First-principles calculations of the structural and electronic properties of AlN, GaN, InN, AlGaN and InGaN

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Abstract

First principles calculations are carried out for AlN, GaN, InN, AlGaN and InGaN in various crystal structures. The computational method used to investigate the structural and the electronic properties is the full potential linear muffin-tin orbital (FP-LMTO) augmented by a plane-wave basis (PLW). Exchange-correlation has been accounted for within LDA using the exchange-correlation potential calculated by Vosko et al. and Perdew et al. The latter parameterisation takes into consideration the generalized gradient approximation (GGA). The results of the calculated properties for the considered compounds in the zincblende and wurtzite phases are discussed and compared to the theoretical works as well as to the experimental data. We have also applied this computational method to AlGaN and InGaN alloys to check its transferability to predict the structural and electronic properties from those of their parent compounds.

Keywords: Electrical Properties, structural Properties, Alloys, (In, Al, Ga) N, LMTO methods.

1. Introduction

Ten years ago, most researchers considered the III nitrides to be laboratory curiosities, unlikely to be of great practical importance. However, after several breakthroughs in growth and doping technologies, the III nitrides have emerged as the leading semiconductor materials for short-wavelength (green, blue, and violet) visible-light-emitting diodes and laser diodes, as well as solar-blind photodetectors, and show promise for high-power, high-frequency, and high-temperature microelectronics. The III nitrides are probably now the third most economically important class of semiconductors, behind only Si and GaAs [1,2]. The InN semiconductor, which band gap is smaller compared to that of GaN and AlN, has been available only in small polycrystalline samples in the past decades. Actually, an important sample of this semiconductor are grown using new techniques. Under normal conditions, these group-III nitrides appear in tetrahedrally coordinated crystal

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structure (the wurtzite structure), but can also be grown in the zinc-blende structure under appropriate conditions [3-5]. There have been many theoretical studies on the structural, electronic and optical properties of these nitride-based compounds. It is found that the alloys based on these group-III nitrides are also technologically promising. However, the crystal growth and the device fabrication for the III-N semiconductors materials are not as simple as the conventional semiconductors materials. Therefore, much effort is still required to learn more about this new materials system. In alloy design it is important to understand the mechanism whereby materials derive their structural and electronic properties and how these can be varied during alloy production. These properties depend on chemical composition, concentration and crystal structure in a complex way which effects can be investigated using computational methods. So, we have interested to the In1-xGaxN and Al1-xGaxN alloys, in order to get a better insight into the mechanism by which the presence of Al or In atoms affect the properties of the gallium nitride. The replacing of Al by In atom gives information about the size effect where the chemical and physical properties are also important in alloying. Among the physical properties of the III-nitride based heterostructures there is the bowing parameter which is one of the most parameters for the characterization of the optical properties.

It is well known that *ab initio* methods for the many-electrons system have been developed since many years, starting from the pioneering works of Hartree and Fock. However, in the last 20-25 years the use of *ab initio* methods in the study of real systems has become more and more frequent, not only because of the availability of powerful computers, but also thanks to the introduction, between the sixties and the eighties, of novel theoretical approaches which have allowed us to simplify substantially the required numerical calculations. The main progress has been done with the Density Functional Theory (DFT), introduced by W. Kohn and Hohenberg in 1964. Through suitable theorems, DFT allows one to shift the attention from the many-body wavefunction (a "monster" quantity for a system of many interacting particles) to the much simpler *electronic density*, i.e. essentially to the squared modulus of the N body wavefunction integrated over (N-1) of its variables.

In its original formulation, DFT only applies to the system's ground state: it can be found as the minimum of a suitable functional, with respect to the variation of the sole density. Only in 1984 DFT has been generalized to Time-Dependent DFT (TDDFT), allowing one to study also the excited state. The electronic properties of nitride semiconductors can be calculated accurately using first principles techniques like density functional theory within the GW approximation, but at the time being, the computational effort of this method is still prohibitive for applications to nanosystems containing a large number of atoms, like wide quantum well structures, quantum wires, or small semiconductor crystallites. Local density approximation (LDA) calculations for III-V semiconductors, until very recently, often led to band-gaps that are typically smaller than the experimental values. The discrepancies between LDA and experimental results have been mostly ascribed to limitations of the local density approximation. The essential differences between the GW results and those of previous LDA calculations are mainly between the conduction (unoccupied) energy bands obtained by the two approaches. There is a reported, surprising agreement, however, between LDA and GW results for the wavefunctions of the valence (occupied) bands.

There are many theoretical studies reported elsewhere for GaN [6-8], for InN [6-9], for AlN [10-12], for InGaN [13-15] and for AlGaN [16-18]. In an attempt to give a more systematic understanding of the structural and the electronic properties of these Group-III nitrides and their related alloys, we have carried out our calculations within the local density approximation (LDA) to density functional theory, using the all-electron full

potential linear muffin-tin orbital (FP-LMTO) augmented by a plane-wave basis (PLW). The exchange-correlation energy of electrons is described in the local density approximation (LDA) using the parameterization of *Vosko et al* [20] and also of Perdew et al. [21]. We have also applied this computational method to AlGaN and InGaN systems greatly used in the heterostructures and the quantum wells to check its transferability to predict the structural and electronic properties from those of their parent compounds.

2. Method of calculation

Let us describe first the details of the (FP-LMTO) method. The full-potential linear muffin-tin (FP-LMTO) method is a specific implementation of density functional theory within the local density approximation (LDA). In this method there is no shape approximation to the crystal potential, unlike methods based on the atomic-spheres approximation (ASA) where the potential is assumed to be spherically symmetric around each atom. For mathematical convenience, the crystal is divided up into regions inside muffin-tin spheres, where Schrödinger's equation is solved numerically, and an interstitial region. In all LMTO methods the wavefunctions in the interstitial region are Hankel functions. Each basis function consists of a numerical solution inside a muffin-tin sphere matched with value and slope to a Hankel function tail at the sphere boundary. The so-called multiple –kappa basis is composed of two or three sets of s, p, d, etc. LMTOs per atom. The extra variational degrees of freedom provided by this larger basis allow for an accurate treatment of the potential in the interstitial region.

In the present work, we use the Savrasov version of the full potential linear muffin-tin orbital (FP-LMTO) method augmented with a plane wave basis (PLW) [19]. The non overlapping muffin tin spheres potential is expanded in spherical harmonics inside the spheres and Fourier transformed in the interstitial regions. The exchange-correlation energy of electrons is described in the local density approximation (LDA) using the parameterization of *Vosko et al* [20] and also of Perdew et al [21].

It is a well-known that the LDA has a tendency to overestimate the bonding. The improvement by the GGA is in fact mainly due to an improvement in the calculation of the atomic reference energies. Since the free atoms contain regions of very low density and strongly varying electronic density, gradient corrections to the exchange and correlation functional are more important for free atoms than for bulk. The lattice constant is usually underestimated with respect to the experimental lattice constant by up to a few percent by the LDA while the GGA sometimes overestimates it. In this work, the orbital $3d^{10}$, $4s^2$, $4p^1$ of Ga, $4d^{10}$, $5s^2$, $5p^1$ of In, $2s^2$, $2p^3$ of N , and $3s^2$, $3p^1$ of Al are all included into the self-consistent treatment, i.e viewed as valence electrons. The present calculation methods is implemented in the available computer code lmtART [19, 22].
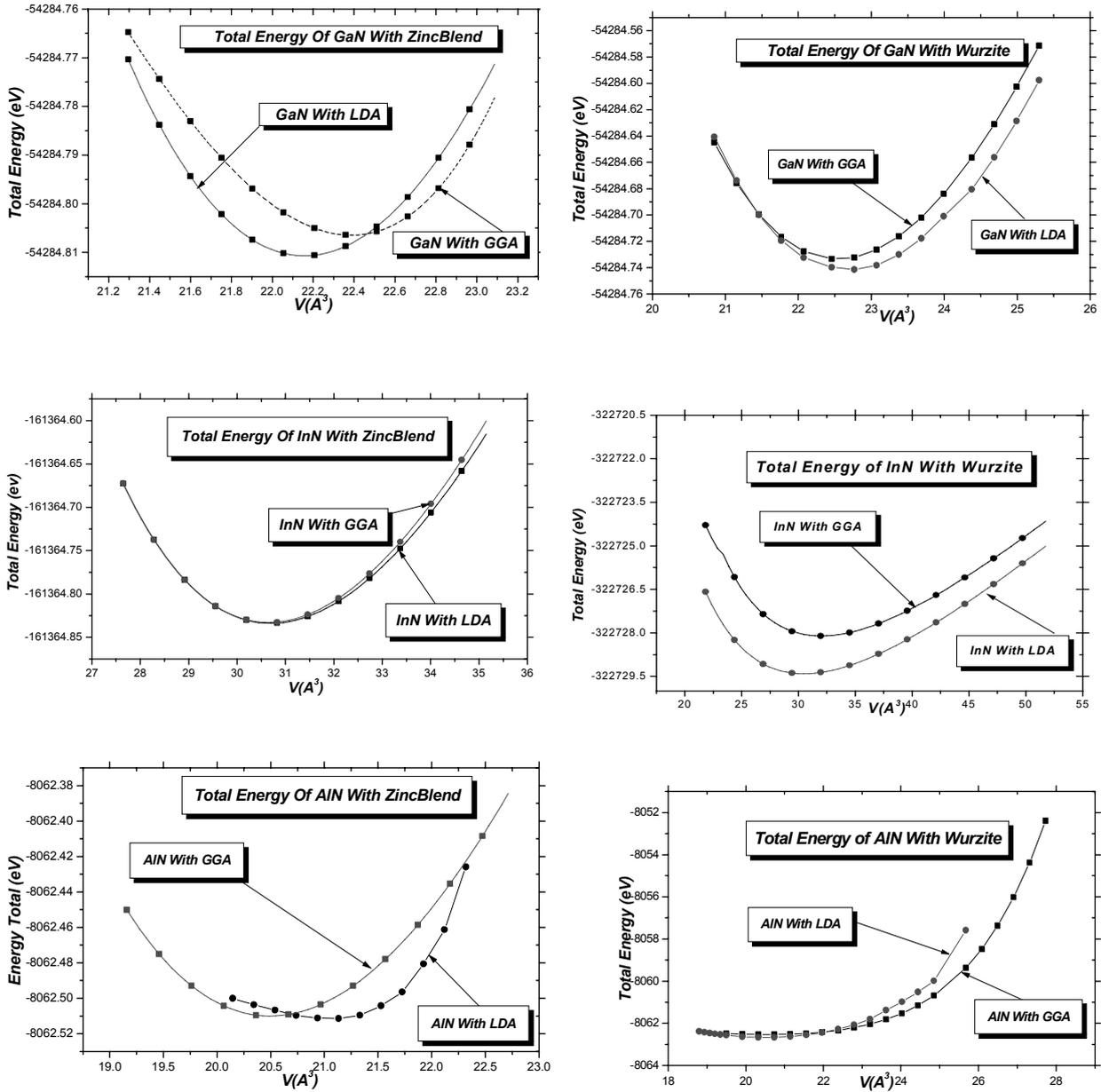
Fig. 1: Calculated total energy versus relative volume for GaN, AlN and InN.

Basis functions, charge density, and potential were expanded inside the muffin-tin spheres in spherical harmonic functions with cut-off l_{max}, and in Fourier series in the interstitial region. In the muffin-tin spheres (MTS) of radius RMT, the upper limit on the angular momentum expansion of the smoothed Hankel functions about a given atomic site is carried out up to lmax=6.

In order to achieve convergence of energy eigenvalues, the wave functions in the interstitial region were expanded in plane waves with a cut-off at K_{max}. We use for GaN, AlN and AlN the value 8 for the parameter RMK_{max} which determines the matrix size, where K_{max} is the PW cut-off and RM (R_{Ga}, R_N are muffin-tin radius equal to 8 for the Ga and N atoms, respectively with RGa = 1.59 and RN=1.87), for the ternary alloys (example: InGaN,

AlGaN) the value (R_N are muffin-tin radius equal to 8,75 au for the Ga and N atoms, respectively with RGa = 2.*08*, RIn = 2.*08* and RN = 1.71). In this code the unit cell is divided into no overlapping muffin-tin spheres (MTS) of radius R_M and an interstitial region, where the Kohn-Sham wave functions are expressed in spherical harmonics within spheres and in plane waves in the remaining space of the unit cell. The k-integration over Brillouin zone is performed up to a (6,6,6) grid by means of an improved tetrahedron method.

3. Results and Discussions

To analyze the structural properties, the equilibrium lattice parameters are calculated within the method seen previously using the habitual minimization procedure. The total energy was calculated for different values of the lattice constant, and the ground state corresponds to the lowest value of the total energy. Figure 1 shows the total energy as a function of volume for GaN, AlN and InN in both the zincblende and the wurtzite structures.

The curves were obtained by calculating the total energy E at many different volumes around equilibrium and by fitting the calculated values to the Murnaghan/Birch [23] equation of state. In order to make easier the comparison of our results, we have plotted the E-V diagram for the zincblende form in the left side and in the right side that of the wurtzite phase. It is clear from the E-V curves for the three compounds that the wurtzite form is slightly lower in energy than that of the zincblende form, in agreement with the experimental result showing that the wurtzite structure is the ground state for these group-III nitrides. Also we notice that the results with and without the (GGA) are different. We show for the GaN in the zincblende form that the E-V curve is shifted upwards and the equilibrium volume is then larger to that of the LDA only. For the wurtzite phase, the equilibrium volume is preserved in spite of the total energy is shifted. For the InN, we found that the effect of the GGA is very small for the zincblende phase compared to that of the wurtzite structure. For the bulk AlN, we notice for the zincblende structure that the equilibrium volume obtained with the GGA is lower to that of the LDA. The situation is quite different for the wurtzite form where the minimum of the total energy is shifted but the equilibrium volume is preserved. One can notice that the difference between the minima of the two phases is smaller compared to that of Ref. [24,25].

Our results are consistent with the fact that the total energy of the system is written as a functional of the density where the exchange and correlation energy, which is generally not known appears. For purposes of practical calculations, an approximation of this term has to be introduced. The traditional one is referred to as the local-density approximation (LDA).

It is based on the assumption that the relation between the exchange-correlation energy and the density is locally the same as for a free-electron gas of identical density, which is quite accurately known. But in regions of low electron density, the exchange correlation is underestimated. Corrections to the LDA have been developed to correct this deficit.

		Wutrzite				
		Current work		Calculations		Experimental
		LDA	GGA	LDA	GGA	
GaN	a (A°)	3.154	3.15	3.095-3.193a	3.245b	3.18-3.192c
	c(A°)	5.134	5.121	5.0-5.228a	5.296	5.166-5.185c
	c /a	1.628	1.626	1.622-1.639a	1.632	1.624-1.627c
	u	0.3764	0.376	0.375-0.378a	0.3762	0.375-0.377c
	B(GPa)	203.13	171.52	195-213a	172b	188-220e
	B'	4.85221	3.83722	4.2-4.5a	5.11b	3.2-4.3e
AlN	a (A°)	3.092	3.136	3.057- 4.114a	3.113- 3.135b	3.111c
	c(A°)	4.95	4.954	4.943 -5.046a	5.022-5.041b	4.978c
	c /a	1.601	1.58	1.604 -1.619a	1.602-1.6193b	1.601c
	u	0.3811	0.381	0.380-0.383a	0.7898-0.381b	0.385c
	B(GPa)	211.22	191.85	195-215a	192b	185-212d
	B'	4.38471	1.65928	3.63-3.82a	3.96b	5.7-6.3d
InN	a (A°)	3.52	3.612	3,544 a	3.614 b	3.544c
	c(A°)	5.677	5.873	5.762 a	5.88 b	5.718c
	c /a	1.613	1.626	1.626a	1.628 b	1.613c
	u	0.384	0.379	0.377a	0.377 b	-----
	B(GPa)	120	117.28	7.33a	116.1b	126.139c
	B'	4 .96	4.8689	6.03a	7.33b	-----

a: Ref. [24,26-28], b: Ref. [29,30], c: Ref. [31-33], d: Ref. [31,34], e: Ref. [31,35, 36].

		Zincblende				
		LDA	GGA	LDA	GGA	
GaN	A (A°)	4.4738	4.47940	4.446-4.537a	4.55-4.59b	4.5c
	B(GPa)	203	171	191-202a	156b	185d
	B'	4.09801	3.60796	3.9-4.14a	4.25b	--
AlN	A (A°)	4.382	4.353	4.31-4.376a	4.39-4.42b	4.37c
	B(GPa)	212.4	196	213-216a	191b	--202
	B'	3.09163	3.35188	3.2-3.86a	3.86a 3.81b	--
InN	A (A°)	4.97	4.77	5.004a	5.109b	4.98c
	B(GPa)	139	115	140a	116.96b	--137
	B'	4.71043	4.49895	4.38a	4.4305b	--

a: Ref. [37,38], b: Ref. [29,30, 39], c: From wurtzite structure Ref. [30,32], d: Ref. [40].

Table 1: The structural parameters of GaN, AlN and InN in the two phases (V_0 is the equilibrium volume, a_0 the lattice constant, B_0 the bulk modulus and B'_0 is its pressure derivative). V_0 is taken equal to $a^3/4$ for both zinc blende and $1/2.[a^2.c.(3/4)^{1/2}]$ for the wurtzite phase for which the volume per unit formula is taken into account. Both FPLMTO results are presented.

In particular, we use the gradient corrected LDA or generalized gradient approximation (GGA), which relates the exchange-correlation energy also to the gradient of the electron density. For these reasons the (GGA) typically improves the underestimation of lattice parameters in crystals. It is also well known that the reduction of the exchange-correlation energy to a simple local potential generally induces an underestimation of the energy gap. This behavior can be easily deduced from the band structure results.

To confirm all these interpretations we can also analyzed the results of structural parameters. The static properties of the phase under study (equilibrium lattice constant, bulk modulus, and its pressure derivative) for the studied compounds are determined using the Murnaghan/Birch [23] equation of state to fit our calculated E-V data. The results compared to experiment and other works are given in Table 1.

We can see from table 1 that our calculated structural parameters for both structures are in good agreement compared to others theoretical works and the experiment. The correction obtained with the GGA gives results different from that of the LDA. Although as a general trend, GGA overestimate the lattice parameter, LDA underestimate it. We notice from our results that GGA is seen to decrease the bulk modulus compared to the LDA. These behaviors agree well with the above physical considerations seen within this calculation method. We also note that our value of the internal parameter u = 0.3764 for the B2 phase agrees well with that of Ref. [24, 25] (u = 0.38) but not with that of Ref. [27,28].

Let us discuss now the results of the band structure calculation. In Fig. 2, the band structure of these materials in the Zincblende (B1) phase for the equilibrium volume is shown. We notice that the bands below the Fermi level correspond to valence bands and above correspond to the conduction bands.

The band structure of InN shows a direct band gap at Γ, closely similar to that of GaN. This is very different from what we have found for AlN, where we notice a small indirect Γ–X fundamental band gap. Our calculated band gaps obtain with the LDA for the zincblende form are Eg=3.33eV, Eg=0.6eV and Eg=5.76 eV for GaN, InN and AlN, respectively. These values are in good agreement compared to the experimental bands gaps found by M. Marques et al. [41] (3.3 eV for GaN, 0. 9 eV for InN and 5.94 eV for AlN) and those of Munoz et al. [42]. However, these band gaps are underestimated by other theoretical works as PWPP method [43] and the FP-LAPW method [44]. It is well known that in the wurtzite case of GaN and AlN , the lowest conduction band and the top of the valence bands are situated at the Γ point in the BZ. Without spin-orbit interaction they are related to an s-like Γ_{1c} state and to p-like Γ_{6v} and $\Gamma 1v$ states. The two latter states are separated by a crystal-field splitting $\Delta cr = \varepsilon_{\Gamma 6v} - \varepsilon_{\Gamma 1v}$. Two energy gaps can be defined by $E_{A/B} = \varepsilon_{\Gamma 1C} - \varepsilon_{\Gamma 6v}$ and $E_C = \varepsilon_{\Gamma 1C} - \varepsilon_{\Gamma 1v}$ according to the optical transition $\Gamma_{6v} - \Gamma_{1c}$ and $\Gamma 1_v - \Gamma_{1c}$ .In GaN, $E_{A/B}$ is the fundamental gap, whereas in AlN it is the C transition gap due to the negative crystal field splitting [45,46]. In Fig. 3, we illustrate the calculated density of states for studied compounds. We may divide the density of states into three general regions. The first region is the most tightly bounded energy band. Electron states corresponding to this band are strongly localized on the anion and are descendants of the atomic N $2s$ states. The next region of note is a peak arising from the onset of the second valence band. The band shows almost no energy variation along the X-U symmetry direction; in fact, it is very flat over the entire square face of the Brillouin zone. This energy band configuration results in a sharp onset of states above the antisymmetric gap. The character of state associated with the second valence band changes from predominantly cation s-like states at the band edge to predominantly anion p-like states at the band maximum. The third region of interest in the density of states extends from the onset of the third to valence band maximum.
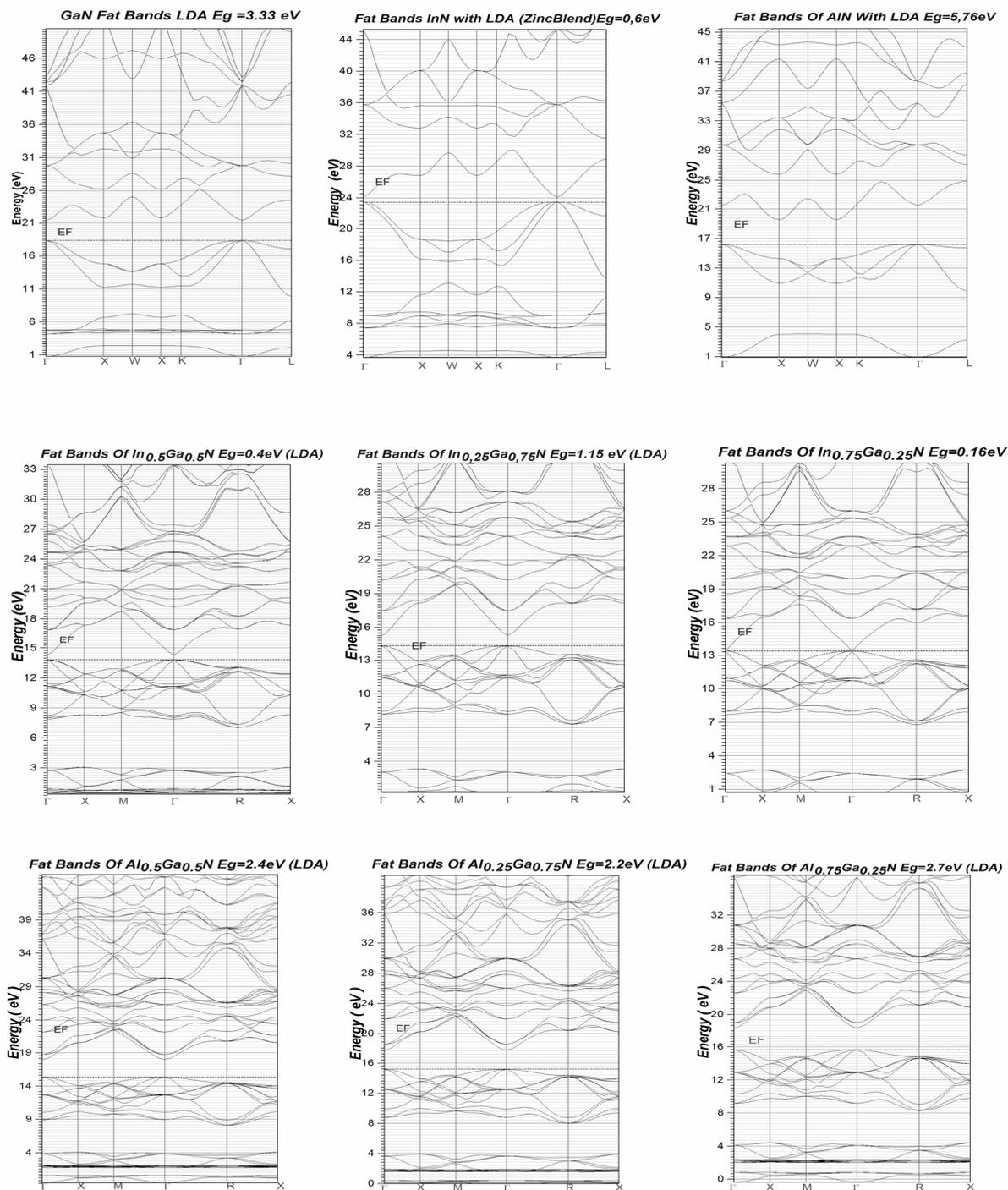
Fig. 2: The band structure of GaN, InN, AlN, InGaN and AlGaN in the equilibrium phase for the equilibrium volume.
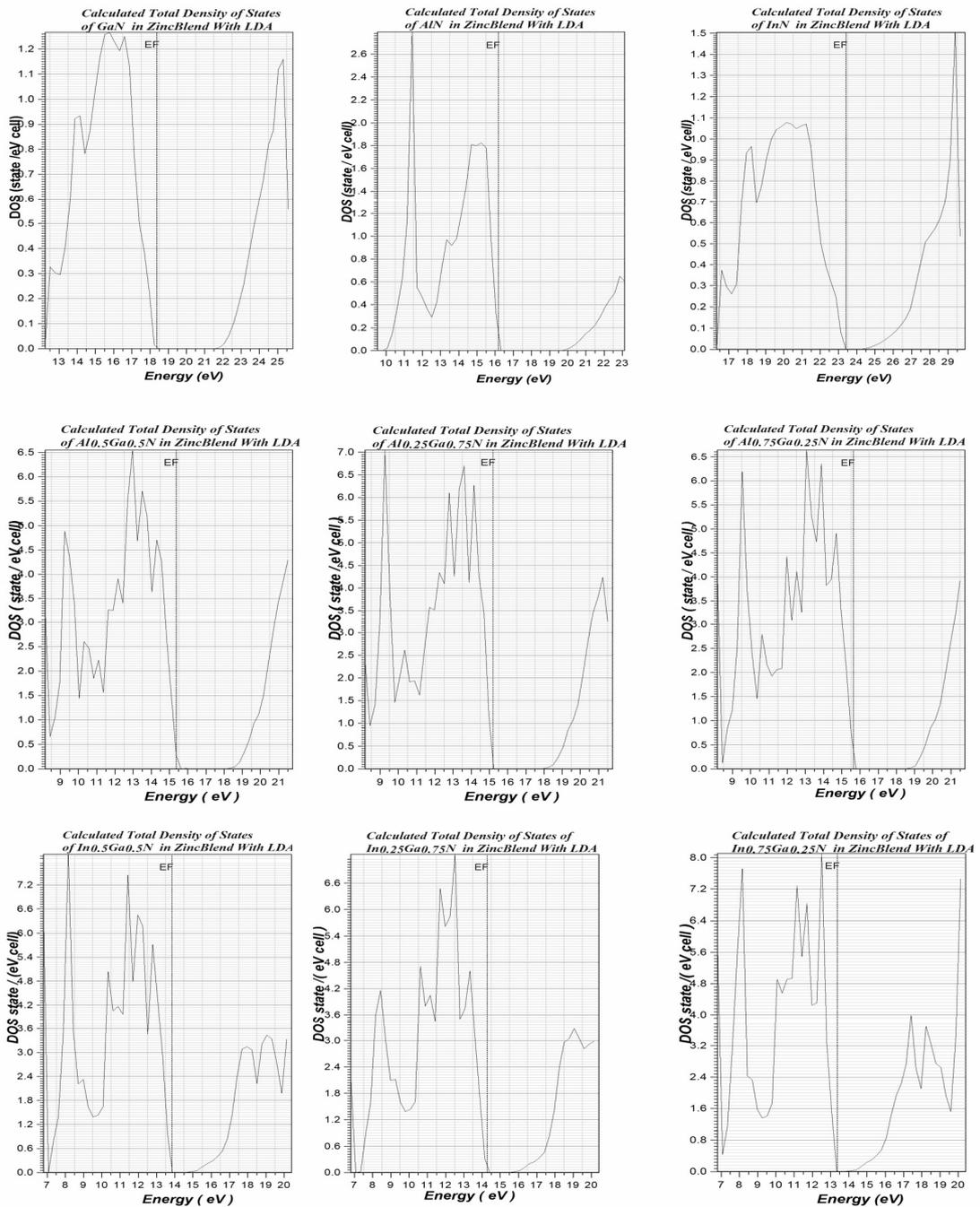
Fig. 3: The DOS of GaN, InN, AlN, InGaN and AlGaN in the equilibrium phase for the equilibrium volume.

This region encompasses the top two valence bands and is predominantly *p*-like and is associated with nitrogen state. The nonuniformity of the density of states arises from hybridization among the atomic orbital and the difference seen in the shape of the peaks for he three compounds arise from the effect of the Ga, In and AlN cations, respectively.

It is a well known that the cation-substituted alloys are attractive candidates for optoelectronic, high-temperature, and high-power device applications because of the flexibility they offer to tune both the lattice constant and band gap. While alloys can be formed by mixing constituents on the cation and/or sublattice, most attention has been

focused on alloys where the substitution is on the cation sublattice—for example, GaInN and AlGaN which form the basis for blue and green LEDs and laser diodes [6]. Calculating the properties of random alloys is, in general, a far more difficult task than calculating the properties of the compounds, and several calculation approaches are generally applied to the problem. In the virtual crystal approximation (VCA), the alloy is modeled by replacing the varying potential due to the alloy disorder by an average potential, approximated by a compositional-weighted average of the potentials of the constituents. Such a crude approximation can be expected to produce poor results in predicting the properties of the nitride alloys, particularly those of the anion-substituted alloys for which there are large chemical and bond length differences. Strong scattering theories such as the coherent potential approximation (CPA) build upon the VCA by including a complex self-energy to describe the alloy inhomogeneities (see Ref. [47] and references therein). The CPA theory can include both on-site disorder arising from differences in diagonal terms in the potential, and offsite and off-diagonal disorder arising from differences in bond lengths. Finally, averaging over samplings of random configurations can also be used to predict the composition dependent properties of alloys [48]. To check the transferability of the present calculation method and to develop a better understanding of how chemical composition and compositional inhomogeneity affect the electronic properties, we have carried out the results of the $In_{1-x}Ga_xN$ and $Al_{1-x}Ga_xN$ alloys DOS and band structure (Fig.2 and Fig.3). As was shown from the profiles of the DOS, the effect of the cation sublattice is clear because the peaks are different from those of the binary compounds. To analyse the quantitative change causes by the alloying effects we have plotted in Fig. 2 the electronic band structures of the two alloys. The band gaps calculated for different concentrations are also shown in the same figure. The calculated band gaps for $Al_{0.75}Ga_{0.25}N$, $Al_{0.5}Ga_{0.5}N$ and $Al_{0.25}Ga_{0.75}N$ are in close agreement with the LDA results of Ref. [49] obtained for ordered $Al_{0.75}Ga_{0.25}N$, and $Al_{0.25}Ga_{0.75}N$ alloys. When comparing these band structures, we observe that the trends in the second band gaps are the same as in Ref. [30]. The ordering changes significantly the crystal-field splitting, which is found positive for all ordered structures, while it was shown to be negative in random Al-rich Al-GaN alloys [50,51]. The $In_{1-x}Ga_xN$ alloys exhibit direct-gap characteristics as a consequence of being formed by the direct-gap binary compounds GaN and InN. In contrast, a direct to indirect gap transition is obtained for $Al_{1-x}Ga_xN$ at x near 0.40. From these results we confirm that the presence of Al or In atoms affect the properties of the gallium nitride due to the fact that Al exhibits a small atom compared to the In atom.

4. Conclusion

Full potential linear muffin-tin orbital method (FP-LMTO) within the density functional theory has been applied to study the structural and electronic properties of GaN, InN, AlN and their related ternary alloys in various phases. The local density approximation has been used with and without generalized gradient correction based on exchange-correlation energy optimization. The calculated energy allowed us to investigate several structural properties such as lattice parameter, bulk modulus and its pressure derivative. Our calculated lattice parameter is found to be in reasonable agreement with other theoretical works as well as the experimental result. From the E-V curves we found that for the studied compounds the wurtzite form is slightly lower in energy than that of the zincblende form. Hence, for the low pressure, these compounds show the new equilibrium phase which is the zincblende structure. At high pressure we can predict that the new phase is probably the rock salt structure. We have also applied this computational method to

AlGaN and InGaN alloys to check its transferability to predict the structural and electronic properties from those of their parent compounds. As a function of composition the alloys of GaN and InN should cover the entire spectral region from the very near UV to the red while AlGaN covers a wide range in the near UV. On the other hand, the band discontinuities in valence and conduction bands are the key parameters governing the behavior of heterojunctions; these junctions are essential for the device properties of optoelectronic devices. The large lattice mismatch between the nitride semiconductors (AlN, GaN, InN) complicates determination of these offsets, which are strongly affected by strain.

Acknowledgements

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