Physica B 407 (2012) 2739–2743

Contents lists available at SciVerse ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Predicted electronic and structural properties of $B_xIn_{1-x}As$

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ARTICLE INFO

Article history:
Received 29 February 2012
Received in revised form
2 April 2012
Accepted 3 April 2012
Available online 10 April 2012

Keywords:
BAs
InAs
Boron alloy
Tight binding
Bowing
Elastic constants

ABSTRACT

Structural and electronic properties of the $B_xIn_{1-x}As$ ternary alloy are studied using the tight binding method. The optical band gap bowing is calculated for the first time in the full range of Boron composition *x*. It is found to be strong. A small deviation from virtual crystal approximation is found for the bond length. New results on elastic constants are reported. The obtained results are in good agreement with the available data in the literature.

1. Introduction

III–V wide band gap semiconductors like BAs, BP, BSb and BN compounds provide good basis for many technological applications in electronic and optoelectronic devices such as high temperature applications and electro-optical devices in the short-wave length range of the visible spectrum.

Boron Arsenide (BAs) has attracted increasing research interest both theoretically and experimentally in recent years. Several theoretical studies have been performed to understand and predict elastic, electronic and optical properties of BAs [1–5]. Because it is difficult to synthesize, the experimental studies of BAs properties are very rare; an experimental value for a small indirect gap of 0.67 eV and a direct gap of 1.46 eV, was reported more than 30 years ago [6], which has not been confirmed recently. Theoretical studies have shown that BAs is an indirect semiconductor which crystallizes in the zinc-blende structure. The conduction band minimum is located along the Δ line [1], the direct band gap is found to be in the 3.0–4.0 eV energy range by various semi-empirical and ab-initio methods [1–5].

Indium Arsenide (InAs), the other compound of the present work, is direct narrow band gap semiconductor with a value of 0.36 eV. Under normal conditions, this compound crystallizes in the zinc-blende structure. The high electron mobility of InAs, which is due to its narrow band gap, makes this compound useful for very high-speed and low-power-electronic and infrared optoelectronic devices [7–9].

Boron Arsenide due to its strong covalent character possesses a peculiar behavior compared to InAs [1]. So, in the present work, we have aimed to combine BAs and InAs compounds having different structural and electronic properties in order to obtain new materials, $B_xIn_{1-x}As$ ternary alloy, with intermediate properties.

In the literature, III–V alloys have been the subject of various theoretical investigations [10–13], while there are only a few theoretical studies on ternary alloy $B_xIn_{1-x}As$ and any experimental work. The aim of this study is to improve this situation through an investigation of optoelectronic and structural properties of this alloy.

We have organized this paper as follows: after a brief introduction in Section 1, we briefly describe the computational details in Section 2. In Section 3, the obtained results are discussed and compared with the available data. Finally, conclusions are given in Section 4.

2. Computational method

The empirical tight-binding (TB) method has been used extensively to study III/V compounds and appears to be well suited for the study of boron compounds BN, BP and BAs [2] and ternary III/V alloys [14]. Our approach for the ternary alloy $B_xIn_{1-x}As$ is based on a semi-empirical sp^3s^* TB method [15] which is treated within the modified virtual crystal approximation (VCA) that include the effect of disorder [16,17].

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http://dx.doi.org/10.1016/j.physb.2012.04.010

Let us consider ternary semiconductor alloy of the form $A_xB_{1-x}C$. We model the band structure of the constituent semiconductors AC and BC using our adjusted tight binding parameters which generate room-temperature band structures and then we form the VCA Hamiltonian matrix and calculate the fluctuations about the VCA using the Lee et al. formalism:

$$H_{alloy} = H_{VCA} + H_{dis} \tag{1}$$

H_{VCA} is the virtual crystal Hamiltonian matrix and H_{dis} describes the cationic (or anionic) disorder which is caused by the compositional disorder:

$$H_{dis} = -p(ABC)\sqrt{x(1-x)}(H^{BC} - H^{AC}) \tag{2}$$

where the disorder parameter $p(ABC)$ simulates the disorder effect and is treated in our calculations as an adjustable parameter.

In the virtual crystal approximation the diagonal elements are linearly interpolated as function of x:

$$H_{jj}^{VCA} = xH_{jj}^{AC} + (1-x)H_{jj}^{BC} \tag{3}$$

While the first neighbor matrix elements are interpolated assuming that they are scaled as inversely proportional to the square of the bond length:

$$V_{ij}^{VCA}(x) = x\frac{d_{AC}^2(x)}{d_{alloy}^2}V_{jj}^{AC} + (1-x)\frac{d_{BC}^2(x)}{d_{alloy}^2}V_{ij}^{BC} \tag{4}$$

$$d_{alloy} = d_{VCA} + d_{relax} \tag{5}$$

$$d_{relax} = x(1-x)\delta(d_{AC}(x) - d_{BC}(x)) \tag{6}$$

$$d_{VCA} = (1-x)d_{AC}(x) + xd_{BC}(x) \tag{7}$$

$$\begin{aligned} d_{AC}(x) &= d_{VCA} - x\xi_{BC:A}(d_{BC} - d_{AC}) \\ d_{BC}(x) &= d_{VCA} + (1-x)\xi_{AC:B}(d_{BC} - d_{AC}) \end{aligned} \tag{8}$$

$$\delta = \xi_{AC:B} - \xi_{BC:A} \tag{9}$$

where d_{AC} and d_{BC} are the unrelaxed bond lengths of the pure semiconductors AC and BC, respectively. $\xi_{AC:B}$ and $\xi_{BC:A}$ are the dimensionless relaxation parameters, which are computed using the formula of Cai and Thorpe [18]:

$$\xi = \frac{1 + C_1(\beta/\alpha)}{1 + 1 + C_2(\beta/\alpha) + C_3(\beta/\alpha)^2} \tag{10}$$

with $C_1 = 1.25$, $C_2 = 3.60$, $C_3 = 1.17$. α and β are the bond-stretching force constant and the bond-bending force constant, respectively and are listed in Table 1.

3. Results and discussions

In this section, we present the results of our tight binding calculation for the electronic band structure, direct and indirect energy gap, elastic constants and bulk modulus as function of the composition x in $B_xIn_{1-x}As$ alloy with and without taking into account the disorder effect.

Table 1
Bond-stretching force α and bond-bending force β constants [28].

Compound	α (10^2 Pa)	β (10^2 Pa)	β/α
BAs	95.7	25.1	0.263
InAs	28.2	6.89	0.245

3.1. Electronic properties

Table 2 gives our adjusted tight binding parameters and bond lengths of BAs and InAs binary compounds. The calculated band-gap energies of the lowest direct and indirect gaps for these compounds are presented in Table 3.

Figs. 1 and 2 display our calculated band structures of BAs and InAs respectively along high symmetry lines in the Brillouin zone. We notice from these figures that the band structure of BAs compound is more complicated than the InAs one. The calculated minimum band gap for BAs is found to be located approximately at X point. This result agrees well with the results of Ref. [19]. One of the important features of BAs band structure is that the Γ_{15c} band is below the Γ_{1c} band, in contrast to InAs compound where the Γ_{1c} state is below the Γ_{15c} state (see Fig. 2). This could be understood on the basis of the nature of the potential used [2]. The Γ_{15c}–Γ_{15v} direct band gap value of 3.25 eV obtained for BAs is also close to the result (3.3 eV) presented in Ref. [2]. The indirect band gap value is equal to 1.63 eV, this result is in the range of the experimental (1.46 eV) [20,21] and theoretical results (1.76 eV) [19].

The variations of direct band gap at Γ point and indirect band gap at X point are presented as function of the boron composition for $B_xIn_{1-x}As$ alloy in Figs. 3 and 4 respectively.

A significant bowing effect for $B_xIn_{1-x}As$ has been observed in the few existing theoretical investigations [22,23]. Our results show clearly that without disorder potential ($p=0.0$), the TB method coupled with the VCA does not reproduce the true band gap bowing. This bowing is known to be an effect caused by disorder and is not taken into account by the VCA. However, when the disorder potential is added, the figure shows that there is a deviation of the modified VCA energy gap from that predicted by the VCA, and an excellent agreement with predictions of Ref. [22] is obtained.

There is no experimental result for the $B_xIn_{1-x}As$ structure available to us. But Chimot et al. have expected an experimental room temperature direct band gap of the $B_xIn_{1-x}As$ alloy ($x=0.4$) in the 0.47–0.88 eV range. In adding the disorder potential and with tuning the p parameter a good agreement with this theoretical value is reached for the value of $p=0.71$. We have found in our calculation a band gap of $B_{0.41}In_{0.59}As$ equal to 0.50 eV and the bowing parameter b value is 3.10 eV for $B_xIn_{1-x}As$ alloy. The calculated band-gap bowing parameter exhibits strong composition dependence. This is different from most conventional III–V alloys which show a weak (<1 eV) composition-dependent bowing parameter [24]. According to Van Vechten and Bergstresser [25], the disorder contribution (which is related to the difference of electronegativities of the alloyed atoms) plays a dominant role in determining the bowing parameter. Thus, the

Table 2
Tight binding parameters of binary compounds BAs and InAs.

Parameters	BAs	InAs
$E(s,a)$	−9.24	−3.9247
$E(p,a)$	1.1106	3.1249
$E(s,c)$	−2.7404	−3.3247
$E(p,c)$	4.1046	0.1251
$E(s^*,a)$	7.4206	7.5870
$E(s^*,c)$	6.3011	6.2710
V_{ss}	−6.2118	−9.5919
V_{xx}	1.2466	0.6252
V_{xy}	4.2215	6.4004
$V(sa,pc)$	2.9781	3.8870
$V(sa,pa)$	6.1844	4.2789
$V(s^*a,pc)$	3.9276	2.6740
$V(s^*c,pa)$	3.1528	2.2191
d (Å)	2.07	2.61