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Pressure dependence of energy band gaps for $AI_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAI_{1-x}N$

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Abstract. Using a first-principles method, we study the effect of pressure on the band gap energy of wurtzite $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$, and $In_xAl_{1-x}N$. Starting with the binaries, GaN, InN and AlN, the direct band gap is found to increase linearly with pressure but becomes indirect for AlN at 13.88 GPa. The direct band gap pressure coefficients are 31.8 meV GPa⁻¹ for GaN, 18.8 meV GPa⁻¹ for InN and 40.5 meV GPa^{-1} for AlN, which are in good agreement with other calculations. For the ternary alloys, the fundamental band gaps energy are direct and increase rapidly with pressure. The pressure coefficients vary in the range of 31.9–34.5 meV GPa⁻¹ for Al_xGa_{1-x}N, 19.8–24.8 meV GPa⁻¹ for In_xGa_{1-x}N and 16.7–20.7 meV GPa⁻¹ for $In_x Al_{1-x}N$; they depend on alloy composition with a strong deviation from linearity. The band gap bowing of InGaN increases linearly with pressure, but those of AlGaN and InAlN strongly decrease when the AlN band gap becomes indirect.

1. Introduction

The group III nitrides GaN, InN and AlN are characterized by a large gap of 3.5 eV [1] for GaN, 1.89 eV [2] (0.9 eV by recent photoluminescence (PL) measurement [3,4]) for InN, and 6.28 eV [5] for AlN. They have also a large thermal conductivity [6] and breakdown fields [7]. Due to these properties, they are suited for optoelectronic devices such as LEDs, laser diodes, UV detectors, high-temperature and high-power devices. All these applications have stimulated the study of their ternary alloys $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$.

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Notwithstanding the important research activity over the last decade on these compounds, a number of their properties are not yet well understood or agreed on, such as the energy band gap of InN [3], or the band gap bowing parameter of the ternary alloys [8, 9]. Moreover, the band gap pressure coefficients are not well known. Experimental data for GaN are scattered over a relatively large range from 37 to 47 meV GPa⁻¹ [10]–[17]. For AlN and InN, to our knowledge, only one value, 49 [18] and 6 meV GPa⁻¹ [4] respectively, has recently been reported using absorption and PL measurements.

Of course, a large number of theoretical investigations has been carried out: the early work of Van Camp *et al* [19, 20], using first-principles pseudopotential calculations, reported high-pressure properties of wurtzite and rocksalt AlN and GaN. Christensen *et al* [21], using LMTO–ASA calculations, studied the effect of pressure on the structural and optical properties of AlN, GaN and InN. Kim *et al* [22] reported full-potential LMTO calculations of the elastic constants and pressure coefficients of BN, AlN, GaN and InN. Bellaiche *et al* [23] studied the pressure variation of the band gap of InN, using first-principles pseudopotential calculations. Recently, Wei and Zunger [24], using a linearized augmented plane wave (LAPW) method, studied the band gap pressure coefficients of the nitride wurtzite compounds and showed them to be almost the same as those of zincblende structures. The above studies reported pressure coefficients which range for AlN from 36 to 44 meV GPa⁻¹, for GaN from 33 to 39 meV GPa⁻¹, and for InN from 19 to 28 meV GPa⁻¹ (a higher value of 33 meV GPa⁻¹ for InN was reported by Christensen *et al* [21]).

For the ternary alloys, the available experimental studies reported pressure coefficients for a limited composition range: $0.05 \le x \le 0.6$ for Al_xGa_{1-x}N [15, 25], and $0.04 \le x \le 0.14$ for In_xGa_{1-x}N [26]–[28]. These values are almost independent of the composition. Theoretically, to our knowledge only the recent work of Perlin *et al* [29] has reported the pressure coefficients of In_xGa_{1-x}N, by means of the full-potential LMTO method. An important dependence of the pressure coefficient on the alloy composition was shown. For In_xAl_{1-x}N, no results are available.

The AlGaN and InGaN alloys are and will be more and more necessary in LEDs, LDs, as well as in transistor-based strained heterostructures. Therefore it is important to know the pressure dependence of their band gap with a given mole fraction in order to calculate the band alignment for designing and optimizing such devices. The third ternary nitride alloy, InAlN, is less investigated. However, it exhibits the largest variation in the band gap and is a candidate for lattice-matched confinement layers in optical devices.

In the following, we use the full-potential LAPW (FPLAPW) method to study the behaviour of the band gap under pressure for wurtzite $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$. We first studied the binaries, GaN, InN, AlN, and in agreement with the calculations of others, the fundamental band gap increases rapidly and remains direct under pressure for GaN and InN; for AlN it becomes indirect at p = 13.88 GPa. For $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, we investigate the fundamental band gap and band gap bowing dependence on pressure.

2. Method of calculation

The calculations are performed using the nonscalar relativistic FPLAPW approach (WIEN97 implementation [30]) within the framework of the density-functional theory (DFT). The exchange–correlation energy of the electrons is described in the local-density approximation (LDA). The LDA functional from Perdew and Wang [31] is used. We have

included the Ga 3d and In 4d as valence states. No shape approximations are employed for either the potential or the charge density. Basis functions were expanded in combinations of spherical harmonic functions inside non-overlapping spheres surrounding the atomic sites (muffin-tin (MT) spheres) and in Fourier series in the interstitial region. In the MT spheres, the *l*-expansion of the non-spherical potential and charge density was carried out up to $l_{max} = 10$. In order to achieve energy eigenvalue convergence, the wavefunctions in the interstitial region were expanded in plane waves with a cutoff of $k_{max} = 8/R_{mt}$ (where R_{mt} is the average radius of the MT spheres). In the following calculations, we have distinguished the Al (1s²2s²2p⁶), Ga (1s²2s²2p⁶3s²3p⁶), In (1s²2s²2p⁶3s²3p⁶3d¹⁰4s²4p⁶) and N (1s²) inner-shell electrons from the valence electrons of Al (3s²3p¹), Ga (3d¹⁰4s²4p¹), In (4d¹⁰5s²5p¹) and N (2s²2p³) shells. For GaN and AlN we have adopted the values of 1.9, 1.8 and 1.6 Bohr for gallium, aluminium and nitrogen, respectively, as the MT radii. In the case of InN, 2.05 and 1.75 Bohr for indium and nitrogen, respectively, are used. For the ternary alloys, we have chosen the MT radii values of 1.75 Bohr for gallium, aluminium and indium, and 1.65 Bohr for nitrogen.

To model the Al_xGa_{1-x}N, In_xGa_{1-x}N and In_xAl_{1-x}N random wurtzite alloys we have used a small 32-atom $X_nY_{16-n}N_{16}$ supercell (X = Al or In and Y = Ga or Al), which corresponds to a 2 × 2 × 2 supercell which is twice the size of the primitive wurtzite unit cell in both directions of the basal plane and along the *c*-axis. For a given number n = 0, ..., 16of X atoms, different atomic configurations have been optimized structurally. However, it is impossible to treat all different atomic configurations. Therefore, for a given number n of X atoms we usually study only a small number of different configurations in which the X atoms are not really randomly distributed. For each configuration and each atomic number n, the fundamental physical properties (total energy, and band gap) are determined. The configurationally averaged quantity is computed using the Conolly–Williams approach [32] for each given x. The composition-dependent weights are determined for an ideal solid solution. We have used only the $X_{4m}Y_{4(4-m)}N_{16}$ clusters (m = 0, ..., 4) to calculate the quantities for the entire composition region. In spite of the small size of our supercell, the calculations are sufficiently converged, and the obtained results for the band gaps are in good agreement with those of Schilfgaarde *et al* [33].

The k integration over the Brillouin zone is performed using the Monkhorst and Pack mesh [34]. A mesh of eight special k-points was taken in the irreducible wedge of the Brillouin zone for the binary cases; seven special k-points were used for the supercell calculations.

The structural optimization of the wurtzite phase was performed by calculating the total energy as function of the three variables u, c/a and V. The two-dimensional minimization of the total energy versus (u, c/a) for a fixed volume requires that each of the self-consistent calculations is converged, so the iteration process was repeated until the calculated total energy of the crystal converged to less than 1 mRyd. A total of seven iterations was necessary to achieve self-consistency.

For the geometric equilibrium determination of the wurtzite phase we proceeded as follows: we first determined the internal parameter u for a specific volume V and c/a, then by using it we optimized the c/a ratio to obtain $(c/a)_{eq}$ at $(V, (c/a)_{eq}, u_{eq})$. Then, using the two parameters u_{eq} and $(c/a)_{eq}$, we optimized the volume. The equilibrium lattice constants and bulk modulus are calculated by fitting the total energy versus volume according to Murnaghan's equation of state [35].

		a (Å)	c (Å)	c/a	u	B (GPa)	E_g (eV)	
GaN	Expt	3.190 [48]	5.189 [48]	1.627	0.377 [48]	188 [39], 195 [49], 237 [38], 245 [40]	3.5 [1]	
	PP This work	3.162 [50] 3.166	5.142 [50] 5.154	1.626 [50] 1.628	0.377 [50] 0.377	202 [50] 207	2.04 [50] 2.22	
AlN	Expt PP This work	3.110 [48] 3.084 [50] 3.092	4.980 [48] 4.948 [50] 4.954	1.601 1.604 [50] 1.602	0.3821 [48] 0.3814 [50] 0.3823	202 [51] 205 [50] 214	6.28 [5] 4.41 [50] 4.4	
InN	Expt	3.544 [52]	5.718 [52]	1.613	_	126 [38], 139 [49]	1.89 [2], 0.9 [3], 0.8 [4]	
	PP This work	3.501 [5 0] 3.520	5.669 [<mark>50</mark>] 5.675	1.619 [<mark>50</mark>] 1.612	0.3784 [50] 0.3799	139 [<mark>50</mark>] - 152	-0.04 0.17	

Table 1. The lattice constants a and c, internal parameters u, bulk moduli B, and energy band gaps E_g of GaN, AlN and InN compounds in the wurtzite structure. References are given where appropriate.

3. Results

The calculated structural properties (lattice constants a and c, internal parameters u, bulk moduli B) and energy gaps E_g of the binaries are summarized in table 1. We have an underestimation of the lattice parameters and the energy gaps, and an overestimation of the bulk moduli in comparison to those of experiment (table 1), due to the use of the LDA. The pressure coefficient of an interband transition i in a semiconductor is easily calculated. It is given by

$$a_g^i = \frac{\mathrm{d}E_g^i}{\mathrm{d}p}.\tag{1}$$

In the cubic structure, this quantity is related to the volume deformation potential $dE/d \ln V$ and the bulk modulus B by

$$a_g^i = -\left(\frac{1}{B}\right) \frac{\mathrm{d}E_g^i}{\mathrm{d}\ln V}.\tag{2}$$

Since the wurtzite structure has two structural degrees of freedom $(u, \eta = c/a)$, the effect of changes in the structural parameters u and η with volume on the band gap yields a generalization of equation (2) to

$$a_{g}^{i} = \frac{\mathrm{d}E_{g}^{i}}{\mathrm{d}p} = -\left(\frac{1}{B}\right)\frac{\mathrm{d}E_{g}^{i}}{\mathrm{d}\ln V} = -\left(\frac{1}{B}\right)\left[\frac{\partial E_{g}^{i}}{\partial\ln V} + \frac{\partial E_{g}^{i}}{\partial\eta}\frac{\partial\eta}{\partial\ln V} + \frac{\partial E_{g}^{i}}{\partial u}\frac{\partial u}{\partial\ln V}\right]$$
(3)

$$=\frac{\partial E_g^i}{\partial p} + \frac{\partial E_g^i}{\partial \eta}\frac{\partial \eta}{\partial p} + \frac{\partial E_g^i}{\partial u}\frac{\partial u}{\partial p}.$$
(4)

The variation of the energy gap versus volume was calculated using the equilibrium u and η parameters (at p = 0). In fact, for GaN Wagner and Bechstedt [36] and Serrano *et al* [37]

New Journal of Physics 4 (2002) 94.1-94.15 (http://www.njp.org/)



Figure 1. Variation of various band gaps, $\Gamma_c - \Gamma_v$, $M_c - \Gamma_v$, $K_c - \Gamma_v$, $A_c - \Gamma_v$, versus pressure for GaN.

using pseudopotential calculations have shown that the pressure dependence of both c/a ratio and internal parameter u are negligible. Wagner and Bechstedt [36] reported $\frac{\partial \eta}{\partial p}$ and $\frac{\partial u}{\partial p}$ as -4.7×10^{-5} and 5×10^{-6} GPa⁻¹, respectively. This result was confirmed by experiment for the c/a ratio [38]. For AlN, Wagner and Bechstedt [36] reported a slope of $\frac{\partial \eta}{\partial p} = -5.6 \times 10^{-4}$ GPa⁻¹ and $\frac{\partial u}{\partial p} = 1.08 \times 10^{-4}$ GPa⁻¹. This is an order of magnitude larger than that of GaN. For InN, the LAPW investigation of Wei and Zunger [24] reported linear pressure coefficients of $\frac{\partial \eta}{\partial p} = -6.7 \times 10^{-6}$ GPa⁻¹ and $\frac{\partial u}{\partial p} = 2.02 \times 10^{-4}$ GPa⁻¹ (estimated from their results: $\frac{\partial \eta}{\partial \ln V} = -0.001$ and $\frac{\partial u}{\partial \ln V} = 0.03$, B = 148 GPa). Therefore, although the variation of the band gap energy with c/a ratio and internal parameter u is important, the $\frac{\partial \eta}{\partial p}$ and $\frac{\partial u}{\partial p}$ slopes make the second and third terms of equation (3) much smaller than the first.

By the use of our calculated values of the bulk moduli, B, and their first pressure derivatives B', the volume change with applied pressure was calculated using the following equation [35]:

$$V(p) = V(0)[1 + (B'/B)p]^{1/B'}.$$
(5)

The behaviour of the lowest conduction band energies with pressure at a number of highsymmetry points of the Brillouin zone for GaN, InN and AlN is reported in figures 1–3. All the quantities are calculated near equilibrium. For GaN (figure 1) and at pressures up to 28 GPa, the fundamental band gap remains direct. However, at p = 16.1 GPa, there is a band gap crossing of the K_c and A_c conduction bands. For InN (figure 2), the fundamental band gap stays direct for a pressure applied up to 21.5 GPa. In contrast, for AlN (figure 3), at pressures up to 21 GPa, the fundamental band gap becomes indirect (K_c – Γ_v) at p = 13.88 GPa. This is due to the rapid increase of the Γ_c conduction band under pressure, while the K_c conduction band remains nearly constant.

At high pressure, GaN, InN and AlN present a phase transition from wurtzite to rocksalt structure. The experimental data for the transition of GaN range from 37 to 53.6 GPa [38]–[41]. The theoretical investigations reported values from 42.9 to 55 GPa [20, 21, 37, 42]. For InN, the transition pressure is from 10 to 14.4 GPa experimentally [38, 41, 43], and from 11.1 to 21.6 GPa

I



Figure 2. Variation of various band gaps, $\Gamma_c - \Gamma_v$, $M_c - \Gamma_v$, $K_c - \Gamma_v$, $A_c - \Gamma_v$, versus pressure for InN.



Figure 3. Variation of various band gaps, $\Gamma_c - \Gamma_v$, $M_c - \Gamma_v$, $K_c - \Gamma_v$, $A_c - \Gamma_v$, versus pressure for AlN.

theoretically [21, 37]. The experimental values for AlN are from 14.0 to 22.9 GPa [41, 44, 45], whereas the theoretical reports range from 9.2 to 12.9 GPa [19, 37, 46].

So for AlN, a modification of the fundamental band gap from Γ_c to K_c is expected at a pressure of about 13.88 GPa, indicating that AlN probably becomes an indirect band gap material before reaching the phase transition, at least with reference to known experimental data.

In order to calculate the pressure coefficients, we have fitted $E_q(p)$ to a quadratic function:

$$E(p) = E(0) + \alpha \cdot p + \beta \cdot p^2 \tag{6}$$

where E is in eV, p the pressure in GPa, and α and β the first- and second-order pressure derivatives respectively, which are given in table 2 for GaN, InN and AlN. For the first derivatives α of the $\Gamma_c - \Gamma_v$ band gap, our calculations give 31.8 meV GPa⁻¹ for GaN, 18.8 meV GPa⁻¹ for InN, and 40.5 meV GPa⁻¹ for AlN. These results are in good agreement with the FP-LMTO

New Journal of Physics 4 (2002) 94.1-94.15 (http://www.njp.org/)

calculations of Kim *et al* [22] which gave 33, 19, and 44 meV GPa^{-1} for GaN, InN and AlN, respectively. The recent FP-LMTO calculations of Perlin *et al* [29] gave 37 and 23 meV GPa^{-1} for GaN and InN, slightly larger than ours. First-principles pseudopotential calculations gave 37.5 meV GPa^{-1} [20], 28 meV GPa^{-1} [23] and 36.3 meV GPa^{-1} [19] for GaN, InN and AlN, respectively. The earlier LMTO calculations of Christensen and Gorczyca [21] gave pressure coefficients of 39 and 40 meV GPa^{-1} for GaN and AlN, respectively, and 33 meV GPa^{-1} for InN. However, Wei and Zunger [24], using LAPW calculations, have recently repeated the calculation of Christensen and Gorczyca [21] for InN, and reported 21 meV GPa^{-1} . They obtained 33 and 43 meV GPa^{-1} for GaN and AlN, in good agreement with our calculations. The small differences seen in tables 1 and 2 when compared with other results, can be for different reasons, as discussed by other authors:

- (i) the treatment of the Ga 3d in GaN and In 4d in InN as core or as valence electrons;
- (ii) the accuracy of the method used, e.g. pseudopotential and full potential;
- (iii) the choice of the functional for the exchange-correlation energy of the electrons;
- (iv) the computational parameters such as the energy cutoff (which determines the number of plane waves used in the pseudopotential approaches and in LAPW approaches which are used in the interstitial region).

For the other band gaps, when we increase the cation atomic number, e.g. going from AlN, GaN to InN, the linear pressure coefficient of the M_c conduction band increases; it decreases for the A_c conduction band, but remains nearly unchanged for the K_c conduction band. This trend is in good agreement with the calculations of Christensen and Gorczyca [21] for GaN and AlN.

Experimentally, for GaN, Perlin *et al* [16] showed that the presence of sapphire substrate leads to an energy gap pressure coefficient reduction of approximately 5% in comparison to free-standing GaN, due to a compressive-biaxial strain [47]. They reported 38.9 meV GPa⁻¹ for GaN on sapphire, and 41.4 meV GPa⁻¹ for free-standing GaN [16]. For InN, only one study recently reported a value of 6 meV GPa⁻¹ [4], with a fundamental band gap energy (at p = 0) of 0.8 eV. For AlN, to our knowledge, only one value has been reported, 49 meV GPa⁻¹ [18].

For the second-order pressure derivatives β of the different band gaps (table 2), our results agree with the LMTO calculations of Christensen and Gorczyca [21] and the pseudopotential results of Van Camp *et al* [19, 20] for GaN and AlN.

In the ternary alloys, the lattice parameters a and c for $Al_xGa_{1-x}N$ follow Vegard's law. For $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, while the lattice parameters c show an almost linear variation versus concentration, the lattice parameters a deviate from VCA with a slope of -0.09 and -0.16 Å, respectively. This deviation is due to the relaxation of the In–N and Ga–N bond lengths in $In_xGa_{1-x}N$, and the In–N and Al–N in $In_xAl_{1-x}N$. It is important for $In_xAl_{1-x}N$, since the lattice mismatch is larger than that of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$. The band gap bowing parameter is 0.71 eV for $Al_xGa_{1-x}N$, 1.7 eV for InGaN, and 4.09 eV for $In_xAl_{1-x}N$.

For the pressure coefficients of the ternary alloys, we followed the same procedure as for the binaries. Near equilibrium and at each composition, we calculated the electronic band structures at different values of the hydrostatic pressure. The pressure behaviour of the fundamental band energy is shown in figure 4 for $Al_xGa_{1-x}N$, in figure 5 for $In_xGa_{1-x}N$ and in figure 6 for $In_xAl_{1-x}N$. For $Al_xGa_{1-x}N$ (figure 4), the fundamental band gaps of $Al_{0.75}Ga_{0.25}N$ are larger than those of $Al_{0.5}Ga_{0.5}N$ which are larger than those of $Al_{0.25}Ga_{0.75}N$. In the investigated pressure range (0 to ~29 GPa) and for all Al composition (25, 50 and 75%), the fundamental band gap ($\Gamma_c - \Gamma_v$) remains direct. It increases rapidly with pressure, from 2.68 to 3.41 eV for

New Journal of Physics 4 (2002) 94.1-94.15 (http://www.njp.org/)

94.7

Table 2. First- and second-order pressure derivatives of Γ , M, K and A conduction bands with respect to the top valence band at (a) Γ for GaN, (b) Γ for InN and (c) Γ for AlN. The linear term $\alpha = \frac{dE}{dp}$ (meV GPa⁻¹) is given on the first line, and the quadratic term $\beta = \frac{d^2E}{dp^2}$ (meV GPa⁻²) on the second line when available.

GaN	$\Gamma_c - \Gamma_v$	M_c – Γ_v	$K_c - \Gamma_v$	$A_c - \Gamma_v$
Our calc.	31.8	13.2	-1.8	31.3
	-0.23	-0.1	-0.01	-0.23
LMTO-ASA [21]	39.0	14	-1.8	36
	-0.32	-0.17	-0.03	-0.3
First-principles PP [20]	37.5	12.1	-6.5	32.4
F	-0.28	-0.12	0.09	-0.1
Absorption [11]	47			
	-1.8			
PL [13]	44 (47)			
	-11(-16)			
PI [12]	39.0			
	-0.1			
Absorption [10]	37_45			
PI [15]	39.0			
PI [16]	38.0 /1 /			
\mathbf{D} [1/ 17]	<i>J</i> 37			
Full potential I MTO [22]	43.7			
$I \wedge DW [24]$	22			
Eull potential I MTO [20]	33 37			
Full-potential LMTO [29]	57			
InN	$\Gamma_c - \Gamma_v$	M_c – Γ_v	$K_c - \Gamma_v$	$A_c - \Gamma_v$
Our calc.	18.8	28.4	1.5	19.6
	-0.23	-0.27	-0.08	-0.2
LMTO-ASA [21]	33	43	1.9	33
	-0.55	-1.1	-0.08	-0.87
				0.07
Full-potential LMTO [22]	19			0.07
Full-potential LMTO [22] LAPW [24]	19 21			0107
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29]	19 21 23			
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23]	19 21 23 28			
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4]	19 21 23 28 6			
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AIN	$ \begin{array}{c} 19\\ 21\\ 23\\ 28\\ 6\\ \hline \Gamma_c - \Gamma_v \end{array} $	M _c -Γ _v	K _c -Γ _v	$A_c - \Gamma_v$
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AlN Our calc.	$ \begin{array}{c} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \Gamma_c - \Gamma_v \\ 40.5 \\ \end{array} $	<u>Μ</u> _c -Γ _v 8.4	$\frac{K_c - \Gamma_v}{0.6}$	$\frac{A_c - \Gamma_v}{40.4}$
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AlN Our calc.	$ \begin{array}{c} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \Gamma_c - \Gamma_v \\ 40.5 \\ -0.19 \\ \end{array} $	$M_c - \Gamma_v$ 8.4 -0.02	$\frac{K_c - \Gamma_v}{0.6}$	$A_c - \Gamma_v$ 40.4 -0.24
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AIN Our calc.	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \hline \underline{\Gamma_c - \Gamma_v} \\ 40.5 \\ -0.19 \\ 40 \\ \end{array} $	$M_c - \Gamma_v$ 8.4 -0.02 13	$K_c - \Gamma_v$ 0.6 0.02 2.7	
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AIN Our calc. LDA-LMTO [21]	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \hline \hline \hline \hline \hline \hline \hline \hline $	$M_c - \Gamma_v$ 8.4 -0.02 13 -0.24	$K_c - \Gamma_v$ 0.6 0.02 2.7 -0.05	
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AlN Our calc. LDA-LMTO [21] First-principles PP [19]	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \hline \hline \hline \hline \hline \hline \hline \hline \hline $	$ M_c - \Gamma_v 8.4 -0.02 13 -0.24 7.7 $		
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AIN Our calc. LDA-LMTO [21] First-principles PP [19]	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \Gamma_c - \Gamma_v \\ 40.5 \\ - 0.19 \\ 40 \\ - 0.32 \\ 36.3 \\ - 0.18 \\ \end{array} $	$\frac{M_c - \Gamma_v}{8.4} \\ -0.02 \\ 13 \\ -0.24 \\ 7.7 \\ 0.11$		$ \begin{array}{r} A_c - \Gamma_v \\ $
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AIN Our calc. LDA-LMTO [21] First-principles PP [19] Absorption [18]	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \hline \Gamma_c - \Gamma_v \\ 40.5 \\ - 0.19 \\ 40 \\ - 0.32 \\ 36.3 \\ - 0.18 \\ 49 \\ \end{array} $	$\frac{M_c - \Gamma_v}{8.4} \\ -0.02 \\ 13 \\ -0.24 \\ 7.7 \\ 0.11$		$ \begin{array}{r} A_c - \Gamma_v \\ $
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AlN Our calc. LDA-LMTO [21] First-principles PP [19] Absorption [18] Full-potential LMTO [22]	$ \begin{array}{c} 19\\ 21\\ 23\\ 28\\ 6\\ \hline \Gamma_c - \Gamma_v \\ 40.5\\ -0.19\\ 40\\ -0.32\\ 36.3\\ -0.18\\ 49\\ 44\\ \end{array} $	$\frac{M_c - \Gamma_v}{8.4} \\ -0.02 \\ 13 \\ -0.24 \\ 7.7 \\ 0.11$	$ \begin{array}{r} K_c - \Gamma_v \\ 0.6 \\ 0.02 \\ 2.7 \\ -0.05 \\ -6.4 \\ 0.18 \\ \end{array} $	$ \begin{array}{r} A_c - \Gamma_v \\ 40.4 \\ -0.24 \\ 40 \\ -0.33 \\ 35.7 \\ -0.16 \end{array} $
Full-potential LMTO [22] LAPW [24] Full-potential LMTO [29] First-principles PP [23] PL and absorption [4] AlN Our calc. LDA-LMTO [21] First-principles PP [19] Absorption [18] Full-potential LMTO [22] LAPW [24]	$ \begin{array}{r} 19 \\ 21 \\ 23 \\ 28 \\ 6 \\ \hline \Gamma_c - \Gamma_v \\ 40.5 \\ - 0.19 \\ 40 \\ - 0.32 \\ 36.3 \\ - 0.18 \\ 49 \\ 44 \\ 43 \\ \end{array} $	$ \begin{array}{r} M_c - \Gamma_v \\ $		$ \begin{array}{r} A_c - \Gamma_v \\ 40.4 \\ -0.24 \\ 40 \\ -0.33 \\ 35.7 \\ -0.16 \end{array} $



Figure 4. Variation of the fundamental band gap versus pressure for $Al_xGa_{1-x}N$ alloys.



Figure 5. Variation of the fundamental band gap versus pressure for $In_xGa_{1-x}N$ alloys.

Al_{0.25}Ga_{0.75}N, 3.12 to 3.87 eV for Al_{0.5}Ga_{0.5}N, and from 3.70 to 4.50 eV for Al_{0.75}Ga_{0.25}N. This is in agreement with the experimental variation found by Shan *et al* [15, 25], except that our energy gaps are lower than theirs because of the use of the LDA. For $In_xGa_{1-x}N$ (figure 5) and $In_xAl_{1-x}N$ (figure 6), the fundamental band gap decreases when In composition increases. For all In composition (25, 50 and 75% In), the fundamental band gap ($\Gamma_c - \Gamma_v$) increases and also remains direct for all applied pressure (from 0 to ~28 GPa). For InGaN, it increases from 1.29 to 1.78 eV for $In_{0.25}Ga_{0.75}N$, 0.77 to 1.55 eV for $In_{0.5}Ga_{0.5}N$, 0.46 to 0.79 eV for $In_{0.75}Ga_{0.25}N$, and for InAlN from 2.22 to 2.63 eV for $In_{0.25}Al_{0.75}N$, 1.31 to 1.64 eV for $In_{0.5}Al_{0.5}N$, and from 0.72 to 1.03 eV for $In_{0.75}Al_{0.25}N$. This variation is consistent with the experimental one for the InGaN [26]–[28].

The energy band gaps, E_g , first-order α and second-order β pressure derivatives coefficients of the fundamental band gaps, bulk moduli, B, and their pressure derivatives, B', of Al_xGa_{1-x}N,

New Journal of Physics 4 (2002) 94.1-94.15 (http://www.njp.org/)



Figure 6. Variation of the fundamental band gap versus pressure for $In_x Al_{1-x}N$ alloys.

In_xGa_{1-x}N and In_xAl_{1-x}N alloys are given in tables 3–5, respectively. For Al_xGa_{1-x}N (table 3), we note that the pressure coefficients of the fundamental band gap $(\Gamma_c - \Gamma_v)$ increase from 31.9 meV GPa⁻¹ for Al_{0.25}Ga_{0.75}N, to 32.4 meV GPa⁻¹ for Al_{0.5}Ga_{0.5}N and to 34.5 meV GPa⁻¹ for Al_{0.75}Ga_{0.25}N. The introduction of Al in GaN leads to a slow increase of the pressure coefficient. However, this variation is nonlinear with alloy composition. Using the following equation:

$$a_g(A_x B_{1-x} C) = x a_g(AC) + (1-x) a_g(BC) - bx(1-x)$$
(7)

we calculate a pressure coefficient bowing parameter of 15.34 meV GPa⁻¹. From experimental data, our results are slightly smaller than those of optical absorption measurements at room temperature [15] on samples with Al composition range $0.12 \le x \le 0.6$, and near-band-edge PL study of single-crystal Al_{0.05}Ga_{0.95}N and Al_{0.35}Ga_{0.65}N [25]. However, the results of these studies do not exhibit significant dependence of pressure coefficient on alloy composition; the near-band-edge PL study [25] reported 40 meV GPa⁻¹ for Al_{0.05}Ga_{0.95}N and 36 meV GPa⁻¹ for Al_{0.35}Ga_{0.65}N, and that of optical absorption [15] reported 39 meV GPa⁻¹ for GaN, 37.3 meV GPa⁻¹ for Al_{0.12}Ga_{0.88}N, 37.2 meV GPa⁻¹ for Al_{0.2}Ga_{0.8}N, 37.6 meV GPa⁻¹ for Al_{0.4}Ga_{0.6}N and 37.2 meV GPa⁻¹ for Al_{0.6}Ga_{0.4}N (table 3). Further, in the optical absorption study, Shan *et al* [15] reported a correction to their measured values, by taking into account the difference of compressibility between the epitaxial films and sapphire substrate, leading to larger values (between 40.4 and 41.5 meV GPa⁻¹).

For $In_xGa_{1-x}N$ (table 4), there is a decrease of the pressure coefficients with In composition from 24.8 meV GPa⁻¹ for $In_{0.25}Ga_{0.75}N$, to 21.7 meV GPa⁻¹ for $In_{0.5}Ga_{0.5}N$, to 19.8 meV GPa⁻¹ for $In_{0.75}Ga_{0.25}N$. From their PL results, Shan *et al* deduced pressure coefficients of 39 meV GPa⁻¹ for $In_{0.08}Ga_{0.92}N$, 40 meV GPa⁻¹ for $In_{0.11}Ga_{0.89}N$ [28], and 35 meV GPa⁻¹ for $In_{0.14}Ga_{0.86}N$ [27]. In their PL measurements and photomodulation spectroscopy [26] on $In_xGa_{1-x}N$ alloys ($0 \le x \le 0.2$), they reported values of pressure coefficients of 39 meV GPa⁻¹ for $In_{0.04}Ga_{0.96}N$, 35 meV GPa⁻¹ for $In_{0.08}Ga_{0.92}N$, and 40 meV GPa⁻¹ for $In_{0.11}Ga_{0.89}N$. From these data, no clear dependence of the pressure coefficient on alloy composition can be drawn.

		E_g (eV)	α (meV GPa ⁻¹)	β (meV GPa ⁻²)	B (GPa)	B'
This work						
	$\begin{array}{l} GaN \\ Al_{0.25}Ga_{0.75}N \\ Al_{0.5}Ga_{0.5}N \\ Al_{0.75}Ga_{0.25}N \end{array}$	2.22 2.68 3.12 3.70	31.8 31.9 32.4 34.5	-0.23 -0.2 -0.21 -0.21	207 210 211 214	4.37 4.06 4.44 4.09
	AIN	4.40	40.5	-0.19	214	3.88
Expt	$\begin{array}{l} Al_{0.05}Ga_{0.95}N~(295~K)\\ Al_{0.12}Ga_{0.88}N~(295~K)\\ Al_{0.2}Ga_{0.8}N~(295~K)\\ Al_{0.35}Ga_{0.65}N~(10~K)\\ Al_{0.4}Ga_{0.6}N~(295~K)\\ Al_{0.6}Ga_{0.4}N~(295~K)\\ \end{array}$	$\begin{array}{c} 3.52^{\rm a} \\ 3.64^{\rm b} \\ 3.88^{\rm b} \\ 4.33^{\rm a} \\ 4.22^{\rm b} \\ 4.72^{\rm b} \end{array}$	$\begin{array}{c} 40^{\rm a} \\ 37.3^{\rm b}, 40.4^{\rm b} \\ 37.2^{\rm b}, 40.5^{\rm b} \\ 36^{\rm a} \\ 37.6^{\rm b}, 41.2^{\rm b} \\ 37.2^{\rm b}, 41.5^{\rm b} \end{array}$			

Table 3. Energy band gaps, E_g , first-order α and second-order β pressure derivatives of the fundamental band gap, bulk moduli, B, and their pressure derivatives, B', of Al_xGa_{1-x}N alloys.

^a PL measurements from [25].

^b Absorption measurements from [15].

In our case, the introduction of In reduces the pressure coefficient significantly and does not lead to linear variation with alloy composition. We have a bowing parameter of $15.1 \text{ meV GPa}^{-1}$. The recent work of Perlin *et al* [29] reported pressure coefficients of the $In_xGa_{1-x}N$ alloys using FP-LMTO and PL. They showed a dependence of the pressure coefficient of the fundamental band gap $(\Gamma_c - \Gamma_v)$ on alloy composition with a significant deviation from those of linear interpolation, in agreement with our calculations. For $In_x Al_{1-x}N$ (table 5), there is a strong dependence of the pressure coefficients on alloy composition. It varies from 20.7 meV GPa⁻¹ for $In_{0.25}Al_{0.75}N$, to 17.6 meV GPa⁻¹ for $In_{0.5}Al_{0.5}N$, and to 16.7 meV GPa⁻¹ for $In_{0.75}Al_{0.25}N$, with a strong deviation from linearity. It appears that introducing In decreases the pressure coefficient significantly: for 50 and 75% of In, the values are lower than that of InN. From the variation of the fundamental band gap energy with alloy composition for different pressures (between 0 and 20 GPa), and using equation (7) for the energy band gap, we calculated the band gap bowing parameter at each pressure. This is shown in figure 7 for Al_xGa_{1-x}N, In_xAl_{1-x}N and In_xGa_{1-x}N. For Al_xGa_{1-x}N and $In_x Al_{1-x}N$, the bowing parameter increases with pressure until a pressure ~14 GPa, after that it decreases rapidly. The reason is the change of the fundamental band gap in AlN from Γ $(\Gamma_c - \Gamma_v)$ to K $(K_c - \Gamma_v)$; the $\Gamma_c - \Gamma_v$ band gap increases quickly in contrast to that of $K_c - \Gamma_v$ which remains almost constant and smaller than that of $\Gamma_c - \Gamma_v$, after the crossing of the two bands at p = 13.88 GPa. For In_xGa_{1-x}N, the band gap bowing parameter increases continuously with pressure.

Table 4. Energy band gaps, E_g , first-order α and second-order β pressure derivatives of the fundamental band gap, bulk moduli, B, and their pressure derivatives, B', of $\ln_x \operatorname{Ga}_{1-x}$ N. The experimental data are given from PL measurements.

		E_q	α	β	В	
		(eV)	(meV GPa ⁻¹)	$(meV GPa^{-2})$	(GPa)	B'
This						
work	GaN	2.22	31.8	-0.23	207	4.37
	$In_{0.25}Ga_{0.75}N$	1.29	24.8	-0.22	186	4.35
	$In_{0.5}Ga_{0.5}N$	0.77	21.7	-0.21	177	4.05
	$In_{0.75}Ga_{0.25}N$	0.46	19.8	-0.25	157	7.04
	InN	0.17	18.8	-0.23	152	4.45
Expt	In _{0.04} Ga _{0.96} N (10 K)	3.25 [<mark>26</mark>]	39 [<mark>26</mark>]			
	In _{0.08} Ga _{0.92} N (10 K)	3.08 [<mark>26</mark>],	35 [<mark>26</mark>],			
		3.249 [27]	39 [27]			
	In _{0.08} Ga _{0.92} N (295 K)	3.04 [26]	36 [<mark>26</mark>]			
	In _{0.11} Ga _{0.89} N (295 K)	2.86 [<mark>26</mark>]	40 [26, 28]			
	In _{0.14} Ga _{0.86} N (10 K)	3.08 [27]	35 [27]			
Other						
Calc.	In _{0.0625} Ga _{0.9375} N		33.75 [<mark>29</mark>]			
	$In_{0.2}Ga_{0.8}N$		28.8 [29]			
	$In_{0.25}Ga_{0.75}N$		28 [29]			
	$In_{0.5}Ga_{0.5}N$		25 [29]			

Table 5. Energy band gaps, E_g , first-order α and second-order β pressure derivatives of the fundamental band gap, bulk moduli, B, and their pressure derivatives, B', of $In_xAl_{1-x}N$.

		E_g (eV)	α (meV GPa ⁻¹)	β (meV GPa ⁻²)	B (GPa)	B'
This work	AlN	4.4	40.5	-0.19	214	3.88
	$In_{0.25}Al_{0.75}N$	2.22	20.7	-0.18	196	4.24
	$In_{0.5}Al_{0.5}N$	1.31	17.6	-0.14	195	2.14
	$In_{0.75}Al_{0.25}N$	0.72	16.7	-0.2	171	7.79
	InN	0.17	18.8	-0.23	152	4.45

4. Discussion and conclusion

Using the FPLAPW method, we have studied the behaviour of the wurtzite nitride ternary alloys with pressure, starting with the pressure coefficients of the binaries. In the experimental studies, many parameters contribute to the determination of the pressure coefficients and this is probably the reason for scattered values. Such parameters are, among others, the technique of measurement of the band gap (PL and absorption), the effect of the temperature, the number of experimental



Figure 7. Variation of the band gap bowing parameter versus pressure for Al_x $Ga_{1-x}N$, $In_xAl_{1-x}N$, and $In_xGa_{1-x}N$.

points [16], the substrate, and the approximation used to fit $E_g(p)$. For binaries, Kim *et al* using PL-free exciton measurement reported pressure coefficient for GaN at 9 K of 44 meV GPa⁻¹, and 47 meV GPa⁻¹ at 300 K. Shan *et al* using PL-free exciton gave 39 meV GPa⁻¹ for GaN at 10 K. Absorption measurement of Perlin *et al* of bulk GaN gave 47 meV GPa⁻¹ at 295 K. Perlin *et al* [16] showed that the presence of sapphire substrate reduces the pressure coefficient by 5%. The approximation used to fit the $E_g(p)$ also plays an important role, since the linear approximation is observed to be not suitable above 10 GPa [16, 24].

For the ternaries, the reported values of pressure coefficients do not exhibit a dependence on alloy composition. For $Al_xGa_{1-x}N$, Shan and his co-workers reported 39 meV GPa^{-1} for GaN (PL) [15], 40 meV GPa⁻¹ for x(Al) = 0.05 at 295 K (PL) [25], 37.3 meV GPa⁻¹ for x(Al) = 0.12 at 295 K (by absorption) [15], 37.2 meV GPa⁻¹ for x(Al) = 0.2 at 295 K (by absorption) [15] 36 meV GPa⁻¹ for x(Al) = 0.35 at 10 K (PL) [25], 37.6 meV GPa⁻¹ for x(Al) = 0.4 at 295 K (by absorption) [15], and 37.2 meV GPa⁻¹ for x(Al) = 0.6 at 295 K (by absorption) [15]. Further, Shan *et al* in their study [15] corrected the measured values by taking into account the difference of compressibility between the epitaxial films and the sapphire substrate: the reported values are given in table 3 and are larger. For $In_xGa_{1-x}N$, Shan *et al* [26] using PL and photomodulation spectroscopy reported 39 meV GPa⁻¹ for GaN at 10 K, 39 meV GPa⁻¹ for x(In) = 0.04 at 10 K, 35 meV GPa⁻¹ for x(In) = 0.08 at 10 K (with a band gap energy at p = 0 GPa of 3.08 eV), 36 meV GPa⁻¹ for x(Al) = 0.08 at 295 K (with a band gap energy at p = 0 GPa of 3.04 eV), and 40 meV GPa⁻¹ for x(In) = 0.11 at 295 K. In a previous work Shan *et al* [27] using PL reported pressure coefficients of 35 meV GPa⁻¹ for x(In) = 0.14and 39 meV GPa⁻¹ for x(In) = 0.08 with a band gap energy at p = 0 GPa of 3.249 eV which differ from those of photomodulation spectroscopy. In the case of $In_x Al_{1-x}N$, no experimental results on pressure coefficient are available.

In our work, using the same method, we calculated the pressure coefficient of the binaries and the ternaries over a wide range of composition. We see that the introduction of Al in $Al_xGa_{1-x}N$ increases and that of In in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ decreases the pressure coefficient. However, this variation is not linear. We also report the variation of the fundamental band gap bowing with

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pressure. It increases continuously with pressure for $In_xGa_{1-x}N$, and has the same variation for $Al_xGa_{1-x}N$ and $In_xAl_{1-x}N$ until a pressure of ~ 14 GPa—after that it decreases significantly. This pressure is in the range where we see that the fundamental band gap of AlN becomes indirect.

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