SPECTRA OF OPTICAL PARAMETERS OF Bi_2Te_3 FILM IN 1÷6 eV INTERVAL

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Reflection spectra *R(E)* of Bi_2Te_3 film samples in energy interval1÷6 eV of beam falling normally on the surface are measured in work.

Keywords: reflection coefficient, optical conduction.
PACS: 535.3; 539.2/6: 539./.04

1. INTRODUCTION

R(E) reflection coefficients of some materials (amorphous and monocrystalline) Se, Se-S, $InSnTe_2$, $TlIn_{0.9}Ce_{0.1}Se_2$, $TlInSe_2Ce_{0.04}$, $TlInSe_2$, Cu_3GdTe_3, Cu_5GdTe_4, $CuGdTe_2$, $Se_{95}As_5$ (with Sm impurity), Bi_2Te_3(Ni, Cu, Zn), Bi_2Te_3, Bi_2Se_3) are measured by us and their optical parameters such as reflected light phase θ, indexes of absorption κ and refraction n, real $\varepsilon_1$and imaginary ε_2 parts of dielectric constant, α absorption coefficient, function of characteristic $-Img\ \varepsilon^{-1}$ volume and $-Img(\varepsilon+1)^{-1}$ surface electron loss, electro-optical differential functions$(\alpha,\ \beta)$, optical conduction ε_2E, integral function of bound state density ε_2E^2, effective static dielectric constant ε_0(E), effective number of valence electrons $n_{ef}(E)$ [1] taking part in transitions up to the given E energy, are calculated.

Bismuth telluride is known as effective material for thermo-electric transformations. This material is easy to prepare in the form of perfect single crystals and obtain n- and p-types by doping [2,6]. Bi_2Te_3 crystals have the packet structure and the bound between neighbor packets has the mixed Van-der-Waals covalent character [7]. The additional bound because of transition of one p-electron on d-levels and overlapping of some d-levels with valence band takes place between packets. All this facts causes the significant metallic properties and comparably small values of its forbidden band energy in 0,15÷0,35 *eV* interval. Bi_2Te_3 and its analogies are the uniaxial crystals in optical respect. The dielectric constant in them is the tensor of second order and depends on falling wave direction in respect of C optical axis. The optical properties of bismuth telluride are investigated in region of higher frequencies in work [5].

The structure of crystal bands is theoretically calculated in work [5]. The absence of data on value of spin-orbit interaction (Δ) and character complexity of chemical bond between Bi_2Te_3 atoms make significant difficulties. Bismuth telluride and solid solutions on its base apply at preparation of different energy transformers [7].The single-crystal or polycrystalline Bi_2Te_3 and its solid solutions with Bi_2Se_3 are mainly used. The single crystal samples Bi_2Te_3 are easily splitted off by cleavage planes [0001] forming the mirror surface which is stable to oxidation that is very important for carrying out of optical measurements and doesn't require the special chemical treatment.

The study of Bi_2Te_3 band structure hasn't achieved such level as germanium, $A^{III}B^{V}$ compounds that is connected with the complexity of its crystal and band structure [3].This makes necessary for new investigations in this direction. The measurement of crystal reflection coefficient of n- and p-types parallel and perpendicularly to C axis and also its polycrystalline film samples and definition of spectra of their optical parameters on the base of reflection coefficient are the task of the given work.

2. EXPERIMENT TECHNIQUE

The split of Bi_2Te_3 single crystals having the mirror surface is used for measurement of R(E) reflection coefficient. The reflection coefficient is measured by method of two-beam spectroscopy. The crystals are doped by Cl impurities having n-type conduction and Tb impurities having p-type conduction.

The obtaining technology of Bi_2Te_3 single crystals and films is described in works [8,9,10]. The single crystals are obtained by Bridgman method as in [3] and Bi_2Te_3 films by thickness 0,3mkm of polycrystalline on the split of rock salt crystals are its sublimation in vacuum. The definition methods of optical parameters are given in work [11] and procedure is explained in [12].

The special computer programs are used for calculation of optical parameters. The optical parameters of investigated materials are calculated by programs made by work author [13]. These programs are checked at calculation of optical parameters of some materials in works [14 – 18].

3. THE RESULTS AND THEIR DISCUSSION

R(E) reflection coefficients of single-crystal of n- and p-types parallel and perpendicularly to C axis and also its film samples of n- and p-types are measured in the work and spectra of their optical parameters: α absorption coefficient, ε_1 real and ε_2 imaginary parts of dielectric constant, indexes of κ absorption and n refraction, effective number of valence electrons $n_{ef}(E)$ taking part in transitions up to the given E energy, $\varepsilon_0(E)$ effective static dielectric constant, $Img(\varepsilon+1)^{-1}$ surface electron loss, θ reflected light phase, ε_2E optical function of characteristic $-Img\ \varepsilon^{-1}$ volume and –conduction, ε_2E^2 integral function of bound state density and $(\alpha,\ \beta)$ electro-optical differential functions are defined.

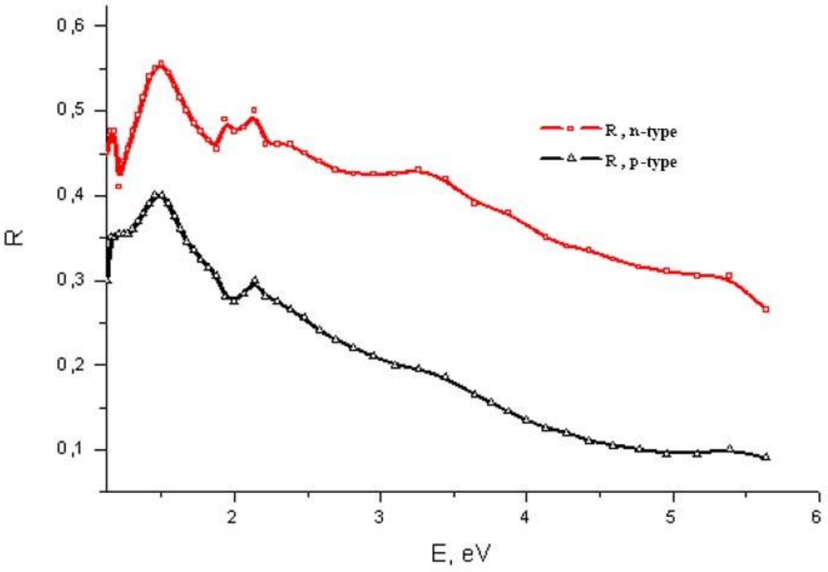

Fig.1. Reflection spectra of film Bi_2Te_3 of n- and p-types.

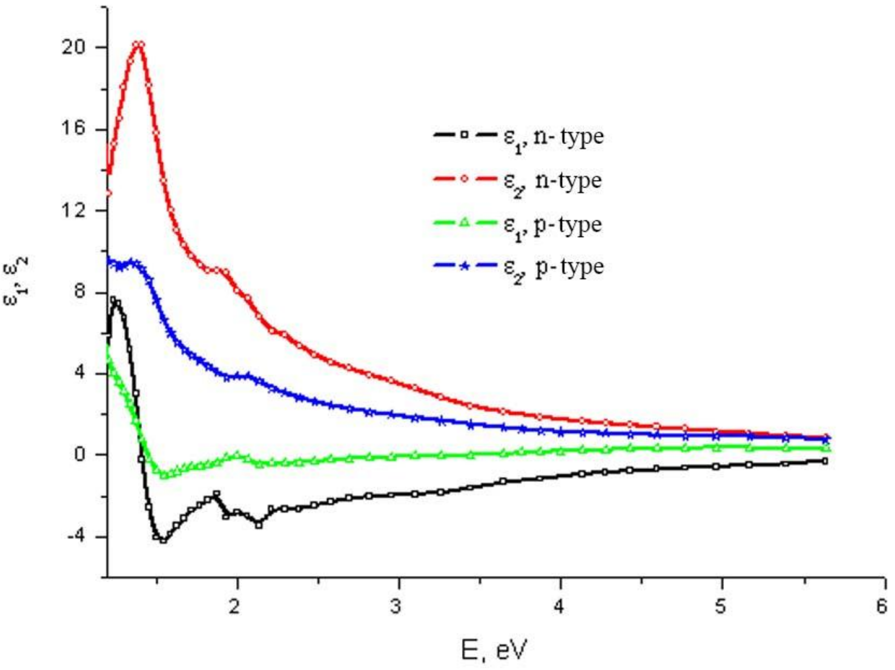

Fig.2. Spectra of coefficients ε_1 and ε_2 of film Bi_2Te_3 of n- and p-types.

Only R(E) reflection coefficients, ε_1 real and ε_2 imaginary parts of dielectric constant, function of characteristic $-Img\ \varepsilon^{-1}$ volume and $-Img(\varepsilon+1)^{-1}$ surface electron loss, spectra of electro-optical differential functions *(α, β)*, spectra of optical conduction of σ massive and film samples correspondingly are presented in fig.1-10 and values of interband optical transitions defined by maximums of σ optical conduction are presented in tables 1 and 2.

The given data give us the possibility to compare the optical spectra, transitions of Bi_2Te_3single crystals and film samples. The transitions 1,4eV and 1,1eV are found by authors of work [5] for the case of high energies for Bi_2Te_3 single crystals. As it is seen from table 1 the same transitions are observed for n- and p-types correspondingly. As it is seen from table 2 the transitions corresponding to energies 1,4eV and 1,15eV are found for Bi_2Te_3 film samples of n- and p-types. From this we can conclude that values of some optical transitions for noncrystalline samples at material transition from crystalline to noncrystalline state are saved.

As it is mentioned in [18] the study of absorption transitions in materials is impossible because of absorption big value in region of interband transition energies $E>E_g$ (E_g is forbidden band width). The reflection is the one effective method.

The analytical singularities of imaginary part of complex dielectric constant $\varepsilon_2(E)$ and dN/dE functions connected by state density almost coincide and interband space gradient makes the main contribution in *dN/dE* functions:

$$\frac{dN_{ij}}{dE} \sim \int \frac{dS_k}{\left|\nabla_k E_{ij}\right|} \quad , \tag{1}$$

where $E_{ij}(k)=E_j(k)-E_i(k)$ is distance between conduction and valence bands. *dN/dE* values near critical points in *k*-space defined by expression and also the position of critical points and transition type can be theoretically calculated from band structure.

The analysis of $\varepsilon_2(E)$, *dN/dE* functions and *R(E)* reflection coefficient shows that disposition and character of maximums in their spectra are similar or very close ones. That's why one can define the values of corresponding interband intervals and band nature with the help of direct comparison of experimental data in $E>E_g$ region with theoretical calculations of *dN/dE* function. As it is mentioned in [18] E_0 resonance frequency presents itself that frequency at which $2nk\cdot E$ conduction achieves maximum by which the interband transitions are defined. The high transparency in wide $E<E_g$ energy region is character for noncrystalline materials and several methods of E_g definition are known.

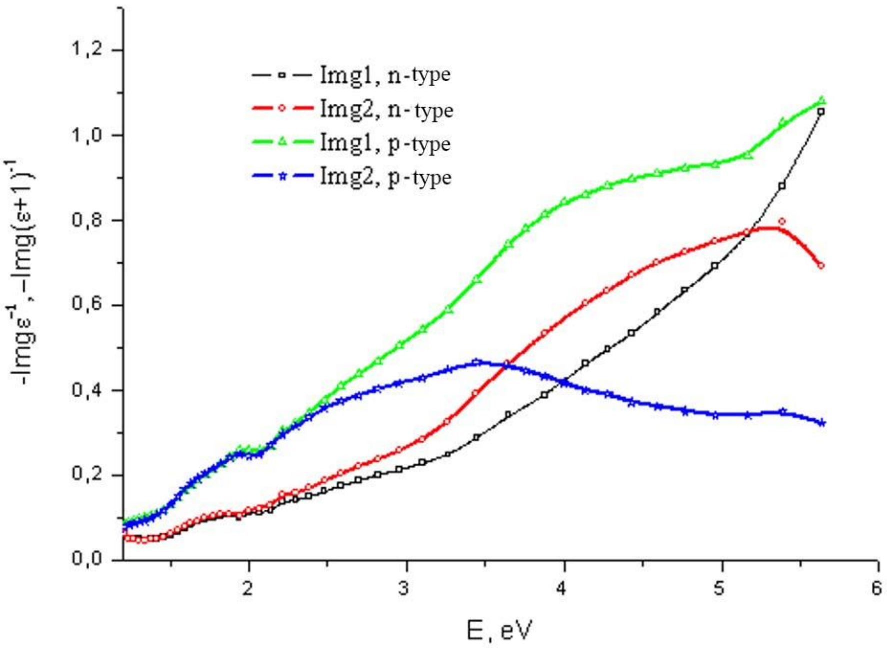

Fig.3. Spectra Img1 ($-\mathrm{Img}\varepsilon^{-1}$) and Img2 ($-\mathrm{Img}(1+\varepsilon)^{-1}$ of film Bi_2Te_3 of n- and p-types.

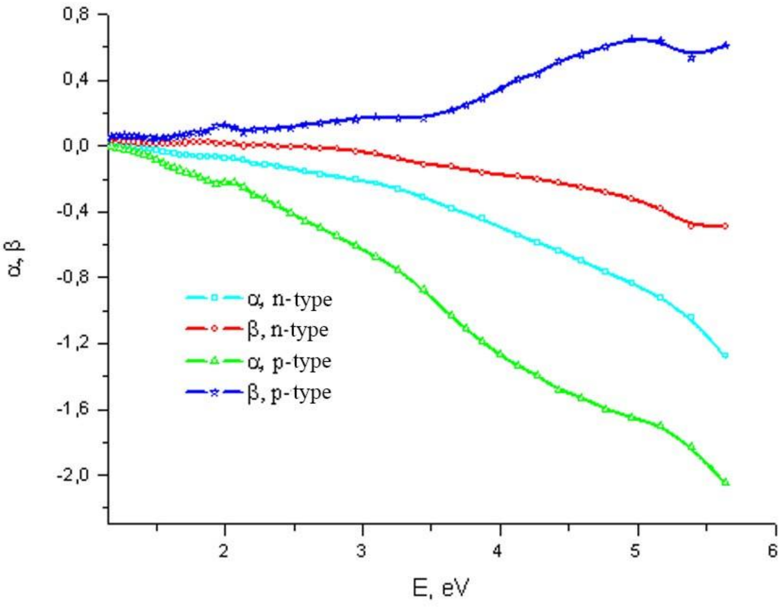

Fig.4. Spectra of electro-optical coefficients α and β of Bi_2Te_3 film of n- and p-types.

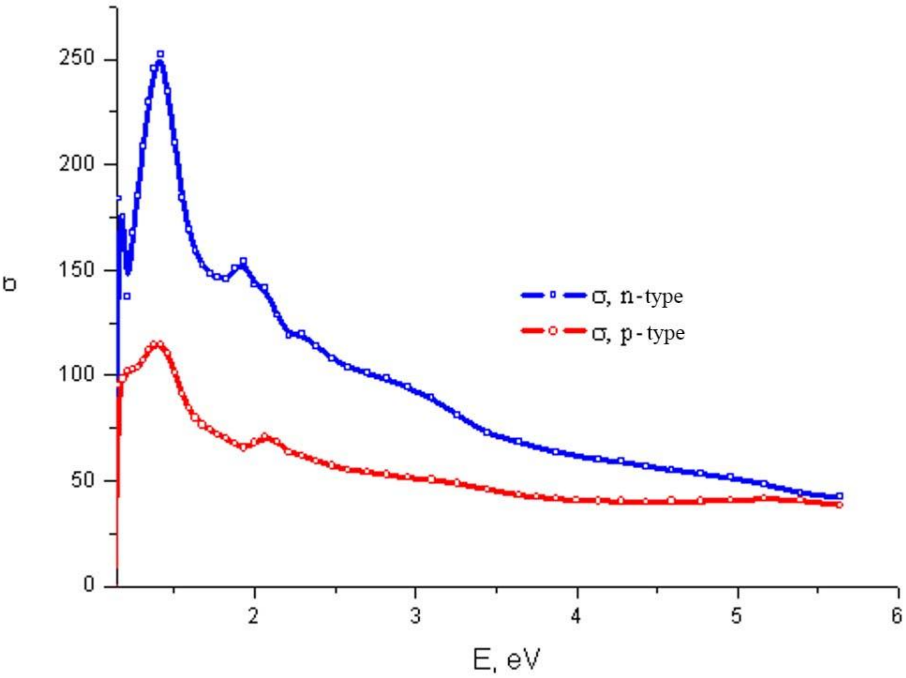

Fig.5. Optical conduction spectraσ of Bi_2Te film of n- and p-types.

Table 1.

Optical transitions in film Bi_2Te_3 in energy interval1÷6 eV of n- and p-types defined by optical conduction maximums.	
n - type	p - type
1.15	1.15
1.37	1.19
1.41	1.37
1.84	1.41
1.93	2.05
2.06	2.13
2.29	-

The transparency estimation by the level of *α(E)* absorption coefficient of long-wave edge is the one of these methods. E_g detail value for noncrystalline semiconductors is discussion one and usually the discussion of *α(E)* spectrum character in Urbach and Tauz models is carried out without E_g estimations [20,21]. E_g is defined by Tauz model for *α(E)* = 10^3cm^{-1} value.

As it is mentioned in [20] N(E) state density is the similarly available conception for crystalline and noncrystalline substances. By existing results of experimental data the step of state density in noncrystalline substance not strongly differs from the corresponding one in crystal. In first case the thin structure can be blurred and local states can appear in forbidden band. The band structure saves as it is defined by short-range order in materials.

The author of work [22] notes that it is impossible to delimit the single crystal, polycrystalline and amorphous substance state. The presence of band structure which are forbidden and conduction bands can be obtained from short-range order and for such conclusion there is no need to require the atom periodic disposition.

As authors show [23 – 25] the structure of disordered binary compound can be considered as the assemblage of different basis clusters presented in structural matrix with different static height and put into effective medium. As authors of work [26] note the short-range order makes the main contribution into electron state density. However, as short-range order in binary compounds can significantly change from node to node in structural matrix of amorphous substance then especially statistics of basis clusters defines the final electron state density.

Thus, low-molecular structural configurations can appear at melt cooling or in process of amorphous substance formation by another way that is accompanied by definite advantage in energy. Such formations can’t serve neither as crystal germs nor as growth centers of solid amorphous phases because of the fact that they are characterized by special symmetry.

The ambiguity of structural ordering in compositional amorphous solid substances of type can be considered as their general property. The peculiarities of short-range ordering near each node are caused firstly by physical methods of A_xB_{1-x} system preparing, secondly by principle of chemical ordering taking into consideration the “rule 8-N” [20] and values of bound energies of neighbor atoms.

The decay of ideal structure in noncrystalline solid substance takes place in systems including atoms with lone-electron pairs. Often at bound breakage the electron pair stay on the one of fragments, i.e. the heterolytic bound breakage takes place. The one positive and one negative charged defect centers in sort-range orders appears. The energy necessary for bound breakage is partly compensated by existing lone-electron pair of atoms being near and number of chemical bounds doesn’t change. Thus, there is structural disordering along with density oscillations and topological disordering of different types in homogeneous noncrystalline materials of stoichiometric composition. It is revealed in the form of positive and negative charged defect centers as in the case of point defects in crystals. As a result the reaction defects the formations of which are characterized by least change of free energy, dominate.

The short-range order idea at formation of electron energy bands is the one of fundamental conceptions in physics of disordered systems. This idea has experimental and theoretical demonstration on example of many noncrystalline solid and liquid semiconductors [27]. The formation mechanism of valence and conduction bands in noncrystalline semiconductors is formed mainly by work authors [28,29]. In works of these authors the similarity of main peculiarities of spectral dependence of imaginary part of $\varepsilon_2(E)$ dielectric constant for noncrystalline semiconductors and their crystal analogues is emphasized. This similarity is shown on example of selenium [28]. The analogous conclusion is made in relation to a-As_2S_3 and a-As_2Se_3 of works [28,29]. For cases of amorphous materials only maximum smoothing takes place in their $\varepsilon_2(E)$, but similarity of curves for amorphous and crystalline samples is saved.

Nowadays it is established that one can directly change the optical, photo-electric and electric properties of noncrystalline semiconductors with change of chemical composition and also by introduction of impurities. The change if concentration of charged defect centers D^+ and D^- (U^{-1}-centers) in them takes place and these defects form from initial neutral defects D^0 by reaction:

$$2D^0 \rightarrow D^+ + D^- , \qquad (2)$$

which can be eigen or impurity and mixed defects which give us the possibility to control by their physical properties.

CONCLUSION

Thus, $R(E)$ reflection coefficients of single crystals and Bi_2Te_3 film samples of n- and p-types in energy interval 1÷6 eV of beam falling normally on surface are measured in work. For case of Bi_2Te_3 single crystals the measurements are carried out parallel and perpendicularly to C axis. It is shown that for noncrystalline samples the values of some optical transitions Bi_2Te_3 from crystal to noncrystalline state are saved.

Only spectra of $R(E)$ reflection coefficients, ε_1 real and ε_2 imaginary parts of dielectric constant, functions of characteristic $-Img\ \varepsilon^{-1}$ volume and $-Img(\varepsilon+1)^{-1}$ surface electron loss, spectra of electro-optical differential functions $(\alpha,\ \beta)$, spectra of optical conduction of σ massive and film samples correspondingly are shown in fig.1-5 and values of interband optical transitions defined by maximums of optical conduction σ are shown in table1.

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Received: 25.01.2018