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THE BAND STRUCTURE AND ELECTRON DENSITY OF $\text{InSb}_{1-x}\text{Bi}_x$ SOLID SOLUTIONS

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A band structure of semiconductor $\text{InSb}_{1-x}\text{Bi}_x$ substitution solid solution is calculated by the empirical pseudopotential method. Spin-orbital interactions are also included in local calculations. Using the virtual-crystal approximation the composition and temperature dependences of energy gap are studied. The results are in good agreement with available experimental data.

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Multicomponent alloys are potentially very important materials for building infrared (IR) detectors, low-noise filters of communication systems, lasers with smooth reorganization of a wavelength [1, 2]. At present the CdHgTe alloys are the most available semiconductor materials for manufacturing far-infrared devices ($\lambda > 8 \mu\text{m}$). However, the properties of these crystals largely depend on technological process, which is not as perfect as, for example, for $\text{A}^{\text{III}}\text{B}^{\text{V}}$ compounds. Many unforeseen factors strongly influence the band gap, and the processes of degradation result in instability of the physical and ecological characteristics [3]. The idea of changing the band gap at the expense of voltage, which arises in appropriate superlattices and heterostructures, is the basis of the latter [4]. Both of the two approaches are characterized by strong and weak legs. The experimental study of the InSb–InBi systems began about 30 years ago in the classical works of Jean-Louis [5–7]. Technological difficulties of growing an indicated substitutional solid solution have been decelerating its broad practical introduction until recently. However, recent achievements in the given field [8, 9] open new possibilities of constructing the solution and its applications. Increasing interest has been noticed in fundamental properties, such as an electronic band structure, relation of the band

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gap to a composition of an alloy and temperature, and optical and photo-electric characteristics of indicated materials.

InBi crystallizes in tetragonal (B10) structure and is a semimetal — which is not characteristic of majority of $A^{III}B^V$ compounds, which are cubic semiconductors. That fact has stimulated the research of the correlation between an anomalous crystalline structure and physical properties [10]. The relation of the lattice constants in InBi is $c/a = 0.9545$ [9]. Physical properties of the solid solution $\text{InSb}_{1-x}\text{Bi}_x$ ($x < 3\%$) were studied in a number of papers. It was shown that substitution solid solution of a zinc-blende structure with a direct band gap forms in a given range of change of composition. The first estimated calculations of the band structure $\text{InSb}_{1-x}\text{Bi}_x$ were developed through three methods: the Hermann relativistic corrections, the empirical pseudo-potential method, and the Van Vechten semiconductor model [7]. These methods have not allowed quantitative explanation of concentration and temperature dependence of the band gap, and, thus, optical properties were not properly explained.

It is necessary to solve the Schrödinger wave equation for calculation of the electronic band structure, where one-electronic pseudo-potential Hamiltonian is written in atomic units as

$$H = -\nabla^2 + V_p(r), \quad (1)$$

where

$$V_p(r) = V(r) + \sum_t (E - E_t) |b_t\rangle \langle b_t| \quad (2)$$

— the crystal pseudo-potential, $V(r)$ — the true crystal potential, $|b_t\rangle$ — the wave function of the fundamental state with the energy E_t . The Fourier transform of the pseudo-potential $V_p(r)$, disregarding its nonlocal part, is written as

$$V_p(r) = \sum_{\mathbf{G}} V_L(\mathbf{G}) \exp(i\mathbf{G} \cdot r), \quad (3)$$

where

$$V_L(\mathbf{G}) = \sum_{\alpha} S_{\alpha}(\mathbf{G}) \nu_{\alpha}(\mathbf{G}), \quad (4)$$

$$S_{\alpha}(\mathbf{G}) = \frac{1}{N_{\alpha}} \sum_j \exp(-i\mathbf{G} \cdot \mathbf{R}_j^{\alpha}), \quad (5)$$

\mathbf{G} is the reciprocal lattice vector, $\nu_{\alpha}(\mathbf{G})$ is the atomic pseudo-potential form-factors, N_{α} is the number of α atoms in the primitive unit cell, \mathbf{R}_j^{α} defines the position of the j -th α atom. In the case of compounds $A^N B^{8-N}$ with zinc-blende structure, middle point of AB was chosen as origin. These equations can be reduced to

$$V_L(\mathbf{G}) = \nu^S(\mathbf{G}) \cos(\mathbf{G} \cdot \boldsymbol{\tau}) + i\nu^A(\mathbf{G}) \sin(\mathbf{G} \cdot \boldsymbol{\tau}), \quad (6)$$

where

$$\nu^S(\mathbf{G}) = [\nu_A(\mathbf{G}) + \nu_B(\mathbf{G})]/2, \quad \nu^A(\mathbf{G}) = [\nu_A(\mathbf{G}) - \nu_B(\mathbf{G})]/2, \quad (7)$$

$\boldsymbol{\tau} = (a/8)(1, 1, 1)$, a is the lattice constant.

In the empirical pseudo-potential method we consider only first four ν^A and ν^S , which can be justified by the effect of truncating the strong spanning potential. The band structure $\text{InSb}_{1-x}\text{Bi}_x$ can be found through solving the secular equation

$$\det \left| [K^2 - E_n(k)] \delta_{GG'} \delta_{ss'} + V_L(G - G') \delta_{ss'} + V_{so}^{ss'}(K, K') \right| = 0. \quad (8)$$

The spin-orbit term is

$$V_{so}^{ss'}(K, K') = (\mathbf{K} \times \mathbf{K}') \sigma_{ss'} \{ -i\lambda^S \cos[(\mathbf{K} - \mathbf{K}') \cdot \boldsymbol{\tau}] + \lambda^A \sin[(\mathbf{K} - \mathbf{K}') \cdot \boldsymbol{\tau}] \}. \quad (9)$$

Here s and s' are the spin states, σ is the Pauli matrix, $\mathbf{K} = \mathbf{k} + \mathbf{G}$, λ^A and λ^S are adjustable parameters. For the substitutional solid solution, in accordance with the virtual crystal approximation (VCA) and the Vegard law, lattice constant and pseudo-potential form-factors $\text{InSb}_{1-x}\text{Bi}_x$ can be constructed as the linear combinations

$$a_{ss} = a_{\text{InBi}}x + a_{\text{InSb}}(1 - x), \quad V_{ss} = V_{\text{InBi}}x + V_{\text{InSb}}(1 - x), \quad (10)$$

where a_{ss} and V_{ss} are the lattice constant and form-factors of the substitution solid solution, respectively. Extensive calculations were made along the high-symmetry directions of the Brillouin zone in the basis of 137 plane waves (the secular determinant with regard to spin states has the dimension 274×274). Figure 1 presents the band structure InSb and InBi , calculated using the theoretical parameters, given in Table I in comparison with parameters of the other works [7, 11]. The

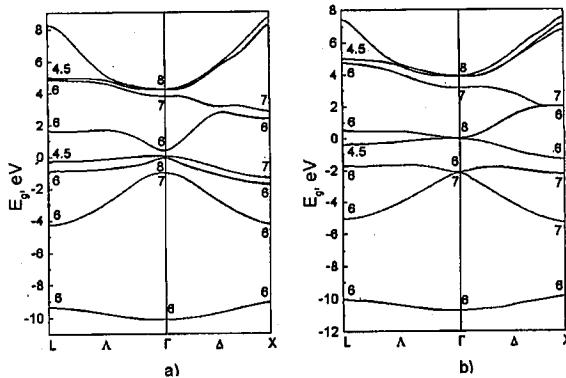


Fig. 1. Band structure of InSb (a) and InBi (b).

calculated energy distances between electronic levels in high symmetry points at the boundary cases $x = 0$ (InSb) and $x = 1$ (InBi) satisfactorily will correlate with known experimental data and results of the pseudo-potential calculations of other authors (Table II).

The s -level of In drops lower than the p -level of Bi at almost 2 eV in the Γ point in InBi as it was indicated in [7, 10]. The temperature influence on the band structure of the examined solid solutions can be studied with the help of the Brooks-Yu theory [13]. For Debye-temperature calculations we assume

TABLE I

Pseudopotential parameters used in calculations.

	InSb		InBi	
	Ref. [11]	Our data	Ref. [7]	Our data
ν^S (3)	-0.2547	-0.2285	-0.22	-0.285
ν^S (8)	0.0188	0	-0.03	-0.0035
ν^S (11)	0.0452	0.0405	0.02	0.0145
ν^A (3)	0.0302	0.06	0.08	0.049
ν^A (4)	0.0012	0.05	0.05	0.035
ν^A (11)	0.0329	0.01	0.02	0.005
λ^S	0.00231	0.00230	-	0.001693
λ^A	0.00028	0.00028	-	0.003443

TABLE II

Interband transitions (eV).

	InSb			InBi	
	Theor. [11]	Our calcul.	Exp. [12]	Theor. [10]	Our calcul.
$\Gamma_{8V}-\Gamma_{6C}$	0.26	0.247	0.2357	1.9	1.97
$\Gamma_{7V}-\Gamma_{6C}$	1.05	1.23	1.216	0	0
$\Gamma_{8V}-\Gamma_{7C}$	3.65	3.6	-	2.56	3.1
$\Gamma_{8V}-\Gamma_{8C}$	3.68	4.21	-	3.10	3.83
$L_{4,5V}-L_{6C}$	2.03	1.89	1.9	1.25	1.18
$L_{6V}-L_{6C}$	2.60	2.48	-	1.75	2.11
$L_{4,5V}-L_{6C}$	5.3	5.71	-	4.12	4.87
$X_{7V}-X_{6C}$	3.95	3.73	-	0.75	0.77
Δ_{CO}	0.82	0.99	0.98	1.9	1.97

$\Theta_{In} = 112$ K, $\Theta_{Bi} = 120$ K, $\Theta_{Sb} = 220$ K [14]. Influence of the lattice thermal expansion was taken into account in corresponding dependences of the lattice constants on temperature. Figure 2 presents the calculated results of temperature and concentration dependences of the band gap of the semiconductor solid solutions $InSb_{1-x}Bi_x$ in comparison to experimentally measured values in optic absorption experiments [6]. The electronic charge densities are shown in Fig. 3.

Satisfactory agreement between the experimental and theoretically derived dependences gives ground to the belief that the chosen model is reasonable for description of the energy band structure of the examined ternary semiconductor solid solutions. This can be the reason for further analysis and prediction of optical properties and right method of approach to solving technological problems for obtaining a more perfect material with desired band gap.

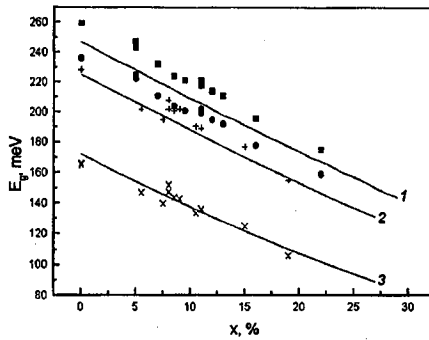


Fig. 2. Variation of energy gap E_g with composition x for $\text{InSb}_{1-x}\text{Bi}_x$. 1 — calculation at 0 K; 2 — calculation at 77 K; 3 — calculation at 300 K; \blacksquare, \bullet — experimental data at 0 K [6]; $+$ — experimental data at 77 K [6]; \times — experimental data at 300 K [6].

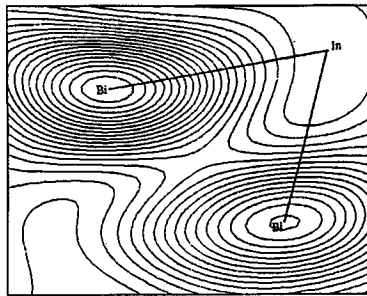


Fig. 3. Electronic charge densities in the (1 1 0) plane of the upper four valence bands.

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