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First principle calculations of the electronic properties and splitting energy of $Al_xGa_{1-x}N$ using GGA and mBJ potentials

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In this paper, we present the first principle calculations of the band structure of gallium nitride (GaN)-based semiconductor alloy of $Al_xGa_{1-x}N$ for x=0.25, 0.50 and 0.75. Our calculations were performed using the density functional theory (DFT) with the generalized gradient approximation (GGA) and modified Becke-Johnson (mBJ) potential of Tran and Blaha, which are based on the optimization of total energy and corresponding potential within the full potential-linearized augmented plane wave (FP-LAPW) method. We have compared our results calculated by GGA and mBJ and we found that mBJ gave better results than GGA. The calculated band gap varies nonlinearly as a function of the composition x. Our calculated direct band gap bowing parameter *b* using mBJ potential is found to be 0.72 eV which is in good agreement with the experimental results as well as the theoretical predictions. However, in the case of GGA, the direct band gap measured has a lower value of 0.55 eV. We also obtained the result on the band structure with the inclusion of spin-orbit interaction (SOI) on both approximations and also compared the results. We have found that the inclusion of SOI affected the band structures and the splitting of the degenerate valence band occurred on high symmetry Γ-point.

Keywords: Gallium nitride (GaN), FP-LAPW, GGA, mBJ, bowing parameter, spin orbit Interaction.

INTRODUCTION

In recent years, Group III nitride-based semiconductors have attracted much attention to researchers due to their potential applications in modern electronics and optoelectronics devices from the UV to the near IR region. Moreover, due to their high chemical and thermal stability, they are most suitable candidates for applications under high temperature, high power and high-frequency electronic devices (Lopez-Apreza *et al*., 2008). Recently, gallium nitride (GaN), aluminium nitride (AlN), indium nitride (InN) and their alloys have been observed to be excellent and promising candidates for laser diodes, short wavelength LED and the absorber layers in solar cells as their absorption edge can be optimized as per the cell efficiency (Lafer *et al*., 2013).

The two commonly used basic crystal structures of Group-III nitrides and their alloys are hexagonal wurtzite structure and cubic zinc blende structure. The wurtzite structure is widely used because of their direct bandgap energy which results in high emitting performance (Pankove *et al*., 1970). The values of band gap in wurtzite structure ranges from 0.17 eV for InN, 2.22 eV for GaN and 4.4 eV for AlN (Dridi *et al*., 2003). Among these compounds, AlN and its alloy $Al_xGa_{1-x}N$ has been considered to be significant for the development of wavelength laser (Miwa and Fukumoto, 1993).

There are many investigations using different methods and technique to calculate the structural, electronic and optical properties of $Al_xGa_{1-x}N$. However, there is still no agreement on the exact values of certain parameters since they exhibit a large scattering. The reported values of the bowing parameter calculated through different experiments range from -0.8 eV to ≈ 1.3 eV (Dridi *et al*., 2003).

In this paper, we analyse the influence of alloying on the electronic band gap of $Al_xGa_{1-x}N$ in the wurtzite structure. All calculations are performed by means of numerical simulation based on first principle calculation using WIEN2k code. We have included the study of SOI and the associated spin splitting for $Al_xGa_{1-x}N$ using LAPWSO method. The SOI contains the Rashba and Dresselhaus effects. Rashba effect is due to the structural inversion asymmetry of confinement while Dresselhaus effect is due to the bulk inversion asymmetry of crystal potential. SOI is the key issue of semiconductor spintronics (Wang *et al*., 2009). Since there is a large spin splitting of a two dimensional electron gas (2DEG) in a wurtzite AlGaN/ GaN heterostructure, GaN based material is a suitable candidate for spintronic applications.

MATERIALS AND METHODS

All our calculations were performed within the framework of the DFT (Hohenberg *et al*., 1964), which states that all of the ground state properties of a system are functional of the electron density and the total energy is expressed in terms of the electron density rather than the wave function. The total energy calculations were based on the FP-LAPW method (Blaha *et al*., 2016). In this method, LAPW is a procedure used to solve the Kohn -Sham equation that is based on the DFT. To minimise the energy, the unit cell is partitioned into non-overlapping spheres called muffin-tin spheres centred at the atomic sites and the interstitial region. Inside these two regions, different basis sets are used. Inside the muffin-tin (MT) sphere, Kohn-Sham orbitals are expanded as linear combination of radial functions multiplied by spherical harmonics.

Inside the interstitial region, plane wave expansion was applied. We distinguished respectively Al ($1s^2 2s^2 2p^6$), Ga ($1s^2 2s^2 2p^6 3s^2 3p^6$) and N ($1s^2$) as inner shell electrons from the valence electrons of Al ($3s^2 3p^1$), Ga ($3d^{10} 4s^2 4p^1$) and N ($2s^2 2p^3$) shells. The different MT-spheres radii used are 1.83 Å for Al, 1.92 Å for Ga and 1.65 Å for N. We used an appropriate set of *k*-points (=500 points) to compute the total energy. The maximum value of *l* for the wave function expansion inside the atomic sphere is taken to l_{max}=10. For energy eigenvalues convergence, the wave function in the interstitial regions are expanded in plane waves with a cut off of (k_{max})(RMT)= 7.

To model the $Al_xGa_{1-x}N$ ternary alloy with different compositions (x=0.25,0.50 and 0.75), we have created 2x2x1 super cell that generates 16-atoms which has twice the size of the primitive wurtzite unit cell in both directions of the basal plane and along *c*-axis at the equilibrium lattice. The analysis of the exchange-correlation energy of the electrons was treated using GGA and mBJ potentials with and without the inclusion of SOI for comparison. SOI is performed using the code LAPWSO. We have used the non-spin polarised calculation since the alloy are non-magnetic in nature. The number of eigenvalues are doubled up since spin orbit couples spin-up and spin-down states, as they are no longer separable.

RESULTS

Electronic properties

For the $Al_xGa_{1-x}N$ ternary alloy, we have calculated the electronic band structures of $Al_xGa_{1-x}N$ using PBE-GGA and GGA-mBJ approximations which are used as exchange-correlation potential and then implemented in the WIEN2k code (Tran *et al*., 2009). The calculated band structures give a direct band gap where the valence band peak and the lowest conduction band are in the same point of symmetry Γ as shown in Figure 1.

We have used the compositions of *x* = 0.25, 0.50 and 0.75. The calculated band gaps of $Al_xGa_{1-x}N$ using the mentioned compositions are shown in Table 1. Using the calculated band gap, we then calculated the band gap bowing parameters by fitting the non-linear variation of the calculated band gap versus composition, *x* which is assumed to follow the simple quadratic form:

$$E_g(A_xB_{1-x}C) = xE_g(AC) + E_g(BC) - x(1-x)b \rightarrow (1)$$

where $E_g(A_xB_{1-x}C)$, $E_g(AC)$ and $E_g(BC)$ are the energy band gaps of the ternary alloy $A_xB_{1-x}C$ and its binary parents AC and BC respectively. The curvature *b* is the so called bowing parameter. It accounts for the deviation from a linear interpolation between the two binaries (Vurgaftman and Meyer, 2003).

The results for the direct band gap using GGA and mBJ potentials without SOI, as shown in Figures 1 and 2 are well fitted using Eqn. (1) which are summarized as follows:

Using GGA approximation,
$Al_xGa_{1-x}N$ (Γ-Γ) = 1.327 + 0.806*x* +0.552 x^2 →(2)

Using mBJ as exchange-correlation potential,
$Al_xGa_{1-x}N$ (Γ-Γ) = 2.852 + 0.462*x* +0.728 x^2 →(3)

Comparisons of the calculated band gap bowing parameter using GGA and mBJ with the other theoretical and experimental works are given in Table 2. We found that for our calculated ternary alloy, mBJ calculation gives more accurate result than GGA.

Spin orbit interaction

We have calculated the band structures of $Al_xGa_{1-x}N$ with the inclusion of SOI through LAPWSO using a second -variation method with the scalar-relativistic orbital (from LAPW) as basis. The calculated band structure of $Al_xGa_{1-x}N$ with the inclusion of SOI is shown in Figure 3. In

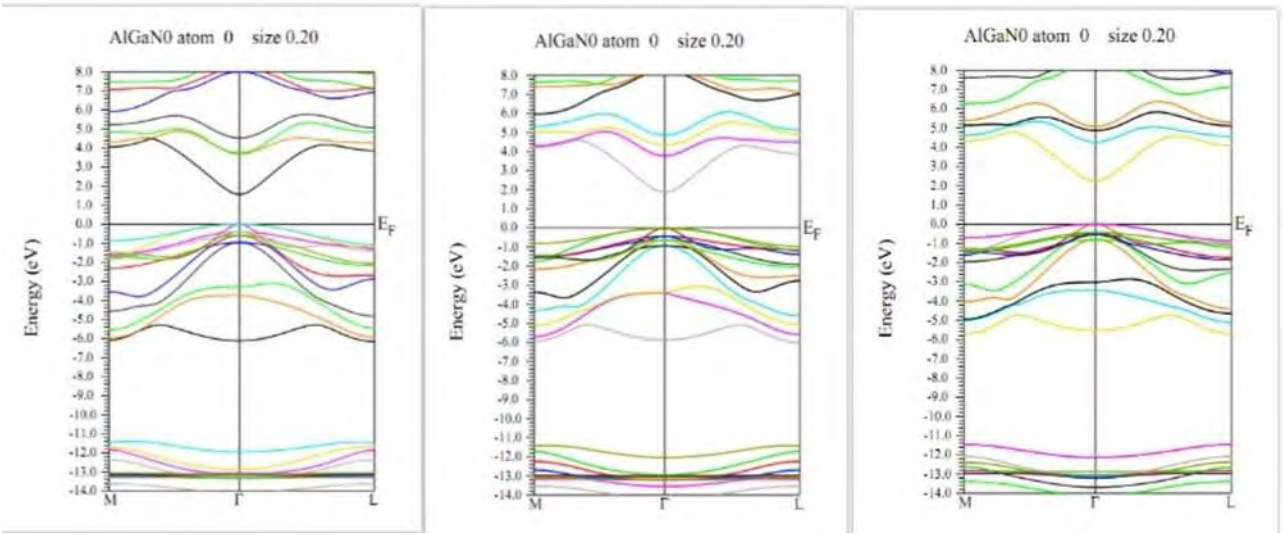

Figure 1: Band structures using GGA for 1) $Al_{0.25}Ga_{0.75}N$ 2) $Al_{0.50}Ga_{0.50}N$ 3) $Al_{0.75}Ga_{0.25}N$ without SOI.

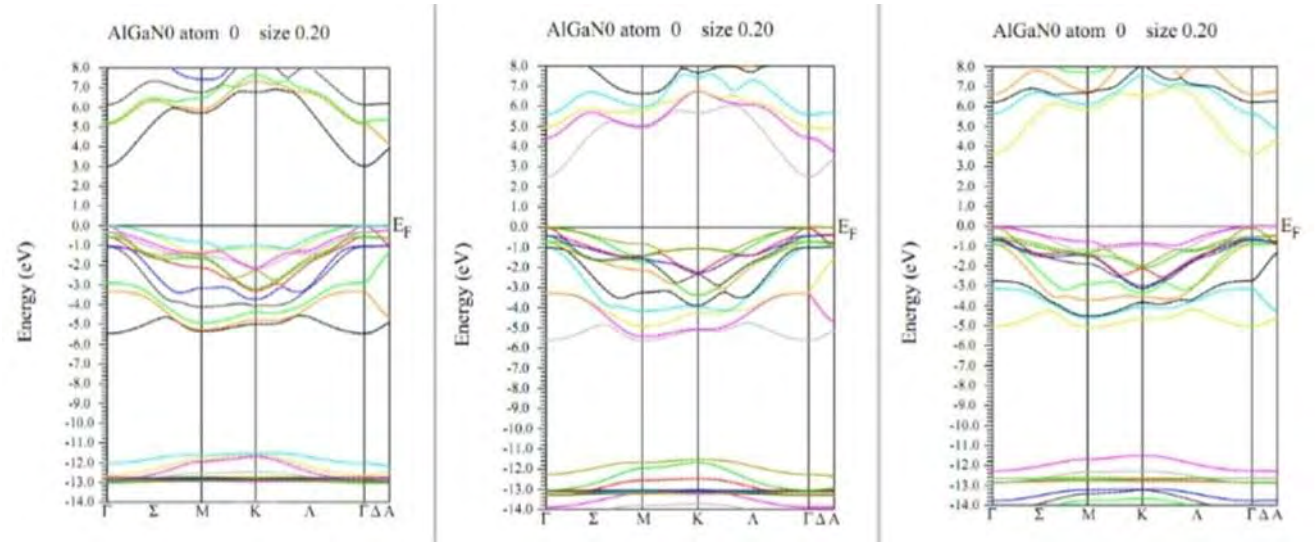

Figure 2: Band structures using mBJ for 1) $Al_{0.25}Ga_{0.75}N$ 2) $Al_{0.50}Ga_{0.50}N$ 3) $Al_{0.75}Ga_{0.25}N$ without SOI.

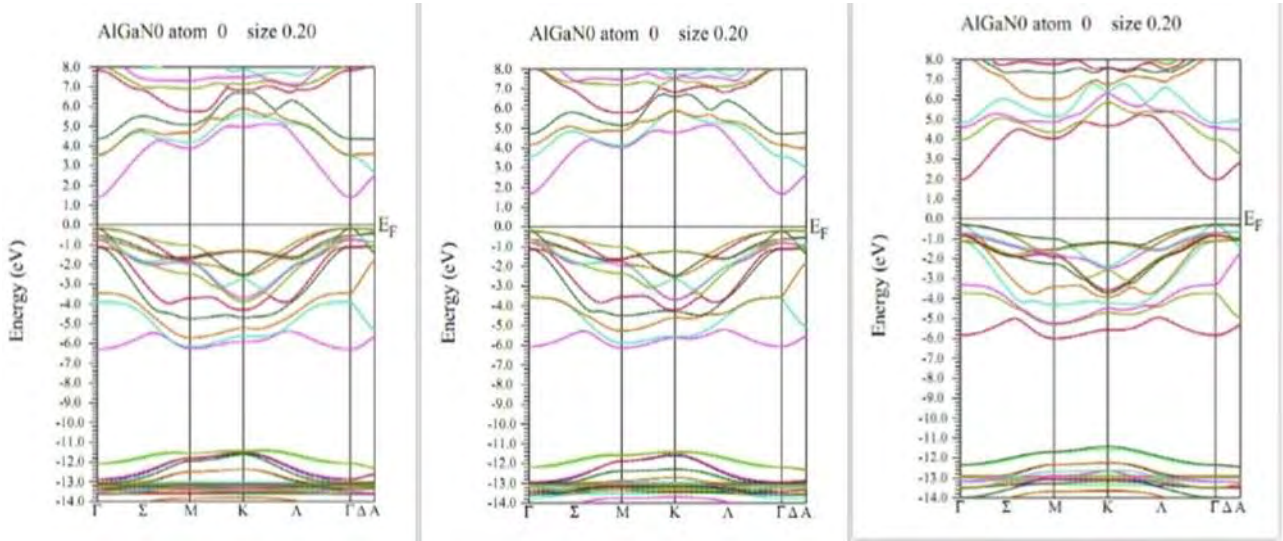

Figure 3: Band structures with the inclusion of SOI for 1) $Al_{0.25}Ga_{0.75}N$ 2) $Al_{0.50}Ga_{0.50}N$ 3) $Al_{0.75}Ga_{0.25}N$ using mBJ.

Table 1: The direct band gap energy (E_g) of $Al_xGa_{1-x}N$ for x=0.25,0.50 and 0.75. ([a]Lopez *et al*., 2010; [b]Liou *et al*., 2005)

Composition	Calculated value of E_g (in eV)		Other works E_g (in eV)
	PBE-GGA	GGA-mBJ	
$Al_{0.25}Ga_{0.75}N$	1.563	3.013	2.319[a] ,4.045[b]
$Al_{0.50}Ga_{0.50}N$	1.868	3.265	2.830[a] ,4.471[b]
$Al_{0.75}Ga_{0.25}N$	2.242	3.608	3.512[a],5.469[b]

Table 2. Band gap bowing parameter '*b*' of AlGaN ([a]Kanoun *et al*., 2005; [b]Dridi *et al*., 2003; [c]Vurgaftman and Meyer, 2003; [d]Liou *et al*., 2005; [e]Wei *et al*., 2004.)

AlGaN	Calculated value of *b* (in eV)		Other work (in eV)
	PBE-GGA	GGA-mBJ	
	0.552	0.728	0.514[a],0.71[b],0.7[c],0.752[d],0.755[e]

Table 3: The valence band splitting energy of $Al_xGa_{1-x}N$ for x=0.25, 0.50 &0.75. ([a]Mourad, 2013)

Composition	Calculated value (in eV)	Other work (in eV)
$Al_{0.25}Ga_{0.75}N$	0.184	0.13[a]
$Al_{0.50}Ga_{0.50}N$	0.162	
$Al_{0.75}Ga_{0.25}N$	0.127	

this calculation, we have found that SOI has no effect on the band energy between the valence band and conduction band and the overall shape in both cases. But due to the interaction, the valence band splits into two parts in both the cases. The lower splitting valence band is called split-off band and the energy calculated lies between (0.12-0.18) eV for x=0.25, x=0.50 and x=0.75

DISCUSSION

In this paper, we have calculated the electronic properties of $Al_xGa_{1-x}N$ ternary alloy using FP-LAPW method within linear density approximation (LDA) and DFT approaches. The exchange–correlation potentials utilised for the calculation are GGA and mBJ. The calculated band gap bowing parameter for $Al_xGa_{1-x}N$ agrees well with other theoretical and experimental works using different approaches (Kanoun *et al*., 2005; Dridi *et al*., 2003; Vurgaftman and Meyer, 2003; Liou *et al*., 2005; Wei *et al*., 2004). It is found that mBJ approach gives higher bowing as compared to GGA. In addition, we also found that there is a strong dependence of the bowing on the Al composition.

We can conclude that mBJ is an efficient theoretical technique for the calculation of band structures as the energy gap is remarkably improved by mBJ over GGA making it closer to the experimental result. It is noteworthy to mention that with the inclusion of SOI, there is a slight decrease in the band gap value on both the approximations. The inclusion of SOI has affected the band structures and splitting of the degenerate valence band occurred on high symmetry Γ-point.

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