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Energy gaps and refractive index of lattice-matched and mismatched $In_xAl_{1-x}As_ySb_{1-y}$ quaternaries

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ABSTRACT

The electronic band structure and optical properties of $In_xAl_{1-x}As_ySb_{1-y}$ quaternaries under conditions of lattice mismatching and lattice matching to InP substrate have been investigated using a pseudopotential approach under the virtual crystal approximation. The extent of the indirect (Γ-X)-to-direct (Γ-Γ) band gap transition in $In_xAl_{1-x}As_ySb_{1-y}$/InP is found to occur at x = 0.38 which agrees reasonably with the data reported in the literature. The lattice mismatch percentage in the range −5%–0% is found to have no effect on the nature of the fundamental band-gap in $In_{0.50}Al_{0.50}As_ySb_{1-y}$ which remains a direct (Γ-Γ) band-gap semiconductor. Trends in bonding and ionicity are discussed in terms of the antisymmetric gap and valence band width. The dependence of the refractive index on both indium concentration x in $In_xAl_{1-x}As_ySb_{1-y}$/InP and lattice mismatch percentage in $In_{0.50}Al_{0.50}As_ySb_{1-y}$ has been examined. Our results showed that more opportunities can be provided for all features of interest by a proper choice of the concentrations x and y ($0 \le x \le 0.52$, $0.56 \le y \le 1$) and/or the lattice mismatch percentage.

1. Introduction

Multicomponent semiconductor alloys based on III-V semiconductor compounds are promising materials for technological device applications. They found a use in numerous optoelectronic and transport devices such as high speed electronic and long wavelength photonic devices [1–5]. In particular, quaternary alloys of these semiconductors open new opportunities for materials engineering [6,7]. This is because they give the possibility of controlling the band-gap energy, lattice constant and conduction-and valence-band offsets independently. As a matter of fact, the physical and chemical properties of these materials depend essentially on their compositions. As compared to ternary semiconductor alloys, these materials have two composition parameters (instead of one in the case of ternaries) which provides more opportunities for the selection of the energy band-gap and the lattice parameter, within the constraints of a given alloy-substrate system.

Among the III–V quaternaries, the $In_xAl_{1-x}As_ySb_{1-y}$ quaternary semiconductor alloys are important materials for use in electronic devices such as p-n junctions and heterojunction bipolar transistors [8]. This in part is due to their wide range of

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Table 1
Experimental band-gap energies at room temperature for InAs, InSb, AlAs and AlSb fixed in the fits.

Compound	$E_{\Gamma\text{-}\Gamma}$ (eV)	$E_{\Gamma\text{-}X}$ (eV)	$E_{\Gamma\text{-}L}$ (eV)
InAs	0.36[a]	1.37[a]	1.07[a]
InSb	0.18[a]	1.63[a]	0.93[a]
AlAs	2.95[a]	2.16[a]	2.36[a]
AlSb	2.30[b]	1.615[b]	2.211[b]

[a] Ref. [13].
[b] Ref. [14].

Table 2
Pseudopotential parameters for InAs, InSb, AlAs and AlSb at room temperature.

Compound	Form factors (Ry)						Lattice constant (Å)
	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$	
InAs	−0.217669	0.011	0.041633	0.054731	0.039485	0.024	6.058
InSb	−0.201294	0.01	0.028338	0.064495	0.03	0.015	6.49
AlAs	−0.212694	0.00	0.092750	0.068833	0.05	−0.0075	5.6611
AlSb	−0.225597	0.028086	0.062230	0.007109	0.058960	0.004544	6.1355

conduction and valence band offsets which makes possible the use of band gap engineering to optimize device performance [8]. In spite of the importance of the material system of interest, only very limited data in the literature were reported in its fundamental properties and/or showed the operation of p-n junctions made with them [8–11]. Recently, Magno et al. [8] made a progress in the molecular beam epitaxy growth of InAlAsSb alloys in order to use them in the development of a low-power, high-frequency heterojunction devices.

In the present paper, a theoretical study has been carried out so as to investigate the electronic properties of the quaternary alloy $In_xAl_{1-x}As_ySb_{1-y}$ lattice matched to InP. Besides, these properties have been also examined for the lattice mismatched alloys under consideration (i.e. in the case of not satisfying the lattice matching condition). The computations are performed using a pseudopotential approach under the virtual crystal approximation (VCA).

2. Computational method

The empirical pseudopotential method (EPM) [12] within the virtual crystal approximation (VCA) have been used so as to calculate the electronic band structure and its related band parameters for the quaternaries $In_xAl_{1-x}As_ySb_{1-y}$ lattice matched to InP substrate. The major virtue of the pseudopotential method is that the valence electrons are assumed to move in a weak one-electron potential, whereas the core electrons are frozen in an atomic-like configuration [12]. Thus, the pseudo-wave function can be expanded into a Fourier series of plane waves.

The EPM involves a direct fit of the atomic form factors to the experimental band structure. In the present work, the experimental energy band-gaps used in the fitting procedure for InAs, InSb, AlAs and AlSb at Γ, X and L high-symmetry points in the Brillouin zone at room temperature are given in Table 1. The optimization of the empirical pseudopotential parameters have been done using the non-linear least-squares method described in Refs. [15–17].

The final adjusted symmetric V_S and antisymmetric V_A pseudopotential form factors along with the used lattice parameters at room temperature for InAs, InSb, AlAs and AlSb parent compounds of the quaternaries of interest are shown in Table 2.

In the case of a quaternary alloy, the formalism can be generalized using the VCA. Thus for $In_xAl_{1-x}As_ySb_{1-y}$ quaternaries, V_S and V_A have been expressed as,

$$V_S^{alloy} = xyV_S^{InAs} + (1-x)yV_S^{AlAs} + x(1-y)V_S^{InSb} + (1-x)(1-y)V_S^{AlSb} \quad (1)$$

$$V_A^{alloy} = xyV_A^{InAs} + (1-x)yV_A^{AlAs} + x(1-y)V_A^{InSb} + (1-x)(1-y)V_A^{AlSb} \quad (2)$$

whereas the lattice parameters of the quaternaries of interest are determined as,

$$a^{alloy} = xya^{InAs} + (1-x)ya^{AlAs} + x(1-y)a^{InSb} + (1-x)(1-y)a^{AlSb} \quad (3)$$

where a^{InAs}, a^{AlAs}, a^{InSb} and a^{AlSb} are the lattice parameters of InAs, AlAs, InSb and AlSb, respectively.

The lattice matching condition for $In_xAl_{1-x}As_ySb_{1-y}$ quaternaries on InP substrate shall be obtained later by using the expression (3).

Generally, 136 plane waves were found to be sufficient for a typical semiconductor system. Once the potential is determined, the electronic structure of the material under consideration can be obtained by solving the secular equation.