases, first some and then other charged particles do not have time to reach localization sites during a quarter period of the applied voltage and, continuously following the change in the electric field, contribute to the conductivity.

In Fig. 5 shows the temperature dependences of the electrical conductivity of TlInSe₂ crystals on alternating current at different frequencies.

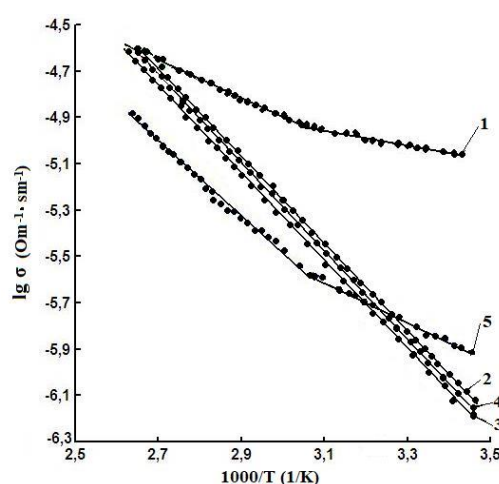


Fig. 5. Temperature dependences of electrical conductivity for TlInSe₂ crystals on alternating current at different values of frequency f , Hz: 1 - 10^6 , 2 - 10^2 , 3 - 10^3 , 4 - 10^5 , 5 - 10^5 [16]

At frequencies of $10^5 - 10^6$ Hz, the dependence $\lg \sigma \sim 10^3/T$ consists of two straight lines with different slopes. From the slopes of these dependences, activation energies (ΔE) are determined, the values of which in the low-temperature region vary in the range of 0.0006 eV, and in the high-temperature region - 0.0029 eV. It follows from this that the magnitude of the activation energy is a function of frequency. The dependence of activation energy on frequency can be explained using the hopping mechanism [15].

It is also known that in TlInSe₂ crystals the temperature dependence of electrical conductivity has an activation character [16]. This means that in the TlInSe₂ compound the conductivity is characterized by band-hopping mechanisms. Thus, the temperature and frequency dependences of the dielectric constant and electrical conductivity of TlInSe₂ crystals on alternating current have been studied. The dielectric constant values were determined.

Conclusion. It is assumed that the increase in ϵ' is associated with an increase in the concentration of defects with increasing temperature. It has been established that in the temperature range 290 - 380 K at frequencies $10^2 - 10^6$ Hz for electrical conductivity the law $\sigma \sim f^S$ ($0,1 \leq S \leq 1,0$) is satisfied. In a TlInSe₂ crystal, the change in electrical conductivity depending on frequency can be explained as follows: in crystals, there are clusters containing localized states with close energies, and electron hopping occurs between them. In the TlInSe₂ compound, conductivity is characterized by band-hopping mechanisms.

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