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СТРОИТЕЛЬСТВО

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## ELECTRICAL PROPERTIES OF TlInSe<sub>2</sub> CRYSTAL

**Abdullayev Adil Polad**- doctor of phy. and math.sc, prof., department of Physics and chemistry, AzUAC

**Akhmedov Valik Ibrahim** – PhD in phy. and math., ass.prof., department of Physics and chemistry, AzUAC

**Gafarova Dilara Mikail**– PhD in phy.and math., ass.prof, department of Physics and chemistry, AzUAC, dgafarova14@gmail.com

**Abstract.** The temperature and frequency dependences of the dielectric permittivity of TlInSe<sub>2</sub> crystals are studied at AC. The dielectric constant values were determined. It is assumed that the increase in  $\epsilon'$  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 TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> compound, conductivity is characterized by band-hopping mechanisms.

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

## TlInSe<sub>2</sub> KRİSTALININ ELEKTRİK XASSƏLƏRİ

**Abdullayev Adil Polad**- f.r.e.d., professor, Fizika və Kimya kafedrası, AzMİU

**Əhmədov Valik İbrahim**– f.r.e.n., dosent, Fizika və Kimya kafedrası, AzMİU

**Qafarova Dilarə Mikayıl**- f.r.e.n., dosent, Fizika və Kimya kafedrası, AzMİU, dgafarova14@gmail.com

**Xülasə.** Dəyişən elektrik sahəsində TlInSe<sub>2</sub> kristallarda dielektrik nüfuzluğun temperatur və tezlikdən asılılıqları tədqiq edilmişdir. Dielektrik nüfuzluğunun qiyməti müəyyən edilmişdir. Təyin olunmuşdur ki, temperaturun artması ilə  $\epsilon'$ -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. TlInSe<sub>2</sub> 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. TlInSe<sub>2</sub> birləşməsində keçiricilik zona-sıcrayış mexanizmləri ilə xarakterizə olunur.

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

**Introduction.** A<sup>3</sup>B<sup>3</sup>C<sub>2</sub><sup>6</sup>-type compounds have been widely studied by researchers because these compounds have unique properties under the influence of various external influences [1-9].

TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> crystal using the method of linear combinations of atomic orbitals.

In TlInSe<sub>2</sub> 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.** TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> 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  $\pm 0.5$ K.

The temperature measurement accuracy was  $\pm 0.5$ K. Measurements of capacitance, dielectric loss tangent and resistance were carried out using digital impedance meters E7-25 (frequencies 25 - 10<sup>6</sup> Hz). A measuring voltage of 1V was applied to the sample. From formulas

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

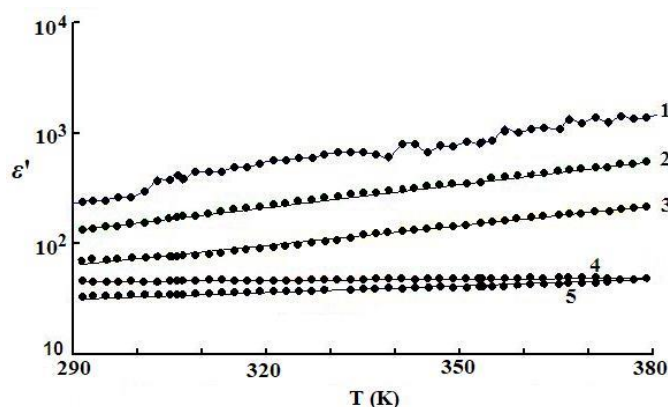
the real and imaginary parts of the dielectric constant were calculated accordingly.

In Fig. Figure 1 shows the temperature dependences of the real part of the dielectric constant ( $\varepsilon'$ ) of TlInSe<sub>2</sub> compounds at various frequencies (f).

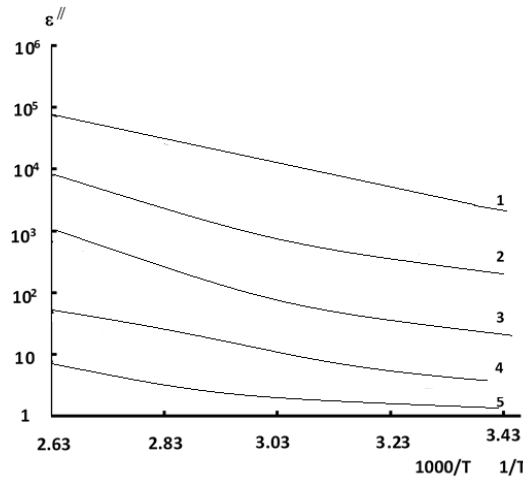
It follows from the figure that in the studied materials, a thermally activated increase in  $\varepsilon'$  is mainly observed. This can be explained as follows. It is known that in the case of parallel connection  $C_R$  and R, the real part of the dielectric constant is described by the relation [14]

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

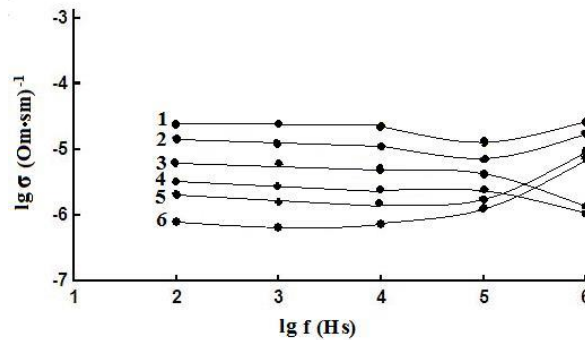
where  $\sigma$  is the electrical conductivity,  $\text{tg} \delta$  is the dielectric loss tangent,  $\omega = 2\pi f$  is the frequency,  $\varepsilon_0$  is the electrical constant. In semiconductors, with increasing temperature, electrical conductivity increases mainly due to the concentration of carriers.



**Fig.1.** Temperature dependences of the real part of the dielectric constant of TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> crystals for measurement frequencies: 1–10<sup>2</sup>, 2–10<sup>3</sup>, 3–10<sup>4</sup>, 4–10<sup>5</sup>, 5–10<sup>6</sup> 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,  $\sigma$  increases and  $\epsilon'$  increases accordingly. In the temperature range 290 - 380 K at frequencies  $10^2 - 10^6$  Hz, the value of the real part of the dielectric constant varies within the range of 33 - 1390. With increasing frequency,  $\epsilon'$  decreases. In Fig. 2 shows the temperature dependences of the imaginary part of the dielectric constant ( $\epsilon''$ ) of TlInSe<sub>2</sub> crystals.

It can be seen that at  $10^2 - 10^6$  Hz frequencies, the dependence  $\lg \epsilon'' \sim 10^3/T$  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 TlInSe<sub>2</sub>. At first, with increasing frequency ( $10^2 - 10^4$  Hz), the electrical conductivity increases, then in the frequency range  $10^4 - 10^6$  Hz the dependence is complex. Electrical conductivity values strongly depend on the frequency of the electric field. Thus, the value of  $\sigma$  increases with increasing frequency. This behavior of the electrical conductivity of TlInSe<sub>2</sub> is apparently due to the peculiarities of the crystal structure. For TlInSe<sub>2</sub> crystals in the frequency range  $10^2 - 10^4$  Hz, with increasing frequency, the electrical conductivity increases according to the law

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

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  $\text{TlInSe}_2$  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].

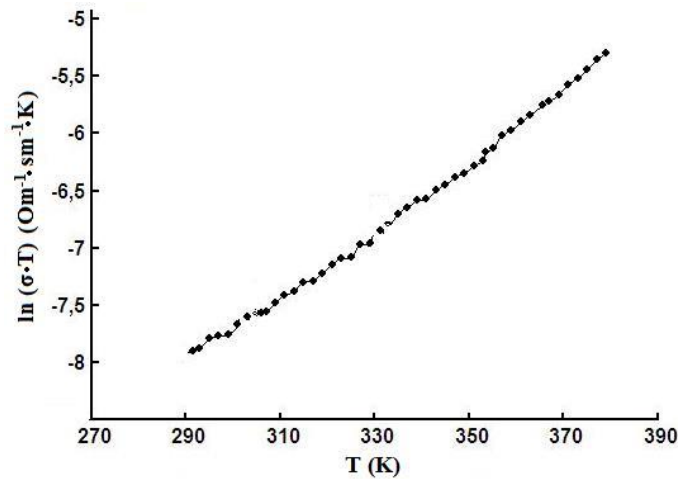
Based on the Debye analysis of the frequency dependence of conductivity, the frequency and temperature dependences of conductivity were theoretically studied [15], where the frequency dependence of conductivity is established as

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

and the temperature dependence of conductivity is determined

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

where  $\nu_f$  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  $\text{A}^3\text{B}^3\text{C}_2^6$  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  $\text{TlInSe}_2$  crystals at  $10^5$  Hz [9]

Therefore, in the  $\text{TlInSe}_2$  crystal, the adoption of the conductivity of the hopping mechanism is natural. In compounds of type  $\text{A}^3\text{B}^3\text{C}_2^6$ , based on the formation of local levels, the following may occur:

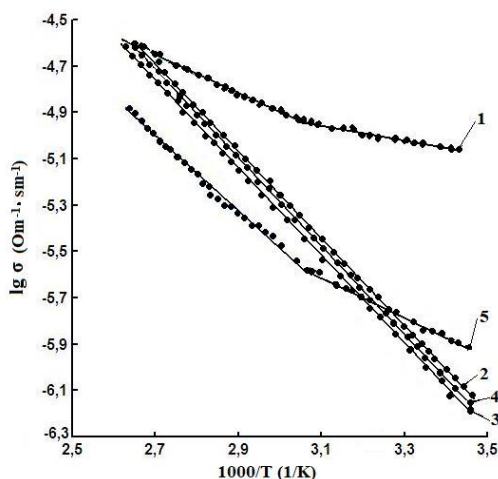
- 1) the formation of antistructural defects based on the mutual substitution of cations;
- 2) violation of the periodic arrangement of stoichiometric voids;
- 3) violation of long-range order;
- 4) content of uncontrolled impurities.

The probability of the formation of antistructural defects based on the mutual substitution of cations in  $\text{TlInSe}_2$  compounds is low, because the ionic radii of Tl and In differ from each other ( $R_{\text{Tl}} = 0,164\text{Å}$ ;  $R_{\text{In}} = 0,92\text{Å}$ ). We believe that the creation of defects in  $\text{TlInSe}_2$  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 TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> crystals on alternating current at different frequencies.



**Fig. 5.** Temperature dependences of electrical conductivity for TlInSe<sub>2</sub> 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 ( $\Delta E$ ) 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 TlInSe<sub>2</sub> crystals the temperature dependence of electrical conductivity has an activation character [16]. This means that in the TlInSe<sub>2</sub> compound the conductivity is characterized by band-hopping mechanisms. Thus, the temperature and frequency dependences of the dielectric constant and electrical conductivity of TlInSe<sub>2</sub> crystals on alternating current have been studied. The dielectric constant values were determined.

**Conclusion.** It is assumed that the increase in  $\epsilon'$  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 TlInSe<sub>2</sub> 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 TlInSe<sub>2</sub> compound, conductivity is characterized by band-hopping mechanisms.

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