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CRITICAL POINTS OF SPECTRUM OF THE DIELECTRIC PERMEABILITY OF THALLIUM-SELENIUM

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The analysis of the lines form of spectra second derivative of main components of the dielectric permeability TlSe tensor near to critical points were carried out. On multy angular method in two orientations of relatively optical axis of a crystal carried out spectraclipsometrical researches at 1,240-3,025eV data were used. The energies of critical points (I), spread parameters (F) and amplitude (A). The majority of the revealed structures are identified and are compared to the earlier found out structures in spectra reflection, thermoreflection and absorbtion.

The optic single-axis crystal thallium-selenium is the most investigated representative of love dimensial semiconductors $TlMeX_2$ (Me= In, Ga; X=Sc, S, Te), having chained structure. In [1,2] the components of tensor of the dielectic permeability of parallel ($E_{||}$) and perpendicular ($E_{\perp}$) optical axis of a crystal are measured by spectroelipsometrical method at room temperature. There are noted the consent of elispometrical data with results of other authors received from measurements of reflection [3, 4, 5], thermoreflection [6] and absorption [7] spectra. Nevertheless, it is required the more detailed analysis, at first, for an establishment types of critical points of observable features in E (ω) spectra, and secondly, for quantitative definition parameters determining the form of spectra lines.

In the present work the analysis of the lines form of spectra dielectric permeability near to Van-Hoffs critical points is carried out, that has allowed to determine energy of critical points (E), spreading parameters (Γ), amplitude (A).

In order to more abruptly to allocate structures in spectra of dielectic permeability and to determine parameters of critical points', second derivative of spectra of the complex dielectric function for both polarization are calculated [8]. Previously data of spectroelipsometric researches are smoothed on part by part most precisely describing an experimental curve polinom. Each subsequent site of a curve is got out so, that the beginning of a site settled down above than end previous one.

The points of connection were fixed. The equality third derivatives' was the tacking. Such procedure is necessary for reception the spectra of second derivative of dielectric function. The spectra second derivative of dielectric function received by differentiation of theoretical expression are shown in Fig. 1 and Fig. 2.

$$E(\omega) = C - Ae^{i\phi}(\omega - E + i\Gamma)^m, \qquad (1)$$

where ω is a frequency of dropping radiation, n is a parametr determining the dimension of Van-Hoff's feature, n=1/2 for three-dimensional feature and n=-1/2 for one-dimensional. It is accepted to consider n=0 for two- dimensional feature. Actually, instead expression (1) we have

$$E(\omega) = C - Ae^{i\phi}\ln(\omega - E + i\Gamma) \qquad (2)$$

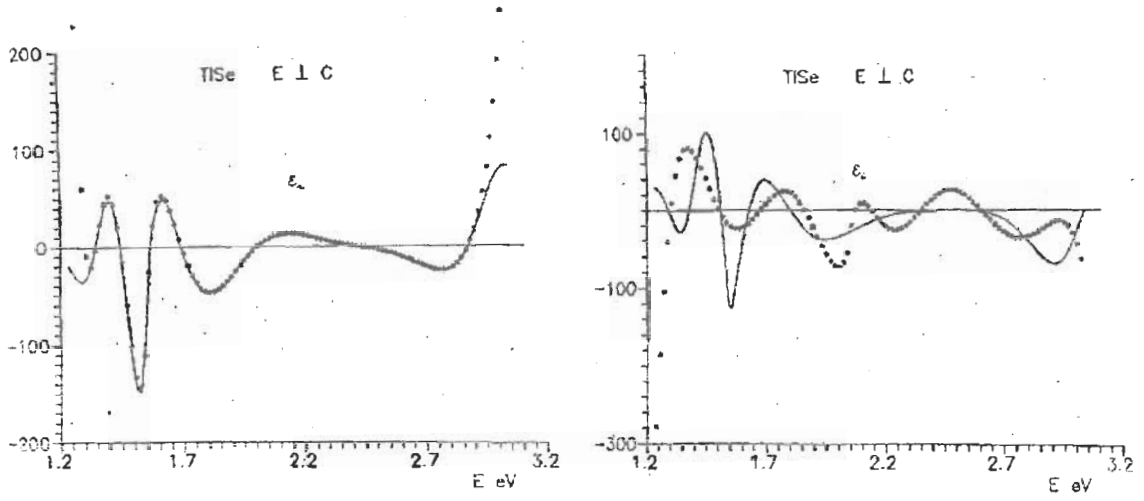

Fig. 1.
Second derivative of real (Er") and imaginary (Ei") part of smoothed dielectric function for E⊥C. The solid line is corresponded to the superposition of functions for real part of second derivative of dielectric function (1) and the dashed line is corresponded to the imaginary part.

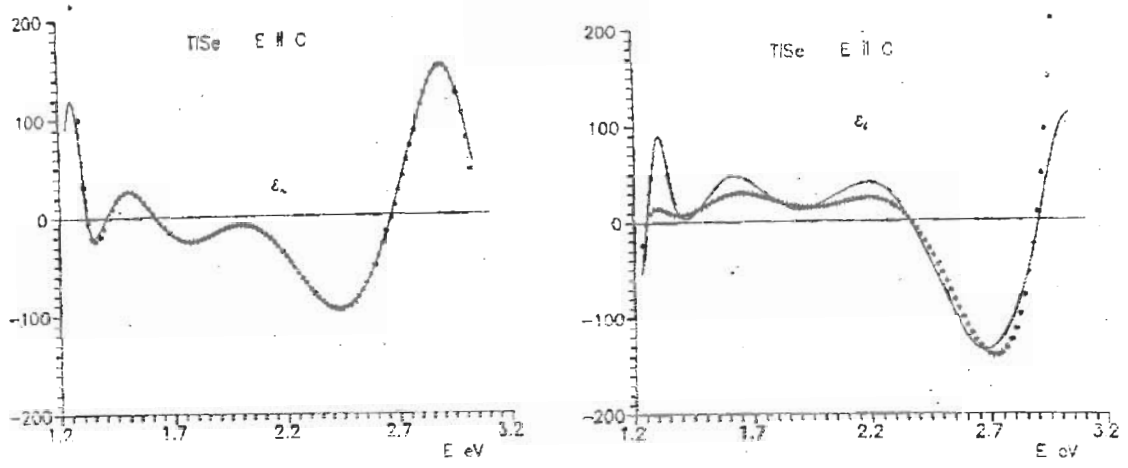

Fig. 2.
Second derivative of real (Er") and imaginary (Ei") part of smoothed dielectric function for EIIC. The solid line is corresponded to the superposition of functions for real part of second derivative of dielectric function (1) and the dashed line is corresponded to the imaginary part

Here and in (1) Γ is a half-width of researched peak, A is a amplitude of a bell of researched peak, and ϕ is a phase angle determining type of Van-Hoff s feature. At this, in a three-dimensional case to a critical point M_0 it is corresponds $\phi=3\pi/2$, M_1- $\phi=0$, M - $\phi=\pi/2$ and M_3 - $\phi=\pi$.

For two-dimensional case we have: $\phi=0$ (2D min); $\phi=\pi/2$ (2D saddles) and $\phi=\pi$ (2Dmax).

For one-dimensional case we have: $\phi=\pi/2$ (1D min), $\phi=0$ (1D max).

At least, the n=-1 case is corresponded an exciton condition.

In Fig. 1 and 2 the solid line is corresponded a superposition values of second derivative of real part function of a kind (1). Second derivative of the imaginary part of dielectric function is shown by dashed line. The parameters of functions (1) were defined by adjustment of second derivative of the real part of a smoothed experimental dielectric function.

Table 1.

Energetic points, polarization and parameters of Van-Hoffs features, comparison with literature data and identification.

E (ev)	*C.P.*	*Γ(ev)*	*Φ (grad)*	*A*	*Translation (3,4,6)*	*E (ev) (3,4,5,6,7)*
1,33(4) ∥	Exiton	0,135	228	0,05		1,291[7]
1,35(0) ⊥	Exiton	0,147	0	0,10		1,291[7]
1,45(2) ⊥	3D(M0+M1)	0,043	296	0,61		-
1,50(2) ⊥	2Dmin	0,075	0	0,57	$P_5 - P_1 + P_4$	1,50[4]
1,53(8) ⊥	3DM1	0,030	0	1,52	$P_5 - P_1 + P_4$	1,55[4]
1,61(4) ∥	2Dmin + saddl	0,337	0	6,55	$T^1_3(T_{12}) - T^1_{10}(T_{14})$	1,61[6]
1,61(6) ⊥	1D(min+max)	0,122	26	0,29	$T^1_3(T_{12}) - T^1_{10}(T_{14})$	1,635[4], 1,618[5]
1,83(5) ∥	3D(M1+M0)	0,156	325	4,13	$G_4 - G_1$	1,95[6], 1,94[5]
1,84(0) ⊥	2Dmin+sedl	0,260	24	3,48	$T^1_6 - T^1_4$	1,895[4], 1,9[6]
2,36(0) ⊥	2Dmin	0,216	0	0,16	$N^1_4 - N^1_5$	2,24[4], 2,4[6], 2,4[5], 2,26[3]
2,36(0) ∥	2Dmin	0,337	0	6,55	$N^1_4 - N^1_5$	2,4[6],2,42[5] ,2,26[3]
2,67(2) ∥	Exiton	0,339	10	1,10		2,78[6], 2,8[5], 2,8[3]
2,93(0) ∥	1D(min+max)	0,263	60	5,44	$N^1_4 - N^1_8$	2,92[5], 2,95[6]
2,98(9) ⊥	Exiton	0,288	65	0,96	$G^1_4 - G^2_1$	3,0[6], 2,96[5], 2,95[3]

For adjustment the second derivative of the real part of an experimental dielectric function it was applied the method of the least squares fitting.

An amplitude, a phase angle, dimension, a spreading parameter, a critical point energy were considered as fitting parameters. The adjustment was made part by part. The chosen site was adjusted using second derivative of functions (1) and (2) kind. The following step was the subtraction value of given function from fitting curve and then again received data were adjusted on the previous' scheme. The error of adjustment does not exceed 1% of value of the second derivative of dielectric functions.

The power points of Van-Hoffs features, a polarization, dimension of features, a phase arigle, a half-veidth and an amplitude are given in Table 1. There are given for comparison found earlier by authors [3-7] the structures in spectra of reflection,

theroreflection and absorption, and also identification of these structures according to the calculated zone structure of TlSe [9] and the selection rule [3, 6].

As is obvious from Table 1., in two cases it was possible to establish the presence of one-dimensional feature in zone structure of TlSe, that was possible to expect because of chained structure of this crystal. In the majority of cases, three-dimensional and a little less often two-dimensional features are observed. The similar situation is typical and for layered crystals [8].

As well the exciton structures in spectra dielectric function are found out above edge of fundamental absorption. Some of them, in particular, a structure at energy 1,33eV for E||C polarization and 1,35eV (E⊥C) was found out in [7] at energy 1,291eV and was interpreted as hyperbolic exiton.

Thus, the energy of critical points, the spreading parameters, amplitudes and dimensions are determined from the analysis of the form of spectra lines of second derivative permeability TlSe near to critical points.

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TALLİUM-SELENİUM DİELEKTRİK FUNKSİYASI SPEKTRİNDƏ BÖHRAN NÖQTƏLƏRİ

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Tallium selenidin kritik nöqtələrin yaxınlıqında olan dielektrik keçicilik tenzorunun ikinci törəmələrinin analizi aparılıb. Analiz üçün enerjinin 1,240 – 3,025eV qiymətləri arasında TlSe-nin çoxbucaqlı metodika üzrə optik oxa nisbətən iki səmtləşmədə aparılmış spektroellipsometrik təqiqatların nəticələrindən istifadə olunub. Kritik nöqtələrin enerjisi (E), enləşmə parametri (Q) və amplitud (A) təyin edilib. Aşkar edilmiş strukturların çoxu müəyyənləşdirilib və əvvəllər aşkar edilmiş strukturlarla qaytarma, termo qaytarma və hopdurma spektrləri tutuşdurulub.

КРИТИЧЕСКИЕ ТОЧКИ В СПЕКТРЕ ДИЭЛЕКТРИЧЕСКОЙ ФУНКЦИИ СЕЛЕНИДА ТАЛЛИЯ

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Проведен анализ формы линий спектров вторых производных главных компонент тензора диэлектрической проницаемости селенида таллия вблизи критических точек. Для анализа использованы данные спектроэллипсометрических исследований TlSe в области энергий 1,240-3,025eV, проведенных по многоугловой методике в двух ориентациях относительно оптической оси кристалла. Определены энергии критических точек (E), параметры уширения (Г) и амплитуды (A). Большинство выявленных структур идентифицированы и сопоставлены с ранее обнаруженными структурами в спектрах отражения, термоотражения и поглощения .