

## Band-Gap Bowing Parameter of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ Derived from Theoretical Simulation

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The band-gap energy and band-gap bowing parameter of the wurtzite AlGaN alloys are investigated numerically with the CASTEP simulation program. The simulation results suggest that the unstrained band-gap bowing parameter of the wurtzite AlGaN alloys is  $b = 0.353 \pm 0.024$  eV. The simulation results also show that the width of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  top valence band at the  $\Gamma$  point decreases when the aluminum composition increases and has a value of 7.331 eV for the GaN ( $x = 0$ ) and 6.132 eV for the AlN ( $x = 1$ ). [DOI: 10.1143/JJAP.41.73]

KEYWORDS: AlGaN, band-gap energy, band-gap bowing parameter, numerical study

Owing to the important application in the visible light emitting diodes (LED) and short wavelength laser diodes, the group-III nitride semiconductor materials have received much attention in the past few years. The group-III nitride semiconductor materials are capable of emitting light efficiently in the visible and ultraviolet spectral range.<sup>1–3)</sup> However, the crystal growth and device fabrication of the group-III nitride semiconductor materials are not as simple as those of the conventional semiconductor materials owing to the lack of a lattice matched substrate. In the mean time, the physics related to the group-III nitride semiconductor materials has not been well developed. Therefore, much effort is still required to investigate the properties of this material system.

The band-gap bowing parameter is important for calculating the band-gap energy of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  material and is usually obtained experimentally. Quite recently, Lee *et al.* investigated the band-gap bowing of the AlGaN alloys and reported that the intrinsic band-gap bowing parameter of the AlGaN alloys was  $b = 0.62 \pm 0.45$  eV.<sup>4)</sup> Several researchers have also investigated the band-gap bowing parameter of the AlGaN alloys; however, different values were achieved.<sup>5–11)</sup> In this paper, we investigate the band-gap bowing parameter of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  alloys ( $0 \leq x \leq 1$ ) numerically with the CASTEP (abbreviation of Cambridge Serial Total Energy Package) simulation program.

The CASTEP simulation program is capable of calculating the energy band structures and the density of electronic states by solving the differential equations based on the quantum mechanics and molecular dynamics. If a set of atoms is given, the CASTEP is capable of calculating the system energy, the distribution of the electrons, and the force undertaken by the atoms at the most stable state. Hence, the CASTEP is capable of accurately describing the interaction among the atoms and predicting the material characteristics in the atomic scale.

Since the energy band structure of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  is direct in the whole range of the aluminum composition, we study the characteristics of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  for the aluminum composition to be between zero and one in this work. In the calculation we assume that the atoms are fixed in space and the lattice constants of the unstrained  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  layer depend linearly on the aluminum composition.<sup>12)</sup> In the mean time, the spin-orbit interaction effects are not taken into account in the calculation. The length of the chemical bonds (in a dimension of Å) used in the CASTEP are as

following:<sup>13)</sup>

$$a(x) = 3.084 \cdot x + 3.162 \cdot (1 - x), \quad (1)$$

$$b(x) = 3.084 \cdot x + 3.162 \cdot (1 - x), \quad (2)$$

$$c(x) = 4.948 \cdot x + 5.142 \cdot (1 - x). \quad (3)$$

The numerical simulation of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  is executed for the situation when the aluminum composition is equal to 0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, and 1. When the aluminum composition is equal to 0 and 1, the ternary compound AlGaN reduces to binary compound GaN and AlN respectively. An aluminum composition of 0.125 means that one eighth of the gallium atoms in GaN are substituted by the aluminum atoms and an aluminum composition of 0.25 means that one quarter of the gallium atoms in GaN are substituted by the aluminum atoms, and so on. Due to the limited dimension of the atomic cluster, the CASTEP simulation results tend to underestimate the band-gap energies of the semiconductor materials. To amend these band-gap energies, we calibrate the results obtained from the simulation to the known band-gap energies of the GaN and AlN. Table I shows the results of the simulation which include the amended band-gap energy, the width of the top valence band at the  $\Gamma$  point, and the crystal-field splitting of the AlGaN alloys. As a typical example, Figs. 1 and 2 show the atomic structure and energy band diagram of the wurtzite AlN (i.e.,  $x = 1$ ) respectively. It is obvious from Table I that the band-gap energy increases and the width of the top valence band at the  $\Gamma$  point decreases when the aluminum composition increases. Specifically, the width of the GaN ( $x = 0$ ) top valence band at the  $\Gamma$  point is equal to 7.331 eV, which is close to those obtained by other researchers,<sup>14–16)</sup>

Table I. Summary of the CASTEP simulation results.

Material	Band-gap energy (eV)	Width of top valence band at $\Gamma$ point (eV)	Crystal-field splitting (eV)
GaN	3.428	7.331	0.0024
$\text{Al}_{0.125}\text{Ga}_{0.875}\text{N}$	3.774	7.216	0.0024
$\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$	4.158	7.053	0.0371
$\text{Al}_{0.375}\text{Ga}_{0.625}\text{N}$	4.499	6.986	0.0150
$\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$	4.854	6.802	0.0223
$\text{Al}_{0.625}\text{Ga}_{0.375}\text{N}$	5.241	6.728	0.0217
$\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$	5.587	6.485	0.1326
$\text{Al}_{0.875}\text{Ga}_{0.125}\text{N}$	6.005	6.371	0.1418
AlN	6.457	6.132	0.1944

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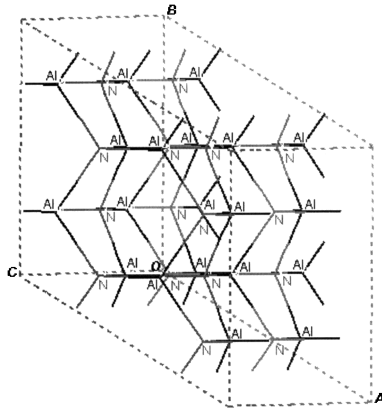


Fig. 1. Atomic structure of the wurtzite AlN.

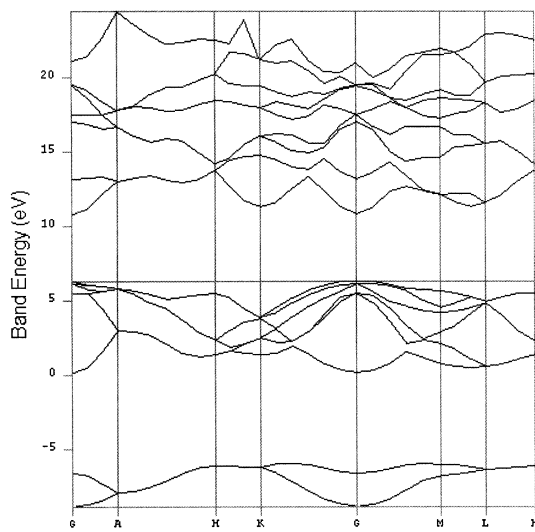


Fig. 2. Energy band diagram of the wurtzite AlN.

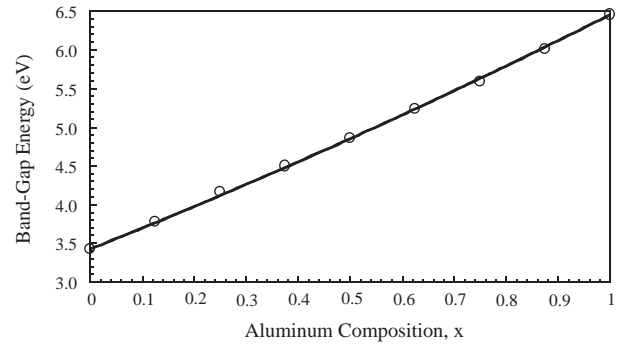
and the width of the AlN ( $x = 1$ ) top valence band at the  $\Gamma$  point is equal to 6.132 eV in our simulation.

The band-gap energy of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  shown in Table I is depicted as a function of the aluminum composition in Fig. 3. The band-gap energy of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  can be approximated by the following formula:<sup>4,17)</sup>

$$E_g(x) = x \cdot E_{g,\text{AlN}} + (1 - x) \cdot E_{g,\text{GaN}} - b \cdot x \cdot (1 - x), \quad (4)$$

where  $E_g(x)$  is the band-gap energy of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ,  $E_{g,\text{AlN}}$  is the band-gap energy of the AlN,  $E_{g,\text{GaN}}$  is the band-gap energy of the GaN, and  $b$  is the band-gap bowing parameter. If we best fit the results shown in Fig. 3 with eq. (4), a band-gap bowing parameter of  $0.353 \pm 0.024$  eV is obtained. This value is similar to that investigated by Lee *et al.*<sup>4)</sup> and other researchers.<sup>5,6)</sup> Note that this band-gap bowing parameter is obtained for an unstrained AlGaN material. Investigation of the band-gap bowing parameter of the strained AlGaN material is still in progress.

In conclusion, the band-gap energy and band-gap bowing parameter of the wurtzite  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  alloys are theoretically investigated with the CASTEP simulation program. The

Fig. 3. Band-gap energy of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  as a function of the aluminum composition.

band-gap energy of the unstrained  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  alloys is studied for the situation when the aluminum composition is equal to 0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, and 1 and a band-gap bowing parameter of  $0.353 \pm 0.024$  eV is obtained. The width of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  top valence band decreases when the aluminum composition increases. The widths of the GaN and AlN top valence bands at the  $\Gamma$  point are determined to be 7.331 eV and 6.132 eV, respectively, in our simulation.

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