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First-principles calculations of the structural, electronic and optical properties of $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys lattice matched to InP and BeS

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ABSTRACT

The structural, electronic, and optical properties of the cubic $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys lattice matched to InP and BeS have been investigated by using the full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). The generalized gradient approximation (GGA) of Wu and Cohen was used as the exchange correlation potential to calculate the structural and electronic properties. In addition, the alternative GGA proposed by Engel and Vosko and the modified Becke–Johnson potential are utilized to calculate the electronic properties. The computed structural and electronic properties of the binary compounds are in good agreement with the available experimental and theoretical data. For the alloys, non-linear variations of composition x and y with the lattice constant, bulk modulus, direct, indirect band gap, dielectric constant and refractive index are found. All the compounds are direct band gap excluding BP and BAs. The energy band gap of $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys lattice matched to InP and BeS substrates is computed. Finally, the band gap of our materials is less than 3.1 eV. Thus the $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys may possibly be used in visible light devices.

1. Introduction

Semiconductors are tremendously important both technologically and economically [1–6]. The III–V and II–VI semiconductor alloys are promising candidates for many device applications such as high speed electronic and long wavelength photonic devices because their band gaps cover a wide spectral range [7]. Recently, the optoelectronic devices of III–V compounds have advantages over II–VI semiconductor devices due to some interesting applications in optical communication systems such as diodes laser, light-emitting diodes, photodetectors, electro-optic modulators and frequency mixing components [8–11]. The major goal of materials engineering is the ability to tune independently the band gap energy and the lattice constant in order to obtain the desired optical properties. One of the easiest methods to change artificially the properties of semiconductors is by forming the alloys; the adapt of two, three or four different binary compounds with different optical band gaps could lead to new semiconductor material with desired band gap and lattice constant over a continuous broad composition range. Hence, we noted in the last decade several researches that led to the development of new material systems based on the incorporation of boron into conventional III–V binary compounds and ternary alloys. These materials have a wide range of technological potentials in the

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field of band gap engineering and optoelectronic integration. This is due to their attractive characteristics which include low ionicities [12–14], short bond lengths [15], excellent physical hardness [15], and high melting point [16]. Consequently, the boron would be a good choice to make new quaternary semiconductors alloys of III–V materials.

$In_{1-x}B_xAs_yP_{1-y}$ alloys belong to this class of new III–V semiconductor materials which are composed by four binary compounds, the indium arsenide (InAs), indium phosphide (InP), boron phosphide (BP), and boron arsenide (BAs). These binary materials crystallize in the zinc blende structure at equilibrium [17]. This paper is the first quantitative theoretical prediction of the fundamental physical properties of the $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys lattice matched to InP and BeS substrates. The aim of this work is to study structural, electronic, and optical properties of the quaternary $In_{1-x}B_xAs_yP_{1-y}$ alloys by using full-potential linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT). Initially, we start the work on binaries to check the accuracy of our approach which is supposed to predict the properties of quaternaries. Then, we compute the lattice constant, bulk modulus, band gap, refractive index, and dielectric function of $In_{1-x}B_xAs_yP_{1-y}$ alloys over the all compositions x and y. Subsequently, we have focused to calculate the gap energy of $In_{1-x}B_xAs_yP_{1-y}$ quaternary alloys lattice matched to InP and BeS.

The paper is divided into four sections. A brief introduction is given in Section 1. The computational method adopted for the calculation is elucidated in Section 2. The most pertinent results obtained for the structural, electronic, and optical properties of the binary compounds, as well as the ternary and quaternary alloys, are presented and discussed in Section 3. Finally, in Section 4, we summarize the main conclusions of our work.

2. Method of calculations

In this study, the calculations are based on the self-consistent first principles full-potential linearized augmented plane wave (FP-LAPW) method [18] within the framework of density functional theory (DFT) [19] as implemented in the WIEN2K computer package [20]. For structural properties, the exchange correlation potential was calculated using the generalized gradient approximation (GGA) in the new form (WC) proposed by Wu and Cohen [21] while the Engel–Vosko (EV-GGA) [22] and the modified Becke–Johnson (mBJ) [23] schemes were used for electronic properties. The latter approximation was designed to reproduce as well as to made possible the exact exchange correlation potential rather than the total energy. In the FP-LAPW method, the space is divided into non-overlapping muffin-tin (MT) spheres centered at the atomic sites (region I) and an interstitial region (region II). In the region I, the wave function solutions of the Kohn–Sham equations are expanded by using the product of the radial functions and the spherical harmonics. However, in the region II, the expansion is carried out using plane waves. The wave functions in the interstitial region were expanded in plane waves with a cut-off $R_{MT}\,K_{max}=8$ (R_{MT} is the smallest muffin-tin radius in the unit cell). The values of R_{MT} were assumed to be 2.3, 2.2, 2.1 and 1.8 a.u. for In, As, P and B, respectively. We used $l_{max}=10$ for wave function expansion inside the atomic spheres and the charge density was Fourier-expanded up to $G_{max}=12$ $(Ryd)^{1/2}$. However, we have chosen a value equal to -6.0 Ry for the energy cut-off between the core and valence states for both compounds. The number of a special k points chosen over the irreducible Brillouin zone are 72 k-points for the binary compounds, 36 k-points for the ternary alloys and 27 k-points for the quaternary alloys. Both the plane wave cutoff and the number of k-points were varied to ensure total energies convergence. Our calculations for valence electrons were performed in a scalar-relativistic approximation neglecting spin-orbit coupling, while the core electrons were treated fully relativistic.

3. Results and discussion

3.1. Binary compounds

The quaternary alloys $In_{1-x}B_xAs_yP_{1-y}$ are bordered by the ternary alloys $InAs_xP_{1-x}$, $In_{1-x}B_xP$, $In_{1-x}B_xAs$ and BAs_xP_{1-x} which are bounded, in their turn, by four binary compounds (InAs, InP, BAs and BP). Before handling the main steps of the present work, let us start with a preliminary study of the structural and electronic properties of the binary compounds which crystallize in the 2-atom-unit-cell zinc blende lattice structure. For all binaries the (0, 0, 0) site is occupied by In and B atoms while the (0.25, 0.25, 0.25) site is occupied by As and P atoms.

In order to obtain the equilibrium lattice constant (a) and the bulk modulus (B) for the InAs, InP, BAs and BP compounds, we conducted the structural optimization by minimizing the total energy with respect to the cell parameters. The calculated total energies are fitted to the Murnaghan's equation of state [24]. The structural parameters (a, B) and the band gap energy are shown in Table 1, which also contains the results of previous first principles calculations as well as experimental data. In addition, the equilibrium lattice parameter of BeS lattice matched with the alloys is added to the same table. It is clear from Table 1 that the calculated lattice constant and bulk modulus are in reasonable agreement with the experimental values and there are only slight differences between our results and those calculated in literature. This difference may be due to a different calculation model and also for the approaches used in each study.

The electronic band structures of the InP, InAs, BAs and BP binary compounds are computed along the high symmetry directions in the Brillouin zone within the WC-GGA, EV-GGA and mBJ approaches. The InP and InAs have direct band gap ($\Gamma\rightarrow\Gamma$). However, BP and BAs have indirect band gap ($\Gamma\rightarrow X$) where the conduction band minimum (CBM) is located at the X point. The values of the band gap energies are given in Table 1. The shapes of the band structures obtained using the three approximations are identical. It is clearly seen from Table 1 that the values obtained by the modified Becke Johnson (mBJ) are close to the experimental results. This method gives significantly improved results than the previous theoretical ones. Also, the Engel–Vosko (EV-GGA) method gives values fairly close to the experimental results. It is found for the WC-GGA scheme that the energy band gap is underestimated compared to the experimental and theoretical values. In fact, GGA usually underestimates the experimental energy band gap [48,49]; this is an intrinsic feature of DFT