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The composition effect on the bowing parameter in the cubic InGaN, AlGaN and AlInN alloys

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Abstract. Numerical simulation based on FP-LAPW calculations is applied to study direct and indirect band gap energy of the cubic $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys.The direct and indirect band-gap bowing parameter is also calculated, and the values obtained are very important, as we find a strong dependence of the bowing parameter on the composition.

Keywords: III-V ternary alloys, band-gap bowing parameter, WIEN(2k).

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1. Introduction

III-V nitrides and their alloys are becoming increasingly important for the development of optical and high temperature electronic devices due to their wide band gap. These materials and their quaternary alloys cover the energy band-gap range of 0.7-6.2 eV and high saturation velocity [1-3]. For their potentials in opto-electronics (emitters and detectors) [4-6] and high power electronic devices as have been treated in length and received recently countless weight.

The recent progress in this field led to fabrication of efficient light emitting diodes and laser diodes operating in the green-blue-UV spectral region [7-8]. In contrast to the ternary InGaN and AlGaN alloys [9-11], slight attention has been paid to InAlN, due to the difficulty in growing it [12-14]. The InAlN alloy exhibits a large band-gap variation, and it is expected that the alloy lattice matched to GaN [15] would have a sufficiently large energy.

In this work, we study the influence of the band gap bowing on the structural and electronic properties of the cubic ternary alloys InGaN, AlGaN, and AlInN.

2. Calculation

Total energy calculations are performed using the full potential linearized 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. In these two kinds of regions, different basis sets are used. Inside the atomic sphere, a linear combination of radial functions multiplied by spherical harmonics is used, furthermore, the plane waves are used in the interstitial region.

The Kohn-Sham equation that is based on the density functional theory (DFT) is solved in a self-consistent scheme. For the exchange-correlation potential, we use the local density approximation (LDA) [16-19]. The orbital of Al ($3s^23p^1$), Ga ($3d^{10}4s^24p^1$), In ($4d^{10}5s^25p^1$) and N ($2s^22p^3$) are treated as valence electrons.

In these calculations, the existing WIEN2k code [20] is used. The required precision in the total energy was achieved by using a large plane wave (PW) cut-off. In the linear APW (LAPW) method the relevant convergence parameter is RMT: $K_{max} = 8$.

The ordered cubic alloys were modelled using the Landau-Lifshitz structures [21, 22] in which the binary compounds AlN, GaN, and InN possess a zinc-blende structure, the ternary alloys for the composition $x = 0.5$ $(InGaN)_2$, $(AlGaN)_2$, and $(InAlN)_2$ are modelled using the chalcopyrite structure, which could be considered as a (2,2) zinc-blende superlattice along the ⟨201⟩ direction.

For the composition $x = 0.75$ or $x = 0.25$ (In_3GaN_4 or $InGa_3N_4$), (Al_3GaN_4 or $AlGa_3N_4$), and (In_3AlN_4 or $InAl_3N_4$) we have adopted the luzonite structure.

3. Results and discussion

3.1. Electronic properties

The different values of the band gap at Γ and X point of the binary compound GaN, AlN, and InN are summarized in Table 1, as seen in this table, the FPLAPW method underrates the gap, it is owing to two facts, the first is using LDA and the second is the presence of the states *d* known by their effect on the gap in the GaN and InN compounds.

Table 1. The direct and indirect band gaps of AlN, GaN, and InN by our calculation and those by other researchers.

		E_g^{Γ} (eV)	E_g^{X} (eV)
AlN	Present work	4.25	3.16
	PWPP [23]	4.503	
	Exp. [24]	5.94	
GaN	Present work	1.58	3.2
	PWPP [23]	3.211	
	Exp. [24]	3.3	
InN	Present work	0.0	1.56
	PWPP [23]	0.753	
	Exp. [24]	0.9	

The both compounds GaN and InN present a direct band gap, whilst AlN has an indirect band gap.

In the ternary alloys, InGaN, AlGaN and InAlN, the direct band gap (Γ) and indirect (X) one are existing in Figs. 1, 2, and 3, respectively. Although the gap is underestimated, its variation is well described by the LDA.

In $In_xGa_{1-x}N$ the gap stays direct in the range composition from $x = 0$ corresponding to GaN to $x = 1$ (InN).

In $Al_xGa_{1-x}N$, the direct and indirect band gaps are prearranged in Fig. 2. We witness a rapid variation of the direct band gap with the Al composition; it conforms to the linear change. In contrast, the indirect band gap varies gradually. Nevertheless, there is a direct-indirect switch near $x = 0.573$, when the band gap of AlN dominates. This result is in accord with the values obtained by Albanesi *et al.* [26] and Wen-Wei Lin *et al.* [27], as they found 0.57 and 0.571 with using the ideal structure and CASTEP calculations, correspondingly.

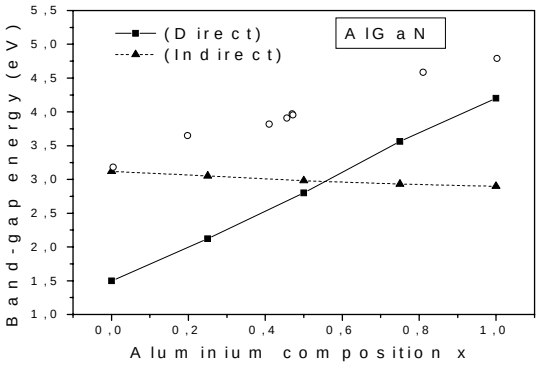

Fig. 2. Band-gap energy of $Al_xGa_{1-x}N$ as a function of indium composition *x*, the open circles are the experimental values of the direct band gap of Takanobu Suzuki *et al.* [28].

For $Al_xIn_{1-x}N$, the direct and indirect band gaps are offered in Fig. 3. There is a swift growth of the indirect band gap through the composition, hence there is a transition from direct (Γ) to indirect (X) band gap for $x = 0.23$, this result agrees well with the calculation of Wen-Wei Lin *et al.* [27], who obtained the transition for $x = 0.244$ with using the CASTEP.

4. Discussions

To be aware on the origin of the direct band gap bowing in III-nitrides alloys AlGaN, InGaN, and InAlN, we have proceed to the calculation of this parameter according to the rule of Zunger [29]. In this law, the bowing parameter is decomposed to three terms, ahead of developing those terms, we consider in the first pace, the beneath reaction:

$$xAC(a_{AC}) + (1 - x)BC(a_{BC}) \rightarrow A_xB_{1-x}C(a_{eq}). \quad (1)$$

Where a_{AC} and a_{BC} are the equilibrium lattice constants of the binary compounds AC and BC, respectively, and a_{eq} is the equilibrium lattice constant of the $A_xB_{1-x}C$ alloy with the average composition *x*.

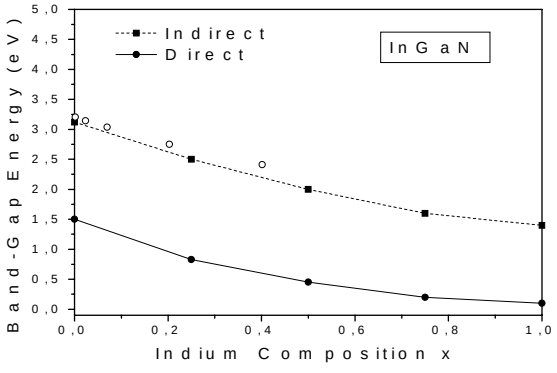

Fig. 1. Band-gap energy of $In_xGa_{1-x}N$ as a function of indium composition *x*, the open circles are the experimental values of the direct band gap obtained by R. Goldhahn *et al.* [25].

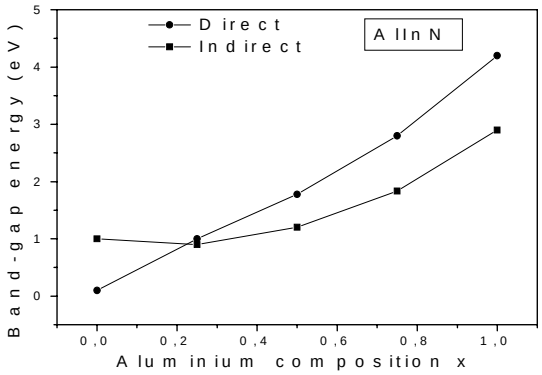

Fig. 3. Band-gap energy of $Al_xIn_{1-x}N$ as a function of aluminum composition *x*.

The second step is to divide the reaction 1 to three parts:

$$AC(a_{AC}) + BC(a_{BC}) \rightarrow AC(a) + BC(a), \quad (2)$$

$$xAC(a) + (1–x)BC(a) \rightarrow A_xB_{1-x}C(a), \quad (3)$$

$$A_xB_{1-x}C(a) \rightarrow A_xB_{1-x}C(a_{eq}). \quad (4)$$

The first equation (2), dealings the volume deformation effect on the gap bowing, the corresponding involvement to the bowing is b_{VD}, it is caused by the effect of the volume deformation. The second reaction (3) is due to charge-exchange (CE) contribution b_{CE}, it reflects a charge transfer effect, it is due to the different averaged bonding behaviour at the lattice constant a. The last part (4), measures amend due to the structural relaxation (SR) in passing from the unrelaxed to the relaxed alloy, it notes b_{SR}, thus, the total gap bowing parameter becomes:

$$b= b_{VD} + b_{CE} + b_{SR}.$$

Table 2. Direct band-gap bowing parameters of AlGaN (a), InGaN (b), and InAlN (c) for different composition, all values are in eV.

a) AlGaN

x composition range	0.25	0.5	0.75
b_{VD}	–0.092	–0.08	–0.08
b_{CE}	0.412	0.73	1.20
b_{SR}	0.56	0.10	0.197
b	0.88	0.75	1.317
Other works:	0.068 [31], 0.05 [32], 0.755 [27], 0.632 [24], 0.068 [34].		

b) InGaN

x composition range	0.25	0.5	0.75
b_{VD}	1.04	0.90	0.67
b_{CE}	0.49	0.94	0.49
b_{SR}	0.14	0.84	0.10
b	1.67	2.68	1.26
Other works:	1.379 [27], 1.89 [30], 1.37 [24], 1.4 [33], 1.36 [34].		

c) AlInN

x composition range	0.25	0.5	0.75
b_{VD}	1.02	1.11	1.21
b_{CE}	2.74	2.32	2.35
b_{SR}	0.42	0.81	0.90
b	4.18	4.24	4.46
Other works:	2.729 [27], 2.914 [24], 1.41 [34].		

The results obtained are depicted in Table 2 (a, b, and c), the value of the bowing linked to the volume deformation b_{VD} depends on the differences between the lattice constants of the binary compounds AlN, GaN, and InN. We imply that b_{VD} is more important in AlInN and InGaN than AlGaN, this is related to lattice mismatching between binary compounds, which is 2.5 % for GaN/AlN, 10 % for GaN/InN and 13 % for AlN/InN. The bowing due to a charge transfer effect b_{CE} is more important in AlInN than AlGaN and InGaN, this is owing to the unlike electronegativities of In and Al atoms. Finally, the contribution due to the structural relaxation is tiny for AlGaN, InGaN, and AlInN, in which the main displacement is due to the anion.

5. Conclusion

Numerical simulation based on first-principle calculations is developed to investigate the band gap of the cubic zincblende $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$, and $Al_xIn_{1-x}N$ alloys. From the simulation results, we found that the band gap sustains an important departure in the AlGaN and InAlN, in which a transition from direct to indirect band gap is ruling. The bowing parameter of band gap is found to be subjugated by the volume deformation and the charge exchange in AlInN. In this case, there is a strong dependence of the bowing on the composition

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