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# OPTICAL PROPERTIES OF MONOCLINIC $In_2Te_5$

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Optical properties of semiconducting compound $In_2Te_5$ with monoclinic structure were investigated: absorption and photoluminescence near fundamental edge at 1.3–1.7 eV were registered and spectroscopic ellipsometry measurements in spectral range of 1–5 eV were performed. It has been concluded that three oscillators in the mentioned spectral range are responsible for the optical singularity in dielectric function of investigated compounds, one of which is very weak. The contributions of other optical transitions were estimated as constants in dielectric function.

A possible ascription of investigated optical transitions for several symmetry points of $In_2Te_5$ Brillouin zone is discussed.

**Keywords:** absorption, photoluminescence, spectroscopic ellipsometry, dielectric function, monoclinic crystals

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## 1. Introduction

The optical properties of monoclinic $In_2Te_5$ (and other $A^3B^6$ compounds such as GaTe, InSe, and GaSe) have not been investigated so far. This is partly due to difficulty in growing single crystals with well defined stoichiometric composition. The crystals with relatively low symmetry are very interesting since their principal axes of dielectric tensors do not coincide with the crystallographic axes. This could cause the polarization singularities of optical spectra. The estimation of $In_2Te_5$ optical parameters is an initial task in solving such a problem. We have investigated the crystals grown earlier by one of the authors [1]. In the other letter [2] we have also presented some photoelectric properties of the mentioned compound.

## 2. Sample preparation and experimental set-up

Single crystals of semiconducting compound $In_2Te_5$ were grown by chemical transport employing iodine as a transport agent. The crystals had a plate-like character with the [100] direction perpendicular to the plane of the platelets. $In_2Te_5$ has a monoclinic structure with dimensions of the base centred cell $a = 13.47$ Å, $b = 16.51$ Å, $c = 4.365$ Å, $\beta = 92°05'$. The space group is $C^6_{2h}$ (or $C_{2/c}$ in Schönflies notation). The optical spectra measurements of investigated samples were performed on the natural (100) surfaces the area of which was $10\times1$ mm$^2$.

The room temperature photoluminescence spectra were measured with common equipment [3], the luminescence was excited with ILA 120 Ar laser light ($\lambda = 488$ nm) incident on the sample at approximately 30° angle and recorded using a conventional lock-in technique.

The ellipsometric measurements were carried out by means of a computer-controlled photometric ellipsometer. A monochromatic light incident upon the sample was linearly polarized at 45° with respect to the plane of light incidence. The reflected light intensity was measured as a function of the analyzer angle, which was varied by steps of 1.5°. The ellipsometric parameters $\Psi$ and $\Delta$ were determined [4] on-line and systematic errors caused by the wandering of the light spot on the detector were taken into account [5] by nonlinear regression analysis. The light incidence angle was 70°. Other experimental details were described elsewhere [6].

## 3. Experimental results and discussion

The low temperature absorption measurements made by us previously show that fundamental absorption edge of $In_2Te_5$ is formed by three optical transitions with energy indicated by arrows in Fig. 1. We could re-

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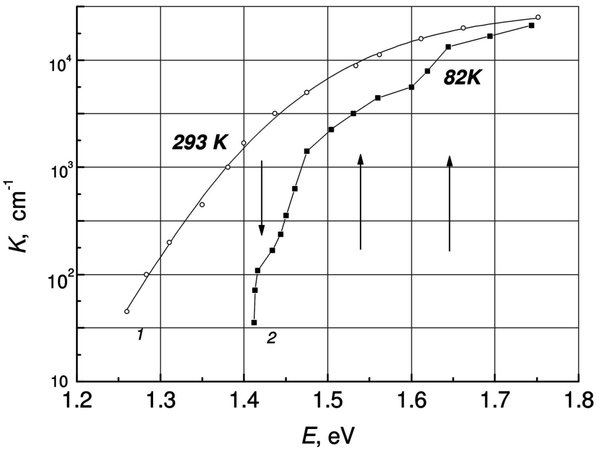

Fig. 1. Absorption spectra of $In_2Te_5$ at 293 and 82 K.

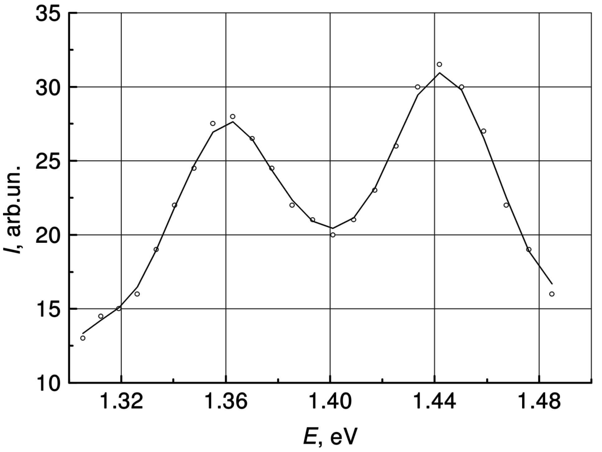

Fig. 2. Photoluminescence spectra of $In_2Te_5$ at room temperature.

solve them only in spectra measured at 82 K temperature, and temperature broadening forbade us to observe it in both room temperature absorption and luminescence (Fig. 2) spectra. Two peaks are detected in weak photoluminescence response signal.

From the measurement data of reflectivity $\rho$, which is the ratio of reflection amplitudes $r_k$ for the components polarized parallel ($k = p$) and perpendicular ($k = s$) to the plane of light incidence, the ellipsometric parameters $\Psi$ and $\Delta$ [7] were determined: $\rho = r_p/r_s = \tan\Psi \exp(\mathrm{i}\Delta)$, where $\Psi = \tan^{-1}|r_p/r_s|$, $\Delta = (\delta_{rp} - \delta_{ip}) - (\delta_{rs} - \delta_{is})$, and $\delta_{kd}$ is the phase of reflected ($k = r$) or incident ($k = i$) light polarized with respect to the plane of light incidence ($l = p, s$).

Experimental investigations of biaxial crystals meet with some difficulties. Therefore, a simplified technique was developed for interpretation of experimental results. The dielectric function of a biaxial crystal with high refraction and small anisotropy was successfully analysed [8] in a simple first-order approximation to pseudo-dielectric function (PDF), which has been calculated from ellipsometric data within the isotropic crystal model. The PDF approximation can be efficiently used for comparison of the optical spectra obtained in the other experimental set-up. The PDF approximation gives reasonable results for the dominant acting component to the optical response of a biaxial crystal. Such component originates from the projection of the dielectric tensor onto the line of intersection between the surface and plane of incidence, when one of the principal axes is normal to the plane of light incidence.

Table 1. Fitting parameters obtained by minimization, using the mean-squares method, of the difference between the experimental and calculated spectra of dielectric function components approximated by Lorentzian lines with amplitude $A_k$ (in $eV^2$), energy $W_k$ (in eV), and half-width $\Gamma_k$ (in eV), along with the effective contribution of higher energy transitions $\varepsilon_0$.

| Components $\varepsilon$ | Energy $W_k$ | Amplitude $A_k$ | Half-width $\Gamma_k$ | $\varepsilon_0$ |
|---|---|---|---|---|
| $\varepsilon_1, \varepsilon_2, \perp c$ | 2.065 | 0.001 | 0.001 | 2.35 |
| | 2.278 | 38.126 | 2.308 | 1.443 |
| $\varepsilon_1, \varepsilon_2, \parallel c$ | 1.47 | 7.2 | 0.75 | 2.473 |
| | 2.54 | 25.24 | 2.186 | 1.139 |

Figures 3 and 4 present the measured spectra of real $\varepsilon_1$ and imaginary $\varepsilon_2$ parts of dielectric function in two orthogonal sample geometries, e. g. with $c$ axes parallel and perpendicular to the plane of light incidence respectively. The experimental spectra of dielectric components were approximated by the contributions of Lorentzian oscillators in order to determine the main optical transitions contributing to the optical response of crystal:

$$\varepsilon_k = \frac{A_k}{W_k^2 - E^2 - \mathrm{i}E\Gamma_k}, \qquad (1)$$

where $A_k$, $W_k$, and $\Gamma_k$ are the amplitude, energy, and half-width of the $k$th Lorentzian line. The effective contribution of higher energy transitions was included in the calculated spectra through the constant term $\varepsilon_0$. The contribution of the free carrier system on the measured functions was taken into account as a Drude-like term. The values of estimated parameters from PDF approximation are presented in Table 1. These fitting parameters are obtained by minimization of the difference between the experimental and calculated spectra of the dielectric function components using the mean-squares method: amplitude of Lorentzian line $A_k$, energy $W_k$, half-width $\Gamma_k$, and the effective contribution of higher energy transitions $\varepsilon_0$.

The absorption, photoluminescence, and photoconductivity [2] measurements have shown that fundamen-

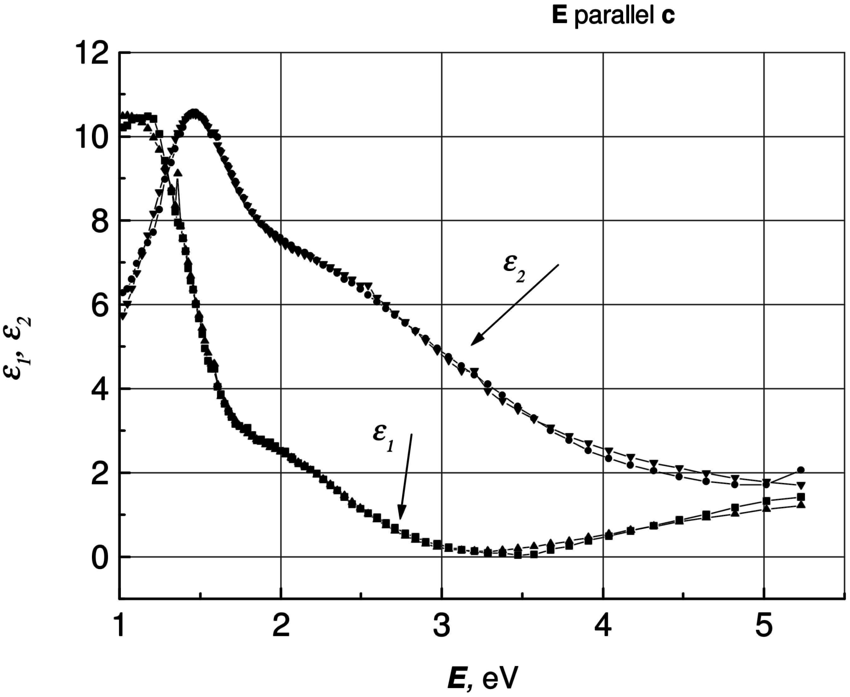

Fig. 3. Real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the pseudo-dielectric function for the sample with $c$ axis parallel to the plane of light incidence and modelled spectra (solid curves). Triangles mark experimental data.

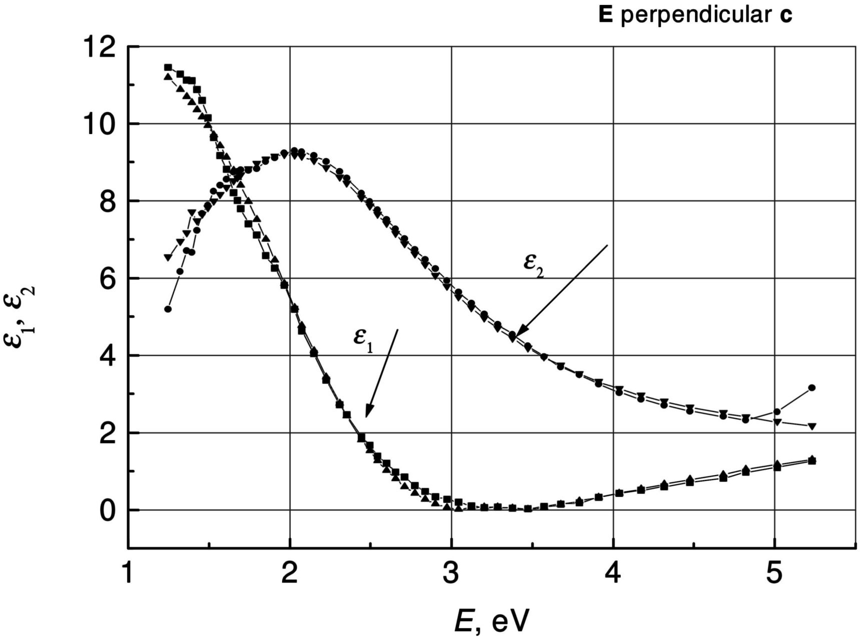

Fig. 4. Real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the pseudo-dielectric function for the sample with $c$ axis perpendicular to the plane of light incidence and modelled spectra (solid curves). Triangles mark experimental data.

tal absorption edge is caused by optical transitions with photons having energy of 1.3–1.4 eV. The second oscillator with the largest amplitude of about 30 $\mathrm{eV}^2$ (in comparison with $\sim$8 $\mathrm{eV}^2$ for transitions at 1.48 eV or 0.001 $\mathrm{eV}^2$ (!) for 2.1 eV) is at 2.4 (between 2.3 and 2.5) eV. Their contributions in formation of the pseudo-dielectric function are the deciding ones.

In many semiconducting compounds the fundamental band edge is caused by optical transitions in the centre of Brillouin zone, i. e. at point Γ (Fig. 2 in [8]). The sampling rules for the investigated space group indicate that transitions with photon energy of 2.4 eV can occur at the border of Brilouin zone in points having symmetry similar to $X$ or $B$ point symmetry. They are

Table 2. Selection rule for $C_{2h}^6$ group dipole transitions and their assigned energy.

| Point | Polarization | | Energy, eV |
|---|---|---|---|
| | $\perp c$ | $\parallel c$ | |
| $\Gamma(A)$ | | $\Gamma_{1,2,3,4} \rightarrow \Gamma_{2,1,3,4}$ | 1.47 |
| | $\Gamma_{1,2,3,4} \rightarrow \Gamma_{4,3,2,1}$ | | 1.34–1.43 (from [2]) |
| X(B,U) | $X_1(B_{1,2}) \rightarrow X_1(B_{1,2})$ | $X_1(B_{1,2}) \rightarrow X_1(B_{1,2})$ | 2.4 |
| $\Lambda$ | $\Lambda_{1,2} \rightarrow \Lambda_{2,1}$ | | 2.1 |

allowed for light polarized both parallel and perpendicular to crystal $c$ axes. We suppose that the weak oscillator with energy near 2.1 eV is related with the lowest symmetry point inside Brillouin zone, such as $\Lambda$. Such transition requires the light to be polarized perpendicular to $c$. The speculative assignment of transitions to the Brilioun zone points is presented in Table 2.

## References

[1] J. Verkelis, Single crystals of $In_2Te_5$, Mater. Res. Bull. **9**, 1063–1066 (1974).

[2] J. Verkelis and R. Bendorius, Poliarizacionnaya zavisimost' spektrov fotoprovodimosti i pogloshcheniya $In_2Te_5$, Fiz. Tekh. Poluprovod. **13**, 1222–1224 (1979) [in Russian].

[3] R.A. Bendorius, J. Sabataitytė, I. Šimkienė, V. Jasutis, H. Tvardauskas, and Z. Martūnas, Luminescence and surface properties of porous GaAs, Lithuanian J. Phys. **40**, 63–66 (2000).

[4] A. Galickas, Nekotorye metody v nelineynom regressionnom analize, Pis'ma Zh. Tekh. **18**, 6–10 (1992) [in Russian].

[5] A. Galickas, Regression analysis in experimental technique, Lithuanian J. Phys. **39**, 149–153 (1999) [in Russian].

[6] G.J. Babonas, L. Leonyuk, A. Galickas, A. Rėza, L. Shvanskaya, L. Dapkus, and V. Maltsev, Optical properties of cuprate crystals with incommencurate structure, Supercond. Sci. Technol. **10**, 496–501 (1997).

[7] R.M.A. Azzam and N.M. Bashara, *Ellipsometry and Polarized Light* (North-Holland, Amsterdam, 1977).

[8] T.N. Sushkevich, Pravila otbora dipolnykh i kvadrupolnykh perekhodov dlya kristallov monoklinnoy singonii, Izv. Vuzov, Fizika **7**, 155–159 (1971) [in Russian].

# MONOKLININIO $In_2Te_5$ OPTINĖS SAVYBĖS

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### Santrauka

Pateikti monoklininės sandaros puslaidininkio $In_2Te_5$ eksperimentiniai sugerties ir fotoliuminescencijos spektrai, išmatuoti ties pagrindinio sugerties krašto (1,4 eV) energine sritimi, bei dielektrinės funkcijos sandų 1,0–5,0 eV srityje elipsometriniai spektrai, taip pat pastarųjų aproksimacija pseudodielektrinės funkcijos (PDF) metodu.

Išmatuotos osciliatorių energinės vertės sugretintos su teoriniais optinių šuolių, galimų įvairiose monoklininės simetrijos kristalų Brijueno (Brillouin) zonos taškuose pagal atrankos taisykles, skaičiavimais. Rasta, kad trys skirtingos amplitudės osciliatoriai lemia tirto junginio optines savybes matuotoje srityje, kai kitų optinių šuolių indėlis formuojant optinius parametrus įvertintas pastoviu dydžiu.