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First principles study of structural, electronic and optical properties of indium gallium nitride arsenide lattice matched to gallium arsenide

Mohamed Issam Ziane [a,*], Zouaoui Bensaad [a], Tarik Ouahrani [b], Hamza Bennacer [a]

[a] Applied Materials Laboratory, Research Center (CFTE), Sidi Bel Abbès Djillali Liabes University, 22000, Algeria
[b] École Préparatoire en Sciences et Techniques, BP 165 R.P., 13000 Tlemcen, Algeria

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ABSTRACT

First principles calculations in the framework of the full-potential linearized augmented plane wave (FP-LAPW) scheme have been carried out. The dilute-nitride zinc blende ($In_xGa_{1-x}N_yAs_{1-y}$) was modeled at selected nitrogen compositions of $y=3.125\%$, 6.25% and 9.375% lattice matched to gallium arsenide (GaAs). We pay attention to the $In_xGa_{1-x}N_yAs_{1-y}$ alloy which can be perfectly lattice matched to the GaAs over its entire compositional range. In our study, this is achieved when a condition $y\sim2.7x$ is maintained. The band structure calculations were performed with and without relaxation by using the generalized gradient approximation of Engel and Vosko (EV-GGA) as well as by the modified Becke–Johnson potential exchange (TB-mBJ). The action of the localized potential of subsisted nitrogen atoms was attributed to effect of relaxation. Increasing both indium and nitrogen compositions leads to decreasing energy band gap. In addition a band anti-crossing model (BAC) was also adopted to study the composition dependence of the direct band gap of quaternary alloys, building a bridge between their electronic and linear optical properties.

1. Introduction

In recent years, III–V semiconductors have attracted both scientific and technological interest, due to their applications in the opto-electronic and technological effort. These semiconductor materials can crystallize in either the cubic zinc-blende phase (space group F43m) or the hexagonal wurtzite phase (space group P63mc). Gallium arsenide (GaAs) is one of the largest important semiconductor among III–V compounds, widely studied due to their significance in the technological application of semiconductor industry. Another novel material system that has attracted considerable interest recently is the dilute nitride semiconductor. The latter is formed by alloying limited quantity of nitrogen into III–V semiconductor hosts [1]. Nitrogen containing GaAs has opened a new opportunity to largely extend the band gap engineering capabilities of III–V semiconductors materials [1]. It has been shown that the introduction of a small amount of nitrogen elements in the III–V hosts such as GaAs reduces the energy band gap by about 150 meV for only 1% of nitrogen [2]. Apart from GaNAs, the closing in the band gap has been remarked also in other ternary and quaternary alloys [3–8]. As explained by Elyukhin et al. [9], this reduction is mainly due to the transformation of the bonds after redistribution of the atoms in their lattice sites.

* Corresponding author. Tel.: +213 774884300.
E-mail address: issam1308@yahoo.fr (M.I. Ziane).

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However, the closure of the electronic band gap induced by nitrogen (N) is then balanced by introducing an atom with high atomic radius such as indium (In) element [10]. An attractive material, which is expected to have significant advantages over the conventional III–V–N materials, is the quaternary InGaNAs alloy [11]. This alloy has received great attention [12–15] because of its direct band gap and relatively high mobilities. The InGaNAs quaternary alloys are the key materials for the fabrication of diverse electronic and optoelectronic components, especially in vertical cavity emitting source above 1.28 μm [16], high performance laser diodes emitting at 1.3 and 1.55 μm optical fiber windows [17,18], visible light emitting diodes (LEDs) [19], photodetector operating at 1.3 μm [20], avalanche photodiodes at 1.064 μm [21], heterojunctions bipolar transistors (HBTs) [22] and high efficiency solar cells [23]. Extensive investigations on InGaNAs lattice matched to GaAs have been reported by various experimental methods [24–26].

One of the most important tasks in the solid-state studies is to understand the atomic structure of a crystalline compound, in which the lattice constant is the key parameter. Therefore, an accurate knowledge of the nitrogen concentration effect on the electronic band gap energy of InGaNAs alloys is very important. Among recently published works on InGaNAs, we can find one theoretical study [27]. In their work M. Aslan and co-workers have calculated the structural and electronic properties of $Ga_{1-x}In_xAs_{1-y}N_y$ quaternary alloys by using PWSCF code based on the plane-wave pseudopotential method within the local density approximation. They have examined the lattice constant and band gap energy for high In and N contents. In this work, we aim to present a theoretical prediction of the structural, electronic and optical properties of dilute-nitride zinc blende ($In_xGa_{1-x}N_yAs_{1-y}$) lattice matched to GaAs with nitrogen contents $y=3.125\%$, 6.25% and 9.375% by carrying out first principles calculation. Although the prediction of physical properties is the subject of our investigation, some aspects of the study of these properties remain controversial. Notably, ignorance persists regarding the scope of the interaction in the Brillouin Zone and hybridization states. This interaction is the source of the strong decrease of the band gap and the appearance of additional transition. Furthermore, the effects of nitrogen are assumed to be negligible at the band valence.

This article is organized as follows. In Section 2, we briefly describe the computational techniques used in this work. Results and discussions of our study will be presented in Section 3. Finally, a summary of this work is given in Section 4.

2. Computational details

The calculations presented in this paper have been performed within the framework of density functional theory (DFT) using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2k code [28]. This is a very accurate and efficient scheme to solve the Kohn–Sham equations [29]. The wave function basis used is mixed atomic functions and plane waves. The exchange-correlation potential is treated within the WC-GGA. However, many calculations for solids [30] have showed that the GGA method constructed by Wu and Cohen in WC-GGA gives, at some extension, a good description of structural optimization. In order to develop and improve the FP-LAPW technique, a considerable effort has been devoted in the last 25 years to go beyond the standard approximations. In 1993 Engel and Vosko analyzed various versions of GGA exchange potentials and argued that, due to their particularly simple forms, GGAs are not able [31] to reproduce a good description of the band gap energy. In addition to the BAC model the generalized gradient approximation of Engel–Vosko (EV-GGA) [32] and the modified Becke–Johnson scheme (TB-mBJ), proposed recently by Tran and Blaha [33], were also used for electronic properties. It is worth reminding that these two latter approximations are not valid for the computations of the equilibrium structural parameters.

In order to simulate our quaternary alloys, we have used a $(2\times2\times2)$ supercell with 64 atoms. The crystal structures of $In_{0.093}Ga_{0.906}N_{0.031}As_{0.968}$, $In_{0.156}Ga_{0.843}N_{0.062}As_{0.937}$ and $In_{0.25}Ga_{0.75}N_{0.093}As_{0.906}$ quaternary alloys are shown in Fig. 1. The unit cell is divided into non-overlapping muffin-tin (MT) spheres around the atomic sites, and an interstitial region. From crystallography and under normal conditions, gallium arsenide (GaAs) and indium arsenide (InAs) have the B3 structure with space group F-43m [34] whereas gallium nitride (GaN) and indium nitride (InN) crystallize under normal conditions in the hexagonal wurtzite phase with the associated space group P63mc. The zinc blende structure (or sphalerite) for GaN and InN has been stabilized by epitaxial growth of the thin films on {011} crystal planes of cubic substrates [35]. In particular, works on zinc blende nitrides have attracted a great deal of theoretical attention due to their potential advantages they offer for optoelectronic applications compared to the commonly employed hexagonal nitrides [36]. The zinc blende structure is considered as a model system for all concerned materials used in this study. The simple cubic super-cell presented in Fig. 1 is constructed with 32 atoms of valency three (In/Ga) and thirty two pentavalent atoms (As/N) used to simulate the present material alloys. The muffin-tin radii R_{MT} were chosen equal to 2.20, 2.10, 1.76, and 2.15 a.u for In, Ga, N and As, respectively. The $R_{MT}K_{max}$ parameter was taken equal to 7.0. To ensure the correctness of our calculations, we have taken $l_{max}=10$ and $G_{max}=14.0$. Also, the self-consistent calculations are considered to be converged when the total energy is stable within 0.1 mRy.

3. Results and discussion

3.1. Volume optimization

In order to calculate the ground state properties of ternary alloys $In_{0.093}Ga_{0.906}As$ and $GaN_{0.031}As_{0.968}$, and quaternary alloys $In_{0.093}Ga_{0.906}N_{0.031}As_{0.968}$, $In_{0.156}Ga_{0.843}N_{0.062}As_{0.937}$ and $In_{0.25}Ga_{0.75}N_{0.093}As_{0.906}$ alloys we must start from volume optimization of the constituent pure binaries. The non-