J Nanostruct 6(4): 273-277, Autumn 2016

RESEARCH PAPER

First-Principles Investigation of Density of States and Electron Density in Wurtzite $In_{0.5}Ga_{0.5}N$ Alloys with GGA-PBEsol Method

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ARTICLE INFO

Article History:
Received 03 August 2016
Accepted 17 September 2016
Published 01 October 2016

Keywords:
InGaN
DOS
DFT
FP-LAPW
GGA

ABSTRACT

In present work, we have calculated the electronic properties including density of states and electron density for GaN, InN and $In_xGa_{1-x}N$ in wurtzite phase for x=0.5. The study is based on density functional theory with full potential linearized augmented plane wave method by generalized gradient approximation for calculating electronic properties. In this report we concluded that $In_xGa_{1-x}N$ band gap, which would be decreased with increasing in concentration and GaN is very sensitive on in content.

How to cite this article
Hashemizadeh S. A, Mohammadi Siavashi V. PFirst-principles investigation of density of states and electron density in wurtzite$In_{0.5}Ga_{0.5}N$alloys with GGA-PBEsol method. J Nanostruct, 2016; 6(4): 273-277. DOI: 10.22052/jns.2016.40758

INTRODUCTION

Group III-Nitride semiconductors are one of the group III-V compound semiconductor, such as InN and GaN, and have long been studied since they have important applications in light emitting diodes (LEDs) [1] and short wavelength laser diodes (LD) [2,3] this is mainly because of their relatively wide band gap corresponding to the visible region to the near ultraviolet region of the spectrum and high emission efficiency. In addition, bright blue LEDs based on III-nitride semiconductors have already paid the way for full-colour displays and also for mixing three primary colours to obtain white light for illumination. The InGaN and AlGaN ternary nitride semiconductors have been studied extensively, because InGaN is the main material of blue-violet light, AlGaN is the material of ultraviolet (UV). The technological importance of GaN and InN particularly for the light-emitting and LDs operating in green and blue spectral regions, has stimulated the study of their alloy $In_xGa_{1-x}N$.

Two basic crystal structures of III-nitride semiconductors are Hexagonal wurtzite (WZ) structure and cubic zincblende (ZB) structure [4-6]. WZ structure is extensively utilized due to exhibiting the direct band gap energy for all conventional nitrides in the WZ phase.

The first approachis to predict the main electronic properties of GaN, InN and$In_{0.5}Ga_{0.5}N$; theoretical calculations have been carriedout in WZ phase. Here we use the wien2k [7] code, which works on DFT [8,9] and also use the full-potential (linearized) augmented plane-wave ((L) APW) plus local orbital (LO) method. The exchange correlation potential was treated by means of the generalized gradient approximation (GGA) [10] within the Perdew–Burke–Ernzerhof solid (PBEsol) [11] exchange-correlation functional.

CALCULATION METHOD

In the framework of DFT, we have employed

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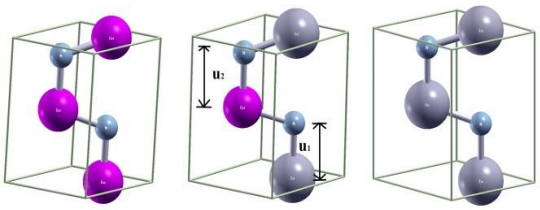

Fig. 1. Wurtzite structure of $In_{0.5}Ga_{0.5}N$, from left to right respectively x=0, 0.5 and 1. The length bond In-N is u_1c and Ga-N is u_2c

the wien2k code which uses augmented plane wave plus local orbital (LAPW + LO) method. Fig. 1 shows the used crystalline structure, which was made with XCrySDen program [12-14], and Table 1 gives position of the atoms in the unitary cell.

The electronic configurations ofGaNandInN are Ga:Ar $3d^{10}4s^24p^1$, In:Kr $4d^{10}5s^24p^1$ and N:H $2s^22p^3$.

In the following calculation, the sub shells of the noble gas cores have been distinguished from the sub shells of valence electrons given explicitly. Basis functions were expanded in combinations of spherical harmonic functions inside non-overlapping spheres surrounding the atomic sites (muffin-tin spheres) and also in a Fourier series in the interstitial region. In the muffin-tin (MT) spheres,thel-expansion of the non-spherical potential and charge density was carried out up to In L_{max}=10 order to achieve energy eigenvalues convergence, (L_{max} is the maximum angular momentum inside the muffin-tin sphere) the wave functions in the interstitial region were expanded in plane waves with a cut-off of K_{max} R_{MT}=8 (where R_{MT} is the average radius of the MT spheres).

There are number of decisions which must first be made for the choice of the particular (and different) muffin-tin radii for the various atoms in compounds and alloys. Our choices for the muffin-tin radius (R_{MT}) are made under some conditions. (i) No core charge leaks out of MT-spheres, (ii) Once we know the nearest neighbor (NN) distances the value for R_{MT} would be specified. Small values of R_{MT} must be less or equal to the NN-distance between cation–anion atoms. (iii) The difference between two atoms should not be too large. Within the allowed ranges of R_{MT}, smaller values give more accurate results, in such case we describe a larger part of the crystal by more flexible plane waves but it take more time (plane waves are expensive). (iv)The final results must not depend on the exact choice of R_{MT}. The choice of particular (and different) muffin-tin radii for various atoms in the compounds and alloys shows small differences that do not affect the present conclusions. However, the use of the full-potential ensures that the calculation is completely independent of the choice of the sphere radii.

For GaNand InNwe have adopted the values of 1.9, 1.8 and 1.6 Bohr radius for indium, gallium and nitrogen, respectively, as MT radius. For the ternary alloy $In_{0.5}Ga_{0.5}N$the MT radius of 1.75 Bohr radiushave been chosen for the gallium and indium, and 1.65 Bohr radius have been chosen for the nitrogen.

Magnitude of the largest vector of potential expansion and charge density which in interstitial region has been used was G_{max}=12. In all calculation convergence was on charge density and energy density and also 0.0001 used as convergence criterion.

We used structural parameters of GaN,$In_{0.5}Ga_{0.5}N$ and InN from theoretical and experimental data as

Table1. Positions in crystal coordinates for the elements of GaN, $In_{0.5}Ga_{0.5}N$ and InN.

Elements	GaN	$In_{0.5}Ga_{0.5}N$	InN
In		$\left(\frac{2}{3},\frac{1}{3},0\right)$	$\left(\frac{2}{3},\frac{1}{3},0\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$
Ga	$\left(\frac{2}{3},\frac{1}{3},0\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$	$\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$	
N	$\left(\frac{2}{3},\frac{1}{3},u_2\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_2\right)$	$\left(\frac{2}{3},\frac{1}{3},u_1\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_2\right)$	$\left(\frac{2}{3},\frac{1}{3},u_1\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_1\right)$

Table 2. Structural parameters which using for calculations.

Elements	GaN	$In_{0.5}Ga_{0.5}N$	InN
In		$\left(\frac{2}{3},\frac{1}{3},0\right)$	$\left(\frac{2}{3},\frac{1}{3},0\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$
Ga	$\left(\frac{2}{3},\frac{1}{3},0\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$	$\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$	
N	$\left(\frac{2}{3},\frac{1}{3},u_2\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_2\right)$	$\left(\frac{2}{3},\frac{1}{3},u_1\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_2\right)$	$\left(\frac{2}{3},\frac{1}{3},u_1\right)$ $\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}+u_1\right)$

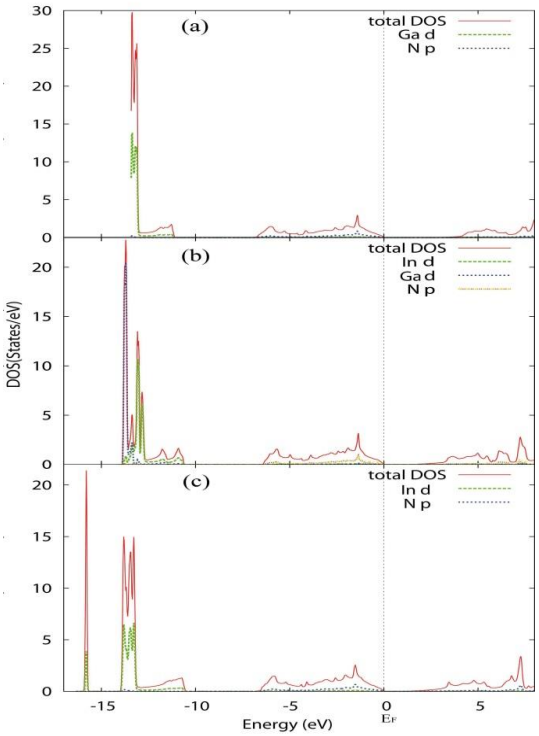

Fig. 2. The total DOS and PDOS in WZ phase for (a) GaN, (b) and (c) InN.

shown table 2.

k integration over the Brillouin zone (BZ) is performed using the Blöchl's tetrahedron method [19]. We use a 12 x 12 x 6 mesh (126 k-points) for InN and GaN and also (234 k-points) for , $In_{0.5}Ga_{0.5}N$in the irreducible wedge of the Brillion zone.

RESULTS AND DISCUSSION

Density of states (DOS)

In order to analyze the electron distribution of each atomic orbital, we calculate total DOS and partial density of states (PDOS). Total DOS and PDOS of configurations [Fig. 2], shows the valence band of GaN and $In_{0.5}Ga_{05}N$ be divided in to three zones and InN be divided in to four zones.

For GaN we find a sharp peak at -13.4eV below the Fermi level (EF), which arises due to Ga-3d states. In the valence region, peaks in the energy range -7 up to 0eV are contributed due to N-2p states and Ga-3d state electrons [Fig. 2(a)]. We also find a pick in conduction band in the energy range 2.095eV up to 8eV are contributed due to N-2p states. Calculated band gap 2.095eV from DOS plot, is in agreement with its value calculated from others in GGA and LDA, as shown in table 3 [17,20,21].

Total DOS of $In_{0.5}Ga_{0.5}N$ shows two sharp peaks in -13.1 and -13.7eV are contributed due to In-4d and Ga-3d, respectively [Fig. 2(b)]. In interval between -6.5 up to 0eV we also observed hybridization of N-2p and very small contribution In-4d and Ga-3d. We note from Table 3 that calculated value for band gap in this Dos plot 0.762eV is in agreement with thecalculated value from others in LDA [17, 20, 21].

Also for InN, Fig. 2(c) shows that the valence band of In can be divided into three zones: a shallow valence band at around -16eV is formed by In-4d bonding states, a middle zone from -14 to -10.5eV is mostly composed of the In-4d states

Table 3. The calculated band gaps (eV) in this work (GGA-PBEsol) and some other work in WZ phase.

Method	Exchange-correlati XC	GaN	$In_{0.5}Ga_{0.5}N$	InN
	GGA-PBEsol (this work)	2.095	0.762	0.572
FP-LAPW	GGA	1.992[20.]		0.192[20.]
	LDA	2.220[17.] 1.87(	0.770[17.]	0.170[17.] -0.340[21.]
Exp.		3.420[22.]	2.001[23.]	1.994[23.] 0.780[24.]

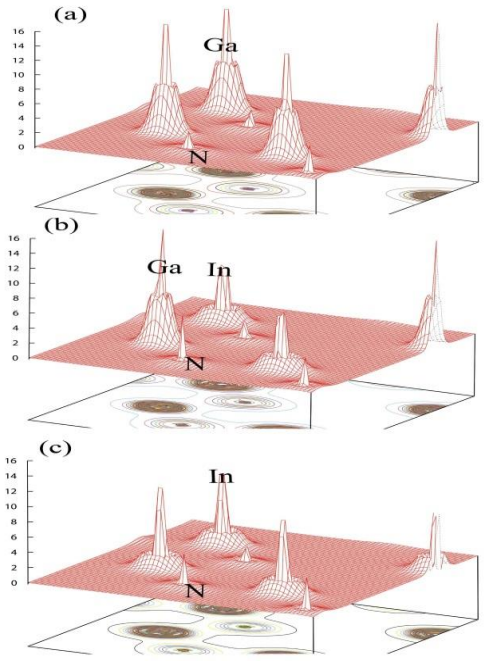

Fig. 3. 3D plot of Electron density for (a) GaN, (b) $In_{0.5}Ga_{0.5}N$ and (c) InN along 110. direction for WZ phase.

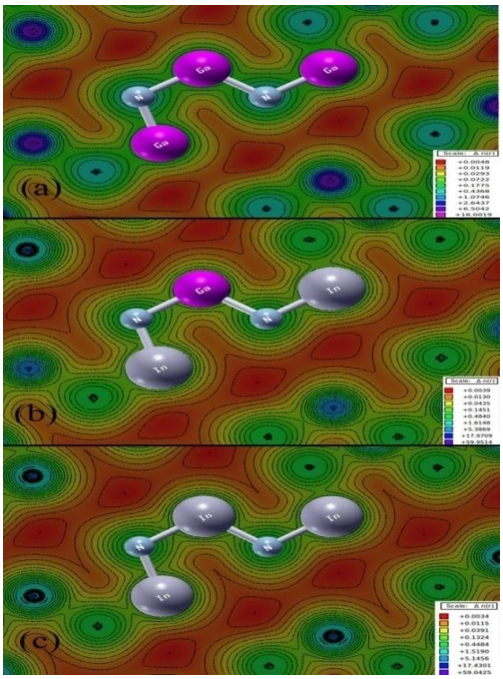

Fig. 4. Electron density for (a) GaN (b) $In_{0.5}Ga_{0.5}N$ and (c) InNalong [110] direction for WZ phase.

which appears to be hybridized with the In and N orbitals and the upper valence band at higher energy, that is from -6.75 to 0eV, is mostly derived from the N-2p states hybridized with the In-4d states. The value of calculated for band gap of InN in this Dos plot 0.572eV is in more agreement with experimental data than LDA and also GGA, as shown in table 3 [17, 20-24].

Electron density

At first principle calculations, the electron density plays an important role in the interpretation of the physical and chemical properties of a compound. Based on the electronic cloud, the bonding nature of compoundsGaN, $In_{0.5}Ga_{0.5}N$, InN is presented in Figs 3(a)-(c) and 4(a)-(c) respectively. These figs show the 3D plots and contour graphs of the electron density on a (110) plane passing through In, Ga and N atoms. Fig. 3 shows that existence a weak covalent bond between In, Ga and N atoms obviously.

Fig. 4 indicates existence Ga-N and In-Nionic bond, and also in Fig. 4(b) it is clearly shows that for, $In_{0.5}Ga_{0.5}N$ the In-N bond is stronger than Ga-N bond, therefore Figs. 4(a)-(c) reveals that the increasing of In concentration varies the bonds, hence We expect the change in the lattice parameters due to these bonds as well as the difference in the size of In atoms. The variation in the lattice constant affects directly the optoelectronic properties of the compound.

CONCLUSION

In present work, FP-LAPW method has been employed to study the electronic properties of GaN, $In_{0.5}Ga_{0.5}N$and InN. The density of state have been calculated by generalized gradient approximation (GGA) within PBEsol and effect of In consentration in density of state has been considered. The band gaps which we acheaved in density of states, specialy for InN is in good agreement with some experimental works, and for GaN is in good agreement with some other computational work, but it doesn`t for the experimental. We conclude that$In_{0.5}Ga_{0.5}N$bandgapwould be decrese with incresing the In concentration from 2.095eV to 0.572eV. Investigation of DOS for this compounds indicate that N-2p, In-4d and Ga-3d orbitals role mainly in this compounds and also electron density indicates that bond of Ga-N and In-N is more ionic than covalent bond and ionic bond in In-N is stronger than Ga-N so.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publicaton of this manuscript.

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