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## Calculation of absorption coefficients of $\text{InSb}_{1-x}\text{Bi}_x$ solid solutions

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**Abstract.** Using local empirical pseudopotential with spin-orbit interaction taking into account the electron band structure of  $\text{InSb}_{1-x}\text{Bi}_x$  in virtual crystal approximation is calculated. For binary compounds InSb and InBi characteristic gaps between energy bands in high symmetry points of Brillouin zone satisfactorily coincide with known experimental results. Temperature dependencies were calculated using the Brooks-Yu method. A satisfactory coincidence of the band structure of  $\text{InSb}_{1-x}\text{Bi}_x$ , temperature and concentration dependencies with experimental data let us to investigate  $\epsilon_1$  and  $\epsilon_2$  dielectrical functions taking into consideration the temperature using integral equations by Kramers-Kronig. Having used them we also calculated an absorption coefficient  $\alpha$  both for binary compounds InSb, InBi and for the triple alloy  $\text{InSb}_{1-x}\text{Bi}_x$ . These results correlate well with experimental ones in the area of the fundamental absorption.

**Keywords:** absorption coefficient, permittivity, solid solution, pseudopotential, band structure.

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Optical functions in a wide range of fundamental absorption (optical fundamental functions) are essential for various semiconductor properties and their applications, when studied theoretically and experimentally. Thus, for instance, investigation of semiconductor fundamental absorption band is powerful way to study energy band structure. Analyzing the edge of fundamental absorption one can determine the minimum gap width between the valency and conduction bands, as well as find out the nature of the transitions (allowed, forbidden, direct, indirect).

The subject of our research was narrow-gap  $\text{InSb}_{1-x}\text{Bi}_x$  substitutional solid solutions, which is promising materials for solid state electronics (fabrication of infrared detectors, low-noise filters for communication systems, lasers with smooth tuning their wavelength [1,2]). The most widely available semiconductor material used for production of far infrared ( $\lambda > 8 \mu\text{m}$ ) devices nowadays are CdHgTe alloys. However, the properties of these crystals are dependent, to some extent, on technological process, which is so perfect as for  $\text{A}^{\text{III}}\text{B}^{\text{V}}$  compound, and on some other unpredictable factors that influence greatly the band gap width [3].

Traditional  $\text{A}^{\text{III}}\text{B}^{\text{V}}$  alloys don't enable us to broaden the wave range over  $7.5 \mu\text{m}$  (InAsSb). That's why, recently, two alternative ways to overcome the drawbacks have appeared. The first one is to obtain new multi-com-

ponent materials on the basis of  $\text{A}^{\text{III}}\text{B}^{\text{V}}$ . Another is based on a band gap width change caused by tensions that arise in appropriate superlattices and hetero-structures [4]. Both, the former and the latter, have good and bad points.

Experimental study of InSb – InBi system started about 30 years ago with classical works by Jean-Louis [5–7]. Technical difficulties of growing mentioned substitutional solid solutions have slowed down their wide practical applications. Nevertheless, recent achievements in this sphere [8–11] reveal new perspectives in obtaining and using them. That's why in the fundamental properties, such as alloy composition and temperature, electron charge density, etc., optical and photoelectrical characteristics of the materials increased.

The main properties of their electron band structure have been investigated in literature [12, 13]. The calculation of the absorption coefficient  $\alpha$  in their fundamental absorption band is represented in this work. It should be pointed out that optical functions studied by Jean-Louis were obtained over extremely narrow frequency range. In present paper we have investigated an absorption coefficient value within 0–10 eV.

Our calculations are based on electron energy  $\text{InSb}_{1-x}\text{Bi}_x$  spectrum calculated using the local empirical pseudopotential method for a virtual crystal, approximation including spin-orbital interaction.

InSb<sub>1-x</sub>Bi<sub>x</sub> band structure can be found by solving secular equation

$$\det \left\{ \left[ K^2 - E_n(\vec{k}) \right] \delta_{\vec{G}\vec{G}'} \delta_{ss'} + V_L(\vec{G} - \vec{G}') \delta_{ss'} + V_{s0}^{ss'}(\vec{k}, \vec{k}') \right\} = 0. \quad (1)$$

Where

$$V_L(\vec{G}) = v^S(\vec{G}) \cdot \cos(\vec{G} \cdot \vec{\tau}) + i \cdot v^A(\vec{G}) \cdot \sin(\vec{G} \cdot \vec{\tau}). \quad (2)$$

Spin-orbital term

$$V_{s0}^{ss'}(\vec{k}, \vec{k}') = (\vec{k} \times \vec{k}') \cdot \sigma_{ss'} \times \left\{ -i\lambda^S \cdot \cos[(\vec{k} - \vec{k}') \cdot \vec{\tau}] + \lambda^A \cdot \sin[(\vec{k} - \vec{k}') \cdot \vec{\tau}] \right\} \quad (3)$$

$\vec{\tau} = \frac{a}{8}(1, 1, 1)$ ,  $a$  is the lattice constant,  $v^S(\vec{G})$  and  $v^A(\vec{G})$  are symmetrical and antisymmetrical formfactors, which are triad parameters,  $s$  and  $s'$  – spin states,  $\sigma$  – Pauli matrix,  $\vec{K} = \vec{k} + \vec{G}$ ,  $\lambda^A$  and  $\lambda^S$  considered as trial parameters. Typical distances between the energetic bands at the high-symmetry points of Brillouine zone for InSb and InBi binary compounds satisfactory coincide with known experimental data. The electron band structure of InSb<sub>95%</sub>Bi<sub>5%</sub> ternary solid solution is shown in Fig. 1.

Temperature dependence was taken into account by the Brucks-Yu method, according to each pseudopotential formfactor corrected by the Debay-Waller factor.

Absorption coefficient  $\alpha$  is given by:

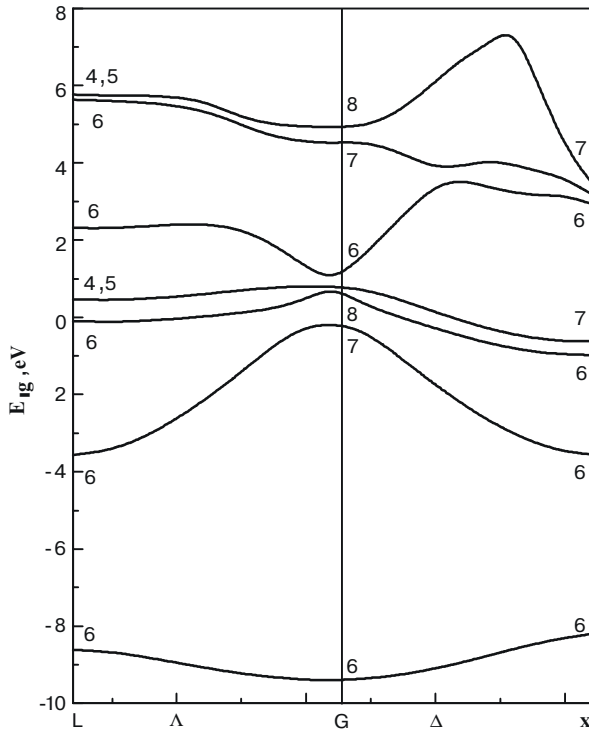


Fig. 1. Band structure of InSb<sub>95%</sub>Bi<sub>5%</sub>.

$$\alpha = \frac{\omega}{nc} \varepsilon_2, \quad (4)$$

where  $n$  is a real part of refraction coefficient,  $N$ ;  $\varepsilon_2$  is an imaginary part of the permittivity,  $\varepsilon$ ;  $\omega$  is a frequency of incident electro-magnetic wave,  $c$  is the speed of light in a vacuum.

The imaginary part of the permittivity is calculated in accordance with [14]:

$$\varepsilon_2(E) = \frac{4\pi^2 \hbar^2 e^2}{m^2 E^2} \times \sum_{vc} \int_{ZB} \frac{2d\vec{k}}{(2\pi)^3} \cdot |\vec{e} \cdot \vec{M}_{vc}(\vec{k})|^2 \cdot \delta(E_c(\vec{k}) - E_v(\vec{k}) - E), \quad (5)$$

where

$$\vec{e} \cdot \vec{M}_{vc}(\vec{k}) = \langle \psi_{ck} | \vec{e} \cdot \vec{p} | \psi_{vk} \rangle = \vec{e} \cdot \int_{V_{crystal}} \psi_c^*(\vec{k}, \vec{r}) (-i\hbar \nabla) \psi_v(\vec{k}, \vec{r}) d\vec{r}, \quad (6)$$

$\vec{e}$  is an unit vector of polarization.

In (5) transition between valency band,  $v$ , and the band of conduction,  $c$ , when the distance between them is equal to the energy  $E = \hbar\omega$ , where summed up.

Integration over Brillouine zone was performed by the tetrahedron method, according to which Brillouine zone was divided into 300 tetrahedrons chosen in its irreducible (1/48) part.

Fig. 2 shows the calculated imaginary part of the permittivity,  $\varepsilon_2$  for InSb at  $T = 300$  K in comparison with experimental curve [16]. Satisfactory correlation between calculated and experimental curves proves that our theory is well applied within the investigated energy range.

Position of experimental peaks  $\varepsilon_2$  ( $E = 1.9, 2.4, 3.9, 5.1$  eV) and their intensity practically coincide with the theoretical ones. Moving from the edge of absorption to the higher energy values, the first maximum is related to transition from valency band  $\Gamma_{v8}$  to the narrowest conduction band  $\Gamma_{c6}$  at  $k = (0, 0, 0)$ . The first peak is followed by almost plane area, which is expected to appear due to enlargement of constant energy range, where transition occur, as owing to the inclusion of  $\Gamma_{v7} - \Gamma_{c6}$  transitions. Increasing the energy in spectrum  $\varepsilon_2$ , a most complex structure, which resembles the structure  $\varepsilon_2$  of the other materials such as crystalline diamond or zinc blende structure, can be noticed. Thus, the next two peaks are correspondent to transitions in highly symmetrical directions  $\Delta_{v4,5} - \Delta_{c6}$  and  $\Delta_{v6} - \Delta_{c6}$ , respectively. Regarding InSb electron structure [12, 13] in direction  $\Delta$  from  $L$  point, two upper valency bands are parallel to the lower conduction band along the considered interval, which causes the arising of these two high peaks. Then, there is a high maximum, the top of which is splitted into two peaks. These peaks are associated with transitions  $\Delta_{v7} - \Delta_{c6}$  and  $\Delta_{v6} - \Delta_{c6}$  respec-

tively. However, experimental curve doesn't show such splitting. There can be explanation given below. As one can see in Fig. 1, at the  $X$  point two upper valency bands are not joint. Therefore, two assumptions can be made: either the empirical pseudopotential method is not valid to describe the energy spectrum of InSb at  $X$  point or these peaks are situated too close to each other, so that resolution in the experiment is not sufficient. The next peaks are not so high. As Fig. 2 exhibits, the first one is accordant to transition in highly symmetrical direction  $\Sigma_{v6} - \Sigma_{c6}$ , while the second maximum is in the vicinity of high-symmetry points  $K_{v6} - K_{c6}$ .

The next step was taken to calculate the real part of the permittivity using the Kramers-Cronig relation. The results of the calculations compared with experimental data [16] for  $T = 300$  K are shown in Fig. 2.  $\epsilon_1$  amounts to its maximum values of 22.4 and 22.3 at 0.3 and 1.8 eV.

Good correlation between calculated curves  $\epsilon_1$ ,  $\epsilon_2$  and experimental curves entitles us to anticipate that the chosen model adequately displays the main optical features. That's why we have used it in investigation of the real and imaginary parts of permittivity for InBi and  $\text{InSb}_{1-x}\text{Bi}_x$  alloys (Fig. 3).

Examining  $\epsilon_1(E)$  and  $\epsilon_2(E)$  dependences, it is possible to derive the other optical functions.

Energy dependence of an absorption coefficient  $\alpha$  are shown in Fig. 4 for both materials. An absorption coefficient

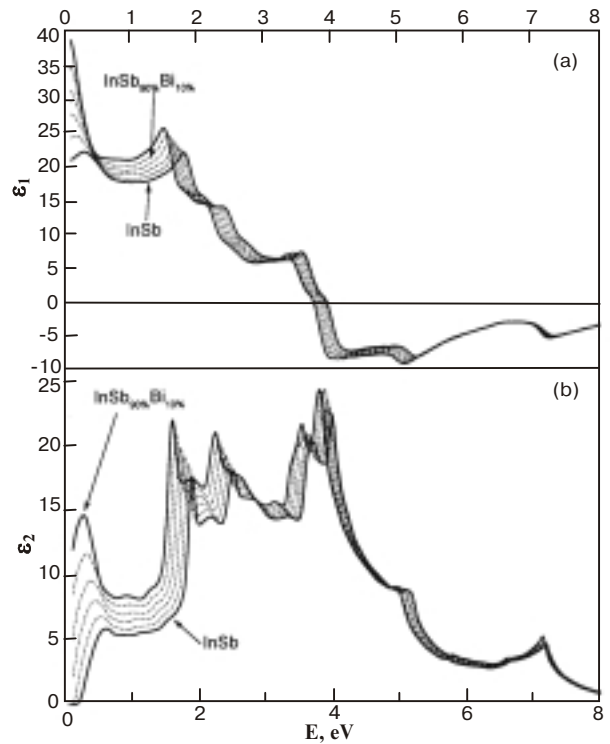


Fig. 3. Energy dependence of  $\epsilon_1$  (a) and  $\epsilon_2$  (b) for  $\text{InSbBi}$ .

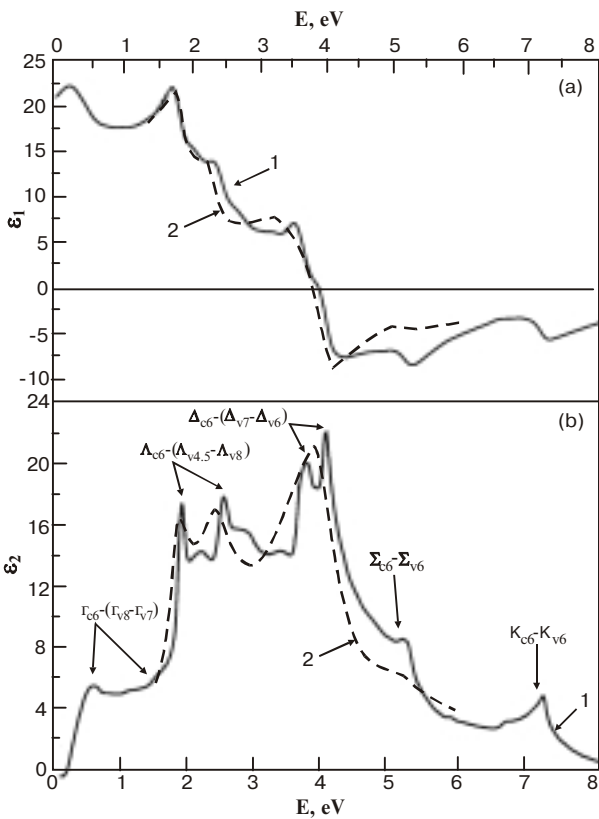


Fig. 2. Energy dependence of  $\epsilon_1$  (a) and  $\epsilon_2$  (b) for InSb.

1 – calculation at 300 K;  
2 – experimental data [16].

for  $\text{A}^{\text{III}}\text{B}^{\text{V}}$  alloys in the vicinity of their fundamental absorption edge rises sharply (see reference to Fig. 4.) and then continues to increase smoothly with increasing photon energy. Bend points and peaks in the graph of absorption coefficient correspond to peaks of the imaginary part of the function connected with corresponding electron transitions.

The highest values of the absorption coefficients for InSb and InBi are equal to: InSb –  $1.475 \cdot 10^6 \text{ cm}^{-1}$  and  $1.655 \cdot 10^6 \text{ cm}^{-1}$  at 4.2 and 5.3 eV; InBi –  $1.558 \cdot 10^6 \text{ cm}^{-1}$  and  $1.814 \cdot 10^6 \text{ cm}^{-1}$  at 3.9 and 5.1 eV.

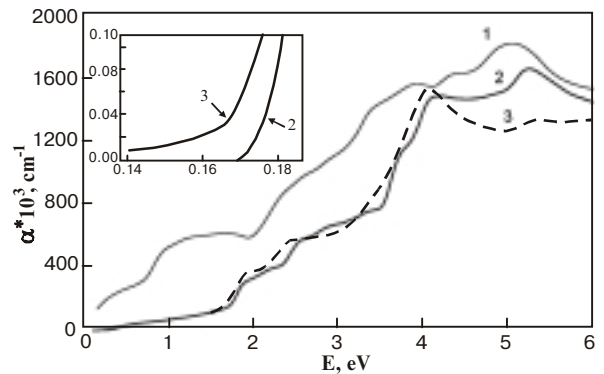


Fig. 4. Energy dependence of absorption coefficient  $\alpha$ .

1 – calculation at 0 K for InBi;  
2 – calculation at 300 K for InSb;  
3 – experimental data for InSb [16].

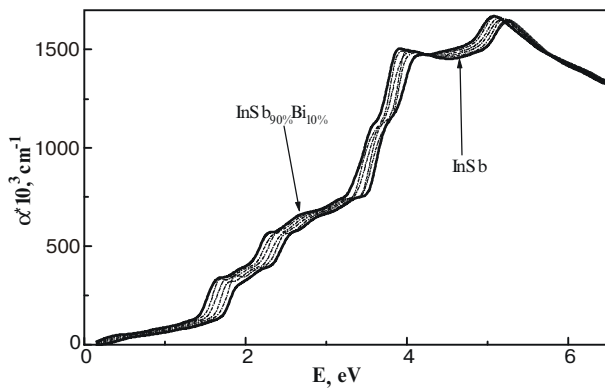


Fig. 5. Energy dependence of  $\alpha$  for  $\text{InSbBi}$ .

Plots of  $\text{InSb}_{1-x}\text{Bi}_x$  absorption coefficient  $\alpha$  versus composition  $x$  are given in Fig. 5. As we can see from this figure, an increase in Bi content in the alloy makes the absorption curve shift to the range of lower energies.

Satisfactory agreement between theoretical and experimental curves enables us to conclude that the empirical pseudopotential method properly indicates the peculiarities of electron spectrum of  $\text{InSb}_{1-x}\text{Bi}_x$  solid solutions and can be successfully applied for the investigation of their optical functions.

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