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Band Gap of Cubic AlN, GaN and InN Compounds Under Pressure

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Abstract

Numerical simulation based on FP-LAPW calculations is applied to study the lattice parameters, bulk modulus and band gap energy of zinc blende binaries AlN, GaN and InN under hydrostatic pressure. The results obtained are in a good agreement with experimental and theoretical values.

Key Words: Lattice parameter, bulk modulus, pressure coefficient, FP-LAPW, WIEN(2k).

1. Introduction

Wide energy gap III-V nitride semiconductors GaN, AlN, InN and their quantum well structures have received considerable attention for their device applications in blue and ultraviolet wavelengths [1–7]. Recently, the successful fabrication of the blue light III-V nitride semiconductor laser was first demonstrated by Nakamura [1]. The vast majority of research on III-V nitrides has been focused on the wurtzite crystal phase. The reason is that sapphire substrates tend to transfer their hexagonal symmetry to the nitride films grown on them. As such, interest in zinc blende nitrides has been growing recently [2–6].

The zinc blende structured GaN has a higher saturated electron drift velocity and a somewhat lower energy gap than wurtzite GaN [7].

The dependence of photoluminescence on pressure is very useful in the understanding of electronic energy band structure and structural properties in semiconductors. The effect of pressure on the electronic properties of III–V compounds can be investigated experimentally in many ways [8–12]. On the other hand, theoretical and technical developments in density-functional theory (DFT) and pseudopotential calculations in recent decades have provided researchers with powerful methods for predicting electronic and energetic properties as revealed by novel experimental techniques. The technical development of epitaxial growth at the end of the last century has provided the possibility for researchers to fabricate synthetic materials with expected compositions and structures. This has stimulated extensive computational studies on high-pressure behavior of various semiconductors [13–17].

In this work, we carry out all-electron full-potential linearised-augmented plane waves (FP-LAPW) calculation to determine band structure of cubic binary AlN, GaN and InN under pressure within the LDA.

2. Calculations

Total energy calculations are performed using the full potential linearised augmented plane wave (FPLAPW). In this method, the unit cell is partitioned into non-overlapping muffin-tin spheres around the atomic sites, and an interstitial region. Among these two types of regions different basis sets are used, the Kohn-Sham equation which is based on the density functional theory (DFT) [18–19] is solved in a self consistent scheme. For the exchange-correlation potential we use the local density approximation (LDA) [20–21] in which the orbitals of Al ($3s^2 3p^1$), Ga ($3d^{10}\ 4s^2 4p^1$), In ($4d^{10}\ 5s^2 5p^1$) and N ($2s^2 2p^3$) are treated as valence electrons. For these calculations the existing WIEN2k code [22] is used and applied to large unit cells.

The muffin-tin radial adopted were 2.0 Å (Ga), 1.60 (N), 2.1 Å (In), and 1.8 Å (Al)

In the following, we use the full-potential LAPW (FPLAPW) method to study the electronic properties under pressure for the binaries zinc blende, GaN, AlN and InN.

3. Result and Discussion

The theoretical lattice constants and bulk modulus in this section are obtained through fitting the total energy data with the Murnaghan equation of state [23]:

$$E(V) - E(V_\circ) = \frac{B_\circ \cdot V}{B'_\circ}\left[\frac{(V_\circ/V)^{B'_\circ}}{B'_\circ - 1} + 1\right] - \frac{B_\circ V}{B'_\circ - 1},$$

where $E(V)$ is the DFT ground-state energy with the cell volume V, V_0 is the unit-cell volume at zero pressure, Bdenotes the bulk modulus, and their first pressure derivative is $B_0^{'} = \partial B/\partial P$ at $P = 0$.

The calculated structural properties (lattice constants a, bulk modulus $B$and B'_0) of the binaries are summarized in Table 1. We have an underestimation of the lattice parameters and an overestimation of the bulk modulus in comparison to those of experiment (see Table1), due to the use of the LDA.

Table 1 shows $B_0^{'}$ ≈4 for AlN, GaN and InN, which is consistent with previous results of EOS studies [24].

Table 1. The lattice constants a, bulk modulus B_0, and their first pressure derivative $B_0^{'}$

		$\boldsymbol{a}$ **(Å)**	$\boldsymbol{B}$ **(Gpa)**	$\boldsymbol{B}_0^{'}$
AlN	Present work	4.353	207.85	4.186
	PWPP[25]	4.323	203.2	4.182
	Other work [26]	4.32	203	-
	Experiment	4.38[27]	202[28]	-
GaN	Present work	4.37[29]	205.38	4.80
		4.475		
	PWPP[25]	4.335	207	4.136
	Other work	4.446[30]	201[26]	-
	Experiment	4.52[27]	190[28]	-
		4.50[2]		-
InN	Present work	4.949	141.16	3.47
	PWPP[25]	4.801	147.6	4.06
	Other work[26]	4.92	139	-
	Experiment	4.98[27]	137[28]	-

By the use of our calculated values of the bulk modulus B_0, and their first pressure derivatives B_0', the volume change with applied pressure was calculated using the equation [29]

$$p = \frac{B_\circ}{B_\circ'}\left[\left(\frac{V_\circ}{V}\right)^{B_\circ'} - 1\right],$$

where p is pressure. The pressure dependence of E_g at the Γ, X and L points of the energy band for the ZB phase from the present energy band structure calculation are plotted in Figures 1, 2 and 3. Since the range of cell volume variation is ±2.0% for all phases in our energy band calculations.

Figures 1, 2 and 3 indicate that the fundamental band gap stays direct for InN (Figure2) and indirect for AlN (Figure 3) a pressure applied up to 21.5 Gpa. In contrast, for GaN (Figure 1), the fundamental gap becomes indirect (X) at pressure 15.53 Gpa. For wurtzite GaN Zhongqin et al. [31]with using semi empirical tight-binding theory found that it pass from direct to indirect band gap under 5% of the strains.

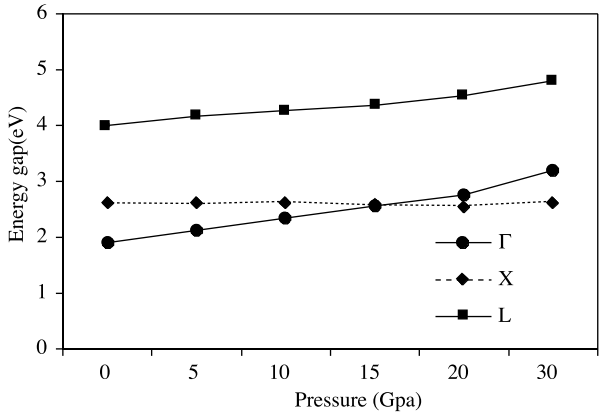

Figure 1. Variation of various band gaps Γ, X and L versus pressure for GaN.

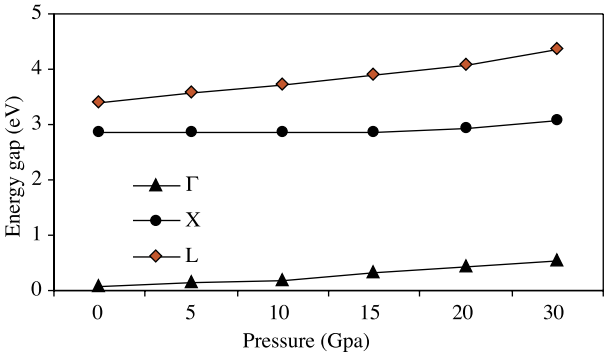

Figure 2. Variation of various band gaps Γ, X and L versus pressure for InN.

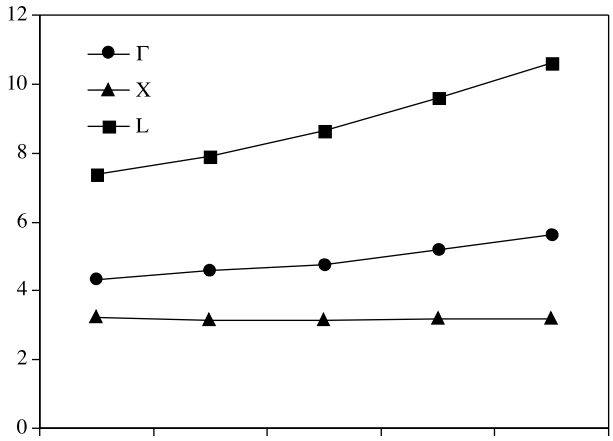

Figure 3. Variation of various band gaps Γ, X and L, versus pressure for AlN.

In order to calculate the pressure coefficients of the fundamental band gap, we have fit $E_g^\Gamma(p)$ data to the linear relation $E_g^\Gamma(p) = E_g^\Gamma(0) + kp$, where $E_g^\Gamma(0)$ is the energy band-gap at the Γ point when $p = 0$ and is given in Table2. Also shown in Table 2 are values of$k$, the pressure coefficient defined by $k = \mathrm{d}E_g^\Gamma/\mathrm{d}p$, along with the theoretical results of others.

Table 2. Band gap at the Γ point and pressure coefficients $k = \mathrm{d}E_g^\Gamma/\mathrm{d}p$ for GaN, AlN and InN.

		E_g^Γ	k (meV·Gpa^{-1})
AlN	Present work	4.24	44.68
	PWPP[25]	4.503	45.0
		5.94[25]	42.0[15]
GaN	Present work	1.80	42.86
	PWPP[25]	3.211	41.7
		3.3[25]	40.0[15]
InN	Present work	0.00	19.94
	PWPP[25]	0.753	34.0
	Others		16[15],
			25.4[13]
		0.9[25]	

For Γ band gap, our calculations give 42.86 meV GPa^{-1} for GaN, 19.94 meV·GPa^{-1} for InN, and 44.68 meV·GPa^{-1} for AlN. These results are in good agreement with the plane wave pseudopotential (PWPP) calculations of Kim et al. [26] for GaN and AlN, which gave 41.7, and 45.0 meV·GPa^{-1}, respectively. For InN, this value is slightly larger than ours, its found 34.0 meV·Gpa^{-1} Christensen and Gorczyca [15], using LMTO calculations, have reported 42 meV·GPa^{-1} for AlN, 40 meV·GPa^{-1} for GaN and 16 meV·GPa^{-1} for InN. The pseudopotential results of Van Camp et al. [13] for InN gives 25.4 meV·Gpa^{-1}.

4. Conclusion

In this work we have reported theoretically calculated electronic properties of zinc blende GaN, AlN and InN under pressure using the FP-LAPW method within LDA. It was shown that, for AlN and InN, the fundamental band gap increases directly with pressure; while for GaN, the fundamental band gap becomes indirect ($\Gamma - X$) at $p = 15.53$ Gpa. So, keeping in mind the fabrication of blue emitting-light devices, it is necessary to diminish stress. However, the pressure coefficient for the fundamental gap obtained is in a good agreement with other investigators.

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