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The optoelectronic properties of the ternary $B_xIn_{1-x}As$ matched on GaAs substrate for laser diode application: Theoretical study with TB-mBJ approximation

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ABSTRACT

The fundamental properties (structural and optoelectronic) of the zinc-blende-type $B_xIn_{1-x}As$ alloys have been theoretically studied employing the full-potential linear augmented plane-wave (FP-LAPW) method within density functional theory (DFT). These calculations are based on the generalized gradient approximation (GGA-WC) of Wu- Cohen to calculate the lattice parameters, bulk modulus, and pressure derivatives. Moreover, the Engel and Vosko GGA formalism (EV-GGA) and Tran-Blaha modified Becke-Johnson (TB-mBJ) approaches were used to improve the bandgap energy values in different compose of Boron in $B_xIn_{1-x}As$ ternary alloys. We have also investigated the densities of states and the variation of the optical properties of the $B_{0.437}$ $In_{0.562}As$ matched on GaAs substrate.

1. Introduction

III–V semiconductors with lattice-matched on GaAs become one of the most important materials for many optoelectronic applications such as a coherent light emitter, lasers, detector devices and solar cell absorber [1]. A new class of III–V alloys commences attracting the interest of researchers, based on the incorporation of boron into conventional III–V binary and ternary compounds specifically for the long-wavelength range applications [2–4].

The goal of this work is to study optoelectronic properties of zinc-blende $B_xIn_{1-x}As$/GaAs ternary alloys to investigate the effect of Boron incorporation in InAs. Let us remember that BAs and InAs are the parent's compounds of our ternary which (BAs) has a small lattice parameter of 4.777A° and indirect band gap of 1.46 eV [5]. The other compounds of the present work, the Indium Arsenide (InAs), is direct narrow bandgap semiconductor with a value of 0.42 eV and a lattice parameter of 6.058 A° [5]. The Boron Arsenide has a strong covalent character causing a strange behavior in comparison with Indium Arsenide [6]. From crystallography, Indium Arsenide (InAs) and Boron Arsenide (BAs) have the B3 structure in under normal conditions, with space group F-43m [7].

There are only a few theoretical and experimental work studies on ternary alloy $B_xIn_{1-x}As$. Experimentally, Tianhe Li et al. have studied the boron incorporation into InAs/GaAs Quantum Dots. The spectra of the room temperature photoluminescence (RT-PL) of BInAs/GaAs QDs show the improvement of the optical properties after the incorporation of Boron atoms [8].

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Table 1
Lattice constant a, bulk modulus *B* and pressure derivative of bulk modulus *B'* for InAs, BAs, and $B_xIn_{1-x}As$ alloys.

compound	a(A°) WC-GGA	Exp.	B(Gpa) WC-GGA	B'(Gpa) WC-GGA
InAs	6.098	6.058[a]	56.796	4.146
$B_{0.0625}$ $In_{0.9375}$ As	5.986	–	69.562	4.247
$B_{0.125}$ $In_{0.875}$ As	5.942	–	70.595	4.417
$B_{0.187}$ $In_{0.8125}$ As	5.895	–	70.725	4.271
$B_{0.25}$ $In_{0.75}$ As	5.845	–	71.983	4.543
$B_{0.325}$ $In_{0.6875}$ As	5.792	–	75.914	4.948
$B_{0.375}$ $In_{0.625}$ As	5.738	–	80.724	4.150
$B_{0.4375}$ $In_{0.5625}$ As	5.677	–	81.687	4.580
$B_{0.5}$ $In_{0.5}$ As	5.617	–	75.252	4.046
$B_{0.5625}$ $In_{0.4375}$ As	5.539	–	75.363	4.938
$B_{0.625}$ $In_{0.375}$ As	5.454	–	84.257	4.120
$B_{0.6875}$ $In_{0.325}$ As	5.363	–	89.340	4.118
$B_{0.75}$ $In_{0.25}$As	5.265	–	94.953	4.398
$B_{0.8125}$ $In_{0.187}$As	5.159	–	103.754	4.127
$B_{0.875}$ $In_{0.125}$As	5.044	–	114.314	3.854
$B_{0.9375}$ In $_{0.0625}$As	4.915	–	125.887	4.511
BAs	4.777	4.777[a]	140.402	4.291

[a] Ref: [5].

The rest of this paper presents the computational method adopter for the theoretical calculations in Section II. Results and discussions will be presented in Section III, and finally, a summary of our work be given in Section IV.

2. Method of calculation

In this work, we have used the first-principles total-energy computations utilizing the full-potential linear augmented plane-wave (FP-LAPW) method in accordance with the density functional theory (DFT) executed in the Wien2K code [9,10] to compute the fundamental properties of the zinc-blende-type BxIn1-xAs/GaAs (Table 1).

In the FP-LAPW method, the potential, charge density and wave functions are developed by spherical harmonic functions within the muffin-tin (MT) spheres (the spheres surrounding the atomic sites) and by the wave base planes in the interstitial region of the unit cell. The wave functions were expanded in plane waves with a cut-off parameter of Kmax = 8/RMT. The RMT values were supposed to be 2.1 a.u. for In, 1.8 a.u. for As, and 1.7 a.u. for B atoms, for all the studied structures. Inside the MT spheres of radius RMT, we took the expansion of the wave function limited to lmax = 10, while for the charge density Fourier-expanded up to Gmax = 12 (Ryd) ^{½}.

The different exchange-correlation potential such as the generalized gradient approximation of Wu- Cohen (WC-GGA), the Engel and Vosko GGA formalism (EV-GGA) and the modified Becke-Johnson (mBJ), were applied to study the material properties for several compose of Boron [11–13].

In this study, the cubic unit cells of $B_xIn_{1-x}As$ alloys ($0 \le x \le 1$) consist of 32 atoms. For the structural and the electronic properties, the integrals on the Brillouin zone are affected with 50 k-points in the irreducible part of the Brillouin zone (IBZ), while for the optical properties, a condensed mesh of uniformly distributed k-points is important to obtain an excellent representation of the optical spectrums. In this case, the Brillouin zone integration is performed up to 500k-points.

3. Results and discussion

We study the structural properties of BAs, InAs and their ternary BxIn1-xAs for $0 \le x \le 1$ in the zinc blende structure using WC-GGA approach to compare them with the lattice parameter of GaAs expected to be a suitable substrate for the BxIn1-xAs ternary. Since the experimental results for the structural properties of BxIn1-xAs alloys are not available, the lattice constants for this ternary can be determined using Vegard's law [14] from the pure binaries parameters of BAs and InAs:

$$a_{(B_xIn_{1-x}As)}(x) = xa_{BAs} + (1-x)a_{InAs} \quad 0 \le x \le 1. \tag{1}$$

The lattice parameter, the bulk modulus and its first derivative with respect to the pressure have been determined by the adjustment of various in Murnaghan equation of state [16]:

$$E(V) = E_0 + \frac{B_0}{B'(B'-1)}\left[V\left(\frac{V_0}{V}\right)^{B'} - V_0\right] + \frac{B_0}{B'}(V - V_0) \tag{2}$$

Where E_0 is the equilibrium energy, B_0 is the bulk modulus and *B'* its first derivative.