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# Photostimulated Tension Effects in $TlInSe_2$ Crystals

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**Abstract**: The paper presents the results of a study of photostimulated strain effects in $TlInSe_2$ single crystals. It was found that the absolute value of the photocurrent in positively (compression) deformed samples increases, and in negatively (stretching) deformed samples – decreases in comparison with the undeformed sample. At the same time, the maximum of the photocurrent does not change, which indicates that the width of the direct transitions of $TlInSe_2$ crystals remains unchanged under various types of deformation.

**Keywords**: photostimulated strain effects, the absolute value of the photocurrent, positively deformed, negatively deformed, and the width of direct transitions of crystals.

## Introduction.

Currently, researchers and practitioners in the world pay great attention to the study of various semiconductor converters, including strain gauges, the main advantage of which is high sensitivity and small size. However, the requirements of modern science and technology are steadily growing, which leads to the search for materials with a variety of properties that meet these requirements.

Therefore, at present, along with the improvement of the properties of existing materials, the search for new semiconductor materials, including ternary and more complex compounds and their solid solutions, and the study of their various characteristics are among the most important tasks of modern condensed matter physics. Of particular value is the creation of new semiconductor materials, if it is possible to obtain them in the form of perfect large single crystals.Among the multicomponent semiconductor compounds of the $A^{III}B^{III}C_2^{VI}$ type, semiconductor compounds $TlInSe_2$ are of particular interest, the regularities of many physical phenomena in which have not received sufficient coverage in the special literature. According to the above, the purpose of our research is to study the tensoresistive characteristics of $TlInSe_2$ single crystals and create highly sensitive strain gauges for electronic technology based on them.

## Samples for research and experimental technique:

For this purpose, we used crystals synthesized by melting the component in accordance with the stoichiometry in evacuated (~$10^{-4}$ mm rt.st) and sealed quartz ampoules.Highly pure elements of thallium (Tl - 000), indium (In - 000) and selenium (Se -OSCH-17-4) were used as initial components for the synthesis. Single crystals were grown by the improved Bridgman method, the crystallization front velocity was varied from 0.5 to 0.9 mm/hour.

Identical crystals required for research are obtained from an ingot by the simplest pressing of a sharp knife, blade thickness ≤ 0.01 mm, onto the loose end of a thin, but wide and long single crystal plate at an angle of 45°.

Thus obtained "acicular" crystals - blanks with mirror edges - without any additional processing are ready for welding contacts and installing them on the base of the substrate.

When soldering "antennae", i.e. creating mechanically reliable ohmic contacts on these workpieces, two methods were used:

a) Fusion of indium in an inert gas flow followed by soldering of copper (or nickel) wires (ø = 0.01 mm).

b) Direct spot welding of the corresponding wires by a capacitor discharge to the ends of a billet heated in an inert gas flow. The second method turned out to be more efficient and reliable (especially for moderate temperatures).

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Plates made of steel 45 with a thickness of 0.5–1.0 mm and a length of 20 mm to 80 mm served as calibration beams for the glued sensors. The surface of the substrate in terms of processing class was not lower than class 7.

**Research results and discussion:**

We found that, as in the case of the study of the photoconductivity of $TlInSe_2$ crystals in [1 - 6], the absolute value of the photocurrent in positively deformed (compression) samples increases, and in negatively deformed (tension) it decreases compared to an undeformed sample. In this case, the photocurrent maximum does not change, which indicates the invariance of the gap of direct transitions of $TlInSe_2$ crystals for various types of deformation. Figure 1 shows the photocurrent spectra normalized to the maximum in the spectral region 0.8–3.2 eV in undeformed (curve 1), negatively deformed (curve 2), and positively deformed (curve 3) samples of pure p-$TlInSe_2$ single crystal in the [001] direction.].

As can be seen from the figure, the photocurrent maxima of all the studied crystals are at 1.20 eV. Under compressive and tensile strains, changes in the spectral distribution of the photocurrent are observed not only in the long-wavelength, but also in the short-wavelength region of the spectrum compared to the photocurrent maximum. This result indicates that there are indirect band transitions in $TlInSe_2$ crystals not only in the low-energy region compared to the photocurrent maximum, as was shown in [7], but also in the high-energy region of the spectrum

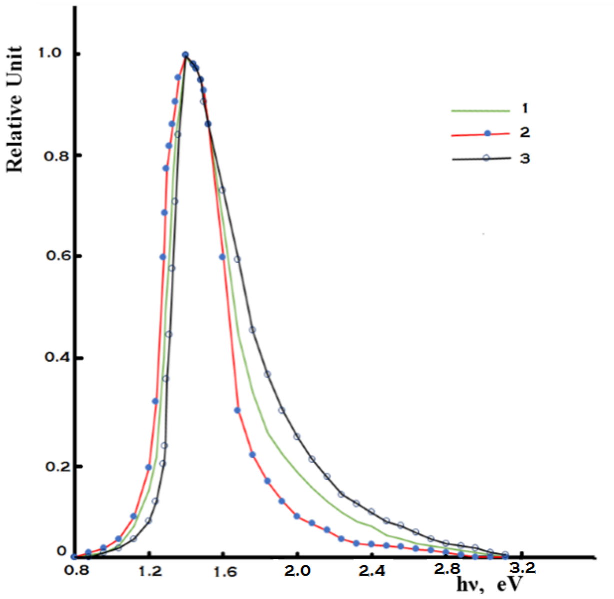


**Fig.1. Spectral distribution of photocurrent in undeformed (1), positively deformed (2), and negatively deformed (3) p-$TlInSe_2$ samples [1].**

Figure 2 shows the spectral distributions of the strain sensitivity of differently deformed crystals illuminated with light in the spectral region 0.8 - 3.2 eV. With a positive deformation (compression) of the crystal, the most intense peak is observed with a maximum at 1.20 eV, a slightly less intense peak with a maximum at 2.10 eV, and some structure in the regions of 1.6 - 1.70 e√. The maximum of the intense peak corresponds to the maximum of the crystal photocurrent (see Fig. 2a). With negative deformation (stretching) of the crystal, the maximum of the intense peak at 1.20 eV remains unchanged. The peak with a maximum at 2.10 eV disappears and a peak with a maximum at 1.70 eV appears clearly (see Fig. 2, b).

It should be noted that in [8], the X-ray photoelectron spectra of $TlInSe_2$ crystals were studied, and theoretically, using the unrestricted Hartree-Fock method (NMHF), the levels of energy states of crystals were calculated, which are in satisfactory agreement with each other.

The results of calculation of the main levels of the valence band (VB) and conduction band (CB) obtained by the authors of [8] are shown in Table 1. In this table, the values of the energy levels are given relative to the Fermi level, where the energy states of the VB have a negative value relative to the Fermi level, and the energies of the CB levels have positive values. Therefore, to determine the energy gap

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between the levels of the CB and VB, it is necessary to add the energy values given in the table. Taking this into account, the width of the energy gap between the top of the air intake (-0.5 eV) and the bottom of the WP (+0.7 eV) is 1.2 eV, which is in good agreement with maximum of the intrinsic photocurrent and the first, most intense maximum in the strain-sensitivity spectrum due to direct band transitions in $TlInSe_2$.

The energy gap between the next VB level (-0.7 eV) and the bottom of the CB (+0.7 eV) is 1.4 eV, which corresponds to the minimum in the strain-sensitivity spectrum of the crystal (see Fig. 3.), located in the high-energy region relative to maximum direct optical transitions.

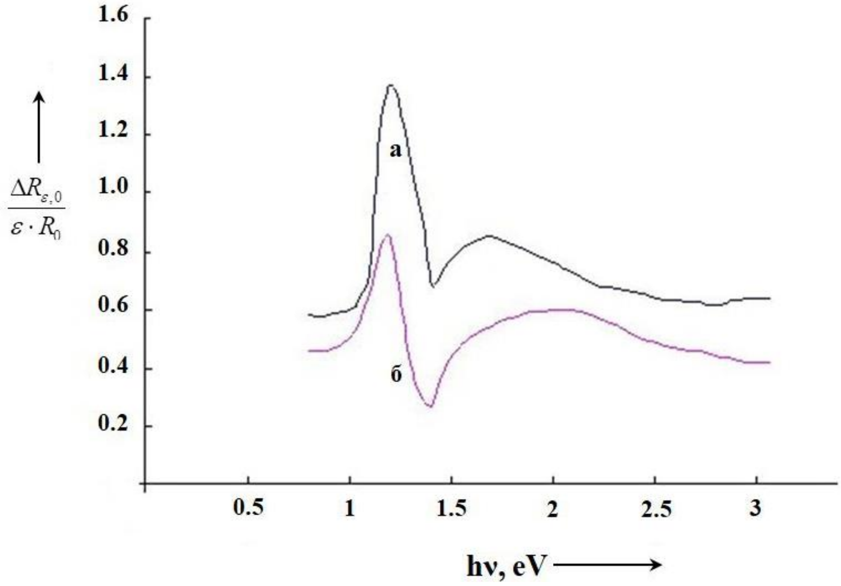


**Fig.2. Spectral distribution of strain sensitivity is positive (a) and negative (b) of the deformed p-$TlInSe_2$ crystal [1].**

The gap between the next level of the air gap VB (1.1 eV) and the bottom of the CB (+ 0.7 eV) is 1.8 eV.If we take into account the fact that the NMHF in the calculations gives a 10% overestimation of the calculated values compared to the experiment [9], then this value coincides well with the maximum of the observed second peak in the strain sensitivity spectrum of the negatively deformed sample.

The gap between the next level VB (-1.4 eV) and the bottom CB is 2.1 eV, which is in good agreement with the maximum of the second peak in the strain-sensitivity spectrum of the positively deformed sample. Thus, the maxima and minima of the spectral distribution of the strain sensitivity of the deformed $TlInSe_2$ crystals under illumination with light of various energies, determined by us, are in good agreement with the values of the band states determined in [8] in the $TlIn_4Se_{16}$ cluster (see Table 2).

A comparison of the spectral distribution of positively and negatively deformed specimens shows (see Figures 3a and 3b) that with positive deformation, strain-sensitivity bands with a maximum of 2.2 eV appear and increase in intensity, and with negative deformation this peak disappears and is observed only peak at 1.7 eV, i.e. when the sign of the deformation changes, the redistribution of the intensities of the individual strain sensitivity peaks occurs. If we take into account that the maximum of the photostimulated strain sensitivity at 1.20 eV is due to direct

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**Table1. Theoretical calculated population values (in %) of the levels of the valence band (VB) in the $TlIn_4Se_{16}$ cluster. $Se_b$ and $Se_s$ are bulk and surface atoms. The binding energies of the VB are negative, while the conduction bands (CBs) are positive [8].**

| $\varepsilon_i$ [eV] | | $MO_i$ | Tl | In | $Se_b$ | $Se_s$ |
|---|---|---|---|---|---|---|
| CB (*p*) | 0,9 | 417 | 4 | 6 | 19 | 71 |
| | 0,7 | 414 | 0 | 4 | 5 | 91 |
| VB (*sp*) | 0,5 | 411 | 1 | 7 | 71 | 21 |
| | 0,7 | 409 | 0 | 6 | 73 | 21 |
| | 1,1 | 404 | 0 | 4 | 90 | 6 |
| | 1,4 | 401 | 1 | 6 | 83 | 10 |
| | 1,6 | 397 | 2 | 16 | 74 | 8 |
| | 1,8 | 394 | 7 | 7 | 72 | 14 |
| | 2,2 | 391 | 0 | 25 | 58 | 17 |
| | 2,5 | 386 | 0 | 14 | 3 | 83 |
| | 2,5 | 385 | 27 | 5 | 65 | 3 |
| | 2,7 | 381 | 0 | 3 | 2 | 95 |
| | 2,9 | 377 | 0 | 6 | 4 | 90 |
| | 3,4 | 373 | 0 | 34 | 14 | 52 |
| VB (*s*) | 6,0 | 369 | 0 | 8 | 91 | 1 |
| | 6,4 | 365 | 0 | 7 | 89 | 4 |
| | 7,0 | 361 | 0 | 4 | 0 | 96 |
| | 7,7 | 357 | 1 | 5 | 5 | 89 |

interband transitions, then it can be argued that all other peaks of strain sensitivity observed in experiments are associated with indirect interband transitions caused from different points of the Brillouin zone.

**Table 2. Theoretically calculated in the $TlIn_4Se_{16}$ cluster (according to [8]) and experimentally determined in $TlInSe_2$ crystals, the band - band electronic transitions.**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Theoretically calculated in the $TlIn_4Se_{16}$ cluster | - | 1,2 | 1,4 | 1,8 | 2,1 | 2,3 | 2,5 | 2,9 |
| Experimentally determined in the $TlInSe_2$ crystal | 1,08 | 1,2 | 1,43 | 1,7 | 2,13 | 2,3 | 2,5 | 2,8 |

Such changes are more clearly manifested in the difference between the normalized spectral distributions of the strain sensitivity coefficients of positively and negatively deformed crystals (see Fig. 3). It can be seen from the figure that with negative deformation of crystals, i.e., in samples subjected to compression, the proportion of transitions with an energy of 1.4 eV is dominant, however, the proportion of strain sensitivity during illumination in the region of all other transitions decreases significantly. In contrast, at positive strain (in stretched specimens), the fraction of transitions with an energy of 1.4 eV is the smallest, while the fraction of strain sensitivity increases noticeably for all other transitions. Based on this, we can conclude that the mechanism of strain-sensitivity of $TlInSe_2$ crystals is indeed due to the flow of charges from one valley to another due to a change in the energy positions of the valleys during deformation.

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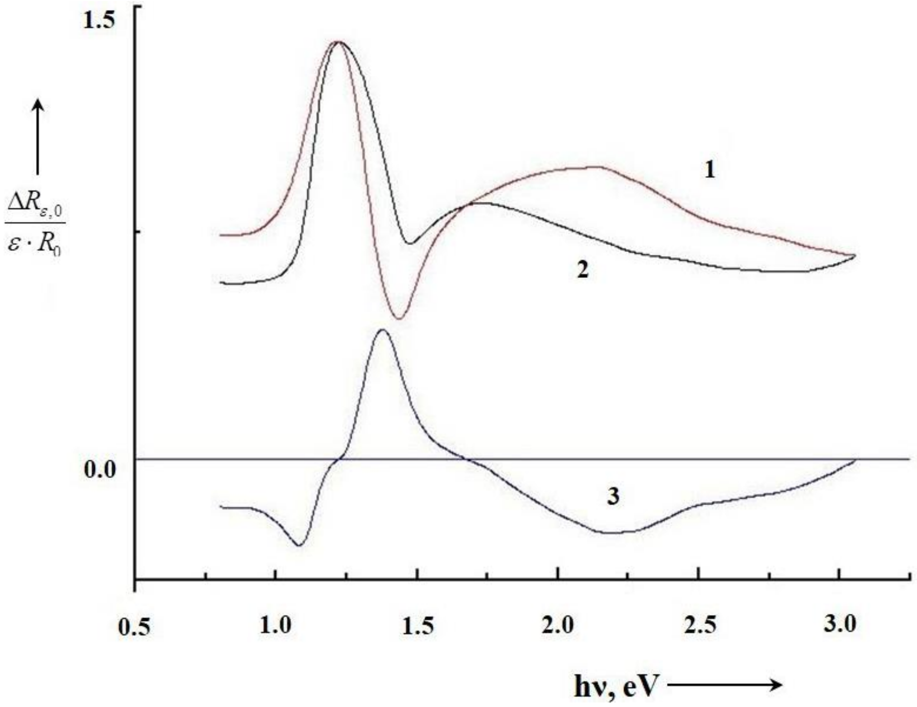


**Fig. 3. Spectral distribution of the strain sensitivity of a negatively deformed (1), positively deformed (2) $TlInSe_2$ crystal and the difference between 1 and 2 (3).**

**Conclusion:**Under uniaxial compression of $TlInSe_2$ crystals along the [001] direction, their band gap decreases. As a result, the Fermi level shifts and the concentration of electrons at r centers increases, which leads to the expansion of the linear sections of the LAH.

It is shown that under compressive and tensile deformations in the [001] direction, a change in the spectral distribution of the photocurrent is observed not only in the long-wavelength, but also in the short-wavelength (compared to the photocurrent maximum) region of the spectrum. This result indicates that there are indirect band transitions in $TlInSe_2$ crystals not only in the low-energy, in comparison with the direct band transition, but also in the high-energy region of the spectrum. It has been established that the band gap decreases under uniaxial compression, and increases under tension.

With positive and negative deformations, the maxima in the spectral distribution of the strain-sensitivity coefficient of $TlInSe_2$ crystals, due to electronic transitions from different valleys, are redistributed, which indicates that the mechanism of strain-sensitivity of $TlInSe_2$ crystals is due to the flow of charges from one valley to another due to a change in the energy positions of the valleys during deformation.

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