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Influence of point defects on optoelectronic properties of $Al_{0.375}Ga_{0.625}N$

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ABSTRACT

In order to study the influence of native point defects on the electronic structure and optical properties of $Al_{0.375}Ga_{0.625}N$, models of $Al_{0.375}Ga_{0.625}N$, $Al_{0.375}Ga_{0.5625}N$, $Al_{0.3125}Ga_{0.625}N$, and $Al_{0.375}Ga_{0.625}N_{0.9375}$ which correspond to Ga, Al, and N vacancies were built. Based on first-principles calculation, formation energies, atomic structures, band structures, density of states, Mulliken charge populations, and optical properties of the crystals with point defects were obtained.

Results show that the $Al_{0.375}Ga_{0.5625}N$ crystal with Ga vacancy and the $Al_{0.3125}Ga_{0.625}N$ crystal with Al vacancy show *p*-type property, meanwhile, the $Al_{0.375}Ga_{0.625}N_{0.9375}$ crystal with N vacancy show *n*-type property. The Fermi level of $Al_{0.375}Ga_{0.5625}N$ and $Al_{0.3125}Ga_{0.625}N$ enter into valence band while the Fermi level of $Al_{0.375}Ga_{0.625}N_{0.9375}$ enters into conduction band. The formation energy of N vacancy is the lowest, showing it is the easiest for N vacancy to exist. The global transfer index values of the defective crystals are all lower than that of the pure one. The bond populations around the defects increase because of the shorter bonds. For the defective crystals, there appear new abnormal dispersion ranges at the low energy region, and the reflectivities of the defective crystals are higher than that of the pure one at the range of 0–2 eV.

1. Introduction

The demand for detectors of deep ultraviolet (DUV) light applications has been increasing in various fields of photolithography, biochemical and engine and flame systems [1]. With the band gap varying from 3.4 eV in GaN to 6.2 eV in AlN, the $Al_{1-x}Ga_xN$ alloy system has great promise as a wide-band-gap semiconductor for DUV optoelectronics [2–4]. Despite the impressive progress in material growth and devices, the role of various defects in the material and their effect on device performance is not yet understood. It is well known that GaN and AlGaN are more difficult to dope *p*-type than *n*-type, which is long suspected to the results of nitrogen vacancies. Ga vacancies and N vacancies have been associated with compensation of highly doped *n*-type GaN and proposed to be the source of the commonly observed "yellow luminescence" [5]. There are many researches on point defects of GaN, meanwhile researches on point defects of AlGaN alloys are inadequate.

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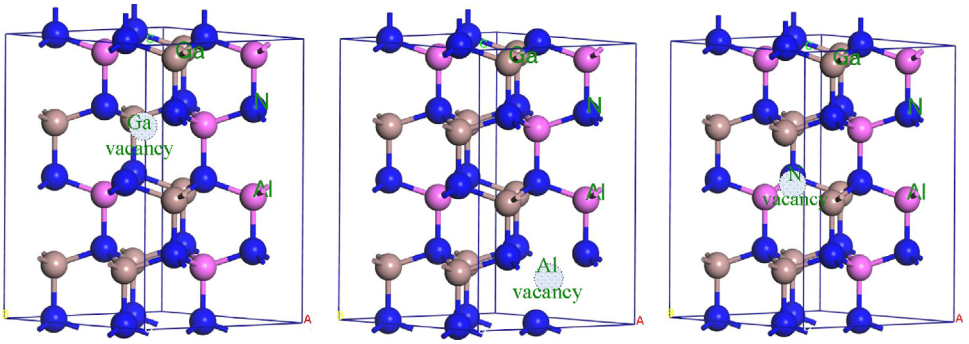

Fig. 1. Computational models (a) $Al_{0.375}Ga_{0.5625}N$ (b)$Al_{0.3125}Ga_{0.625}N$ (c) $Al_{0.375}Ga_{0.625}N_{0.9375}$.

Table 1
Lattice parameters and average bond lengths of $Al_{0.375}Ga_{0.625}N$, $Al_{0.375}Ga_{0.5625}N$, $Al_{0.3125}Ga_{0.625}N$, and $Al_{0.375}Ga_{0.625}N_{0.9375}$.

models	Lattice parameters (Å)		Average bond length (Å)			
	a = b	c	$(Ga\text{-}N)_{\perp 0001}$	$(Ga\text{-}N)_{\parallel 0001}$	$(Al\text{-}N)_{\perp 0001}$	$(Al\text{-}N)_{\parallel 0001}$
$Al_{0.375}Ga_{0.625}N$	3.186	5.189	1.975	1.988	1.914	1.912
$Al_{0.375}Ga_{0.5625}N$	3.148	5.001	1.964	1.804	1.905	1.893
$Al_{0.3125}Ga_{0.625}N$	3.106	5.032	1.961	1.872	1.906	1.819
$Al_{0.375}Ga_{0.625}N_{0.9375}$	3.100	5.084	1.963	1.886	1.901	1.898

In this paper, three models with different types of point defects were built. They are AlGaN models with Ga, Al, and N vacancy defects. Using first principle based on density function theory (DFT), formation energies, atomic geometry, electronic structures, Mulliken charge distribution, and optical properties of the three models were calculated.

2. Theoretical model and calculation method

2.1. Theoretical model

$Al_{0.375}Ga_{0.625}N$ models are obtained by submitting 37.5% Ga atoms for Al atoms based on GaN crystals. Wurtzite GaN belongs to the P63mc(186) space group; the symmetry is C6v-4; the lattice constant is $a = b = 0.3189$ nm, $c = 0.5185$ nm, and $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$ [6]. The Ga vacancy model, Al vacancy model, and N vacancy model are shown in Fig. 1. In the Ga vacancy model, there are 9 Ga atoms, 6 Al atoms, and 16 N atoms. In the Al vacancy model, there are 10 Ga atoms, 5 Al atoms, and 16 N atoms. And in the N vacancy model, there are 10 Ga atoms, 6 Al atoms, and 15 N atoms.

2.2. Calculation method

All calculations were performed with the quantum mechanics program of Vienna Ab-initio Simulation Package (VASP) [7] based on DFT. The *Broyden Fletcher Goldfarb Shanno* (BFGS) algorithm was used to optimize the structures of the crystal models. The final sets of energies were computed with an energy cutoff of 500 eV after a series of convergence test. All calculations were performed with a plane-wave pseudo potential method based on DFT combined with the generalized gradient approximation (GGA) [8,9]. In this calculation, the GGA was parameterized by Perdew, Burke, and Ernzerhof (PBE) [10,11]. The integral in the Brillouin zone was sampled with the Monkhorst-Pack [12] scheme and special k points of high symmetry. The number of k points is $9 \times 9 \times 9$ in the calculation. All calculations were carried in reciprocal space with Ga:$3d^{10}4s^24p^1$, Al:$3s^23p^1$, and N:$2s^22p^3$ as the valence electrons. The scissors operator correction was used for the optical properties calculation to improve the calculation accuracy.

3. Results and discussion

3.1. Atomic geometry

The presence of vacancy makes the atomic geometry change. After geometry optimization, the atomic geometry of $Al_{0.375}Ga_{0.5625}N$, $Al_{0.3125}Ga_{0.625}N$, and $Al_{0.375}Ga_{0.625}N_{0.9375}$ is shown in Fig. 2, and the lattice parameters and average bond lengths of the three crystals are shown in Table 1.

From Fig. 2, it can be found that the lengths of Ga-N and Al-N bonds around the Ga vacancy and Al vacancy decrease significantly, which is caused by the missing of Ga-N bonds. There appear dangling bonds, resulting in the number of valence electrons of the four N neighbors unsaturated, so N atoms move towards other Ga and Al neighbors to overlap electrons.