RESEARCH OF CRITICAL POINTS IN THE ENERGY SPECTRUM $TlInSe_2$

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The present work is devoted to detail study and improvement of the band structure $TlInSe_2$. With this purpose we analyzed the spectroellipsometric measurement results of imaginary and real parts of dielectric function in an energy range E = 1,2- 3,02 eV for detection of Van-Hove singularities. The classification of the found structures, identification to their transitions in the earlier designed band structure $TlInSe_2$ is carried out. The correlation energy position of structures observed in $TlInSe_2$ with the energy position of structures found in base crystal TlSe is found.

INTRODUCTION

Halcogenids of the elements of the third group of a periodic table crystallize in chain and layer structures. TlSe, $TlInSe_2$, TlGaTe, TlInTe crystallizes in a chain structure. Many physical properties of these compounds reveal an anisotropy. In connection with the interest to low dimensional systems the big attention is given to their electron spectra, which determine the above mentioned singularities of physical properties. The band structure $TlInSe_2$ are carried out by the authors [1-5]. So in [1] the spectral dependence of the absorption coefficient is investigated and the conclusion, that E = 1,18 eV and the intrinsic absorption edge is stipulated by direct transitions. In work [2] the opposite conclusion that $TlInSe_2$ -indirectband semiconductor with E = 1,14±0,02eV is done and the energy of phonons participating in the optical transitions0,08eV is estimated. The authors [3] analyzing a spectral dependence of an absorption coefficient have revealed in the energy range 1,45-1,6 eV direct solved transitions with a minimum energy 1,44 eV. In work [4] investigations of a long-wave length absorption edge are shown, that $TlInSe_2$ - indirectband semiconductor with E = 1,21 eV and it is stipulated by phonons with an energy E = 0,045 - 0,005eV, and also, that the weak absorption bands with E = 1,16 eV and E = 1,08 eV at T = 80 K and T = 300 K accordingly are connected with indirect exiton transitions. In same work the spectra of photoconductivity $TlInSe_2$ are investigated. It is shown, that the crystals have high photosensitivity in the energy range 0,95-1,7 eV. A position of a long-wave length maximum at the energy 1,2-1,25 eV the authors assign to indirect optical transitions. Spectroellipsometric measurement in the energy range E = 1,2-3,02 eV, which allow to obtain the imaginary and real parts of dielectric function from experiment are carried out.

CLASSIFICATION OF VAN-HOVE SINGULARITIES

To improve the band structure $TlInSe_2$ we analyze the critical points. For data processing the analytical expression for dielectric function is used

$$\varepsilon(\omega) = C - A\exp(i\varphi)(\omega - E + i\Gamma)^n \quad ,$$

where ω - phase frequency of an incident radiation; n - parameter defining dimension of Van-Hove singularity; φ - phase angle, defining type of Van-Hove singularity; Γ - half-width of researched peak; A - amplitude of a bell of researched peak; E - energy of Van-Hove singularity.

Case n = -1 corresponds to exiton state (Fig.1).

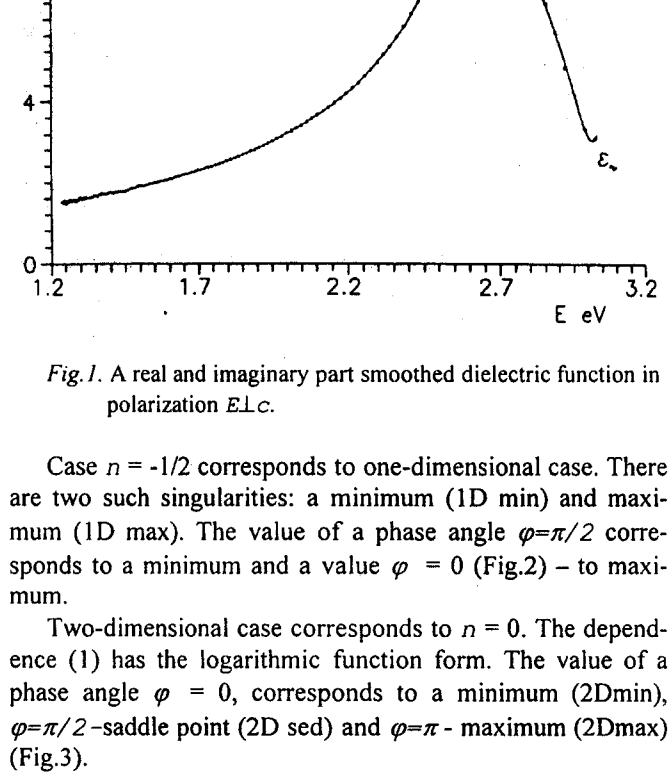

Fig.1. A real and imaginary part smoothed dielectric function in polarization $E \perp c$.

Case n = -1/2 corresponds to one-dimensional case. There are two such singularities: a minimum (1D min) and maximum (1D max). The value of a phase angle $\varphi=\pi/2$ corresponds to a minimum and a value φ = 0 (Fig.2) – to maximum.

Two-dimensional case corresponds to n = 0. The dependence (1) has the logarithmic function form. The value of a phase angle φ = 0, corresponds to a minimum (2Dmin), $\varphi=\pi/2$ -saddle point (2D sed) and $\varphi=\pi$ - maximum (2Dmax) (Fig.3).

For three-dimensional case n = 1/2 the value of a phase angle $\varphi=3\pi/2$ corresponds to minimum (M0), φ = 0 - to saddle point (M1), $\varphi=\pi/2$ – to saddle point (M2) and $\varphi=\pi$ - to maximum (M3) (Fig.4).

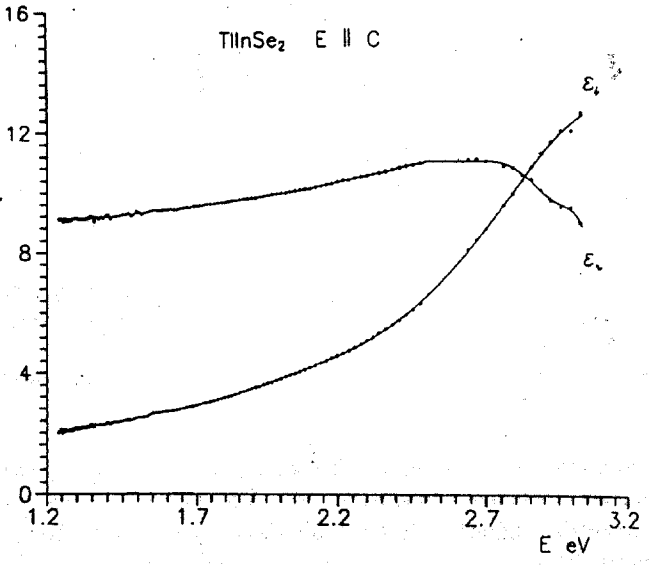

Fig.2. A real and imaginary part of dielectric function in polarization $E \parallel c$.

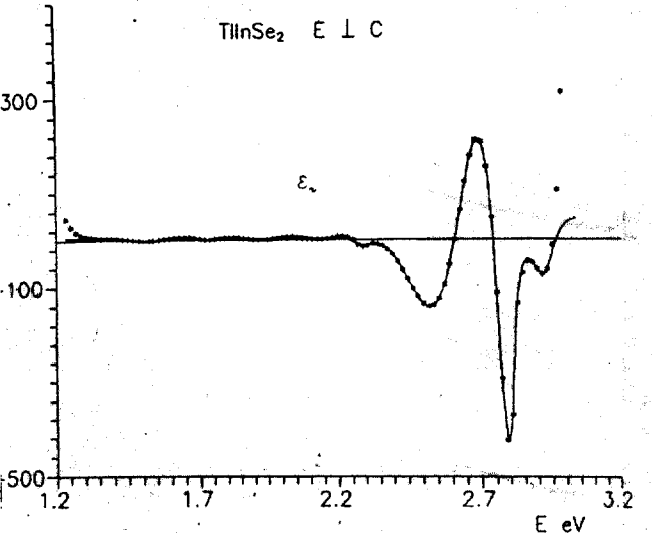

Fig.3. Second derivative of a smoothed real part of dielectric function in polarization $E \perp c$.

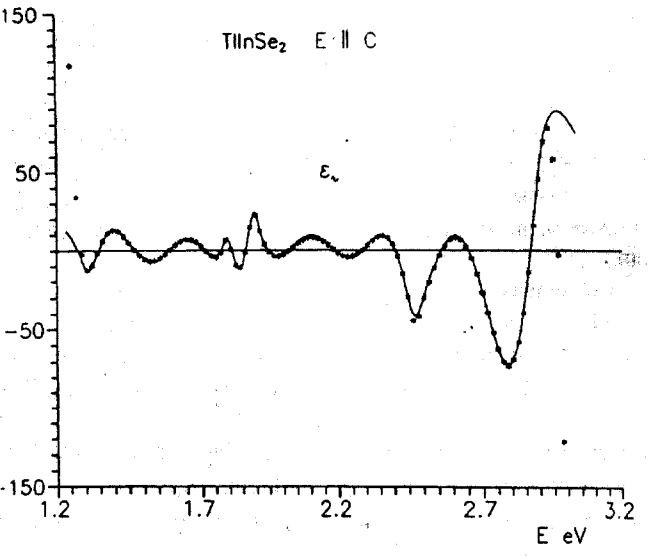

Fig.4. Second derivative of a smoothed real part of dielectric function in polarization $E \parallel c$.

RESULTS

For the correct definition of the energy position of Van-Hove singularities, and also their classification it is necessary to investigate the second derivatives of an imaginary and real part of dielectric function. On (Fig.4) the second derivative of a smoothed real part of dielectric function in polarization $E \perp c$ is represented. On (Fig.5) the second derivative of a smoothed real part of dielectric function in polarization $E \parallel c$ is represented. On (Fig.6) and (Fig.7) the second derivatives of smoothed imaginary part of dielectric function in two polarization $E \perp c$ and $E \parallel c$ accordingly are represented.

As result the energy position of Van-Hove singularities was found, and their classification is made.

The results are shown in a table (1).

Table 1.

$TlInSe_2$			
Energy (eV)	Classification	Polarization	Identification
1.51(7)	3D(M0+M1)	$E \perp c$	P5 - (P1+P4)
1.64(3)	Exiton	$E \perp c$	--
1.72(1)	2Dmin	$E \perp c$	T3 – T10
1.92(8)	2Dmin	$E \perp c$	T6 – T4
2.17(0)	3D M1	$E \perp c$	--
2.39(0)	2Dmin	$E \perp c$	N4 – N5
2.51(1)	3D(M0+M1)	$E \perp c$	--
2.67(1)	1D(min+max)	$E \perp c$	--
2.81(2)	2D min	$E \perp c$	--
2.92(7)	2D (min+c)	$E \perp c$	N4 – N8
1.55(3)	3D M1	$E \parallel c$	P5 – (P1+P4)
1.79(2)	3D(M2+M3)	$E \parallel c$	T3 – T10
1.84(7)	3D M1	$E \parallel c$	G4 – G1
2.25(0)	3D(M0+M1)	$E \parallel c$	--
2.46(8)	2D min	$E \parallel c$	N4 – N5
2.68(2)	2D(max + c)	$E \parallel c$	--
2.84(7)	2D min	$E \parallel c$	N4 – N8
2.90(5)	1D min	$E \parallel c$	--

DISCUSSION

The presence of correlation between singularities observed in base crystal TlSe [6] and $TlInSe_2$ is very interesting. Let's consider in the beginning singularities observed in $TlInSe_2$ in polarization $E \perp c$ and compare them transitions in calculated band structure [5].The singularity at the energy E = 1,51 (7) eV, being superposition of a three-dimensional mixed minimum with a saddle, is interpreted by us as transition P5-P1 + P4, i.e. in polarization $E \perp c$ only one component of a doublet registered in TlSe. The exiton state at the energy 1,64 (3) eV is observed. Observed by us in TlSe exiton peak at energy E = 1,35 (1) eV is shifted respect of above mentioned one approximately on 0,3 eV. It is stipulated by that forbidden band width $TlInSe_2$ almost on 0,3eV more than in TlSe. The energy position of a two-dimensional minimum at E = 1,92 (8) eV will be well agreed with the energy position of critical point being mixing of a two-dimensional minimum with a saddle at E = 1,84 (7) eV in TlSe. We have compared transition T3-T10 and transition T6-T4 to singularities at E = 1,72 (1) eV and E = 1,92 (8) eV accordingly. It is established that the structure observed at E = 2,17 (0) eV is a three-dimensional saddle, and at E = 2,39 (0) eV it is a two-

dimensional minimum and corresponds to transition N4-N5. This structure will be well agreed with the two-dimensional minimum at E=2,36(2) eV in TlSe. It is possible to confirm, that the singularity at E = 2,67 (1) eV is mixing of one-dimensional minimum with a maximum, and the structure at E = 2,81 (2) eV is a two-dimensional minimum. The structure at E = 2, 92 (7) is identified as transition N4-N8. Let's consider now the singularities observed in $TlInSe_2$ in polarization $E \| c$. Structure at E = 1,55 (3) eV being a three-dimensional saddle M1 is interpreted as the transition P5-P1 + P4. As the energy position of this singularity disposes near of the critical point according to superposition of a three-dimensional mixed minimum and a saddle in polarization $E \| c$ then it is reasonably to assume, that it is the same structure. The singularity exhibiting as a mixing of a three-dimensional saddle with a maximum at E = 1,79 (2) eV we are identified the transitions T3-T10, and three-dimensional saddle M1 corresponds to transition G4-G1. The energy position of this singularity also well correlates with a singularity observed in TlSe at energy E = 1,83 (1) eV in the same polarization. It is established, that the structure at E = 2,25 (0) eV is superposition of a three-dimensional minimum with a saddle M1 and can be identified as transition on a line of a symmetry D1-D1. Two-dimensional minimum observed at E = 2,46 (8) eV corresponds to transition N4-N8. The energy position, and also classification of this singularity will be well agreed to the observed critical point at E = 2,36 (7) eV in the same polarization. It is established, that the structures at E = 2,68 (2) eV and E = 2,84 (7) eV are two-dimensional minima, and to a last structure there corresponds to the transition N4-N8. It is possible unequivocally to confirm, that the singularity found at E= 2,90 (5) eV is superposition of one-dimensional minimum and maximum.

CONCLUSIONS

Obtained as result of investigations of structures, and also their found identification allow to improve of the band structure $TlInSe_2$. Transitions between electronic levels univalent thallium are observed both in TlSe, and in $TlInSe_2$ almost at the same values of an energy and represent Van-Hove singularities of one type and dimension.

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$TlInSe_2$ ENERJİ SPEKTRİNDƏ BÖHRAN NÖQTƏLƏRİN TƏDQİQİ

Bu işı $TlInSe_2$-nin quruluşunun dəqiq öyrənilməsi və tə'yininə həsr olunmuşdur. Bu məqsədlə Van-Xov xüsusiyyətlərini aşkar etmək məqsədi ilə E=1,23,02 eV enerji intervalında dielektrik funksiyasının həqiqi və mövhumi hissələrinin spektroellipsometrik ölçülərinin nəticələri analiz edilmişdir. Tapılan strukturların klassifikasiyası aparılmış, $TlInSe_2$-də qabaqcadan hesablanmış zona quruluşundakı keçidlərə aidliyinə baxılmışdır. Baza kristalı TlSe-də müşahidə edilən strukturların enerji vəziyyətləri ilə $TlInSe_2$-də görülən strukturların enerjı vəziyyətlərinin korrelyasiyası müşahidə edilmişdir.

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ИССЛЕДОВАНИЕ КРИТИЧЕСКИХ ТОЧЕК В ЭНЕРГЕТИЧЕСКОМ СПЕКТРЕ $TlInSe_2$

Настоящая работа посвящена детальному изучению и уточнению зонной структуры $TlInSe_2$. С этой целью нами были проанализированы результаты спектроэллипсометрических измерений мнимой и действительной частей диэлектрической функции в интервале энергий E=1,2-3,02 эВ на предмет выявления особенностей Ван-Хова. Проведена классификация найденных структур, идентификация их переходам в ранее рассчитанной зонной структуре $TlInSe_2$. Была обнаружена корреляция энергетического положения структур, наблюдаемых в $TlInSe_2$ с энергетическим положением структур, обнаруженных в базовом кристалле TlSe.

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