International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 19 (2018) pp. 14254-14256
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Study of the Substitution Effects of Carbon on the Electronic Properties of AlN and GaN

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Abstract

In this paper in framework of the density functional theory using the pseudopotential method, the substitution effects of carbon on the electronic properties of AlN and GaN in zincblende structure, were studied. In particular, we analyzed the AlC0.0625N0.9375 and GaC0.0625N0.9375. The density states calculation reveals that, when one atom of N is substituted with one C atom, the two compounds losses their semiconductor character. The GaC0.0625N0.9375 compound acquires a metallic behavior but not magnetic properties. While AlC0.0625N0.9375 acquire a half-metallic ferromagnetic behavior with a magnetic moment of 1.0 μβ/cell. The metallic behavior of GaN and half-metallic character of AlN comes from hybridization and polarization of C-2p states and their neighboring N-2p orbitals.

Keywords: Density Functional Theory, structural and electronic properties, substitution.

INTRODUCTIÓN

AlN and GaN crystalizes in the wurtzite structure in bulk form [1]. These compounds have extraordinariness physical and chemical properties, as high thermal conductivity, stability at high temperature, low thermal expansion, and high resistance to gases and chemicals [2-4]. Actually, AlN and GaN doped with metal transition (MT) has been extensive studied because of its applications as diluted magnetic semiconductor (DMS), with potential application in the field of spintronics [5-17]. To get these applications ferromagnetism a room temperature in necessary. Recently, high-temperature ferromagnetism has been found in several investigations using different types of transition-metal (TM)-doped semiconductors, oxides, and nitrides [6-8]. However, it was found that the TM-doped DMS segregate to form ferromagnetic secondary phases, precipitate or clusters [9-11]. This represents a big obstacle for practical applications of DMS. To avoid this problem, many investigations have focused in the effect of nonmagnetic atom doping in semiconductors in order to obtain high-temperature ferromagnetic. Experimental results have proved that is possible to obtain high-temperature ferromagnetism with nonmagnetic anion, for example nonmagnetic C- and N-doped ZnO, TiO_2 and C-doped GaN [12-14]. In this paper we studied the electronic and magnetic effect in AlN and GaN doped with carbon.

COMPUTATIONAL METHOD

In the framework of the density functional theory [18, 19] within pseudopotential method [20, 21] and using the Quantum ESPRESSO computational code [22], computational calculation was performed. The correlation and exchange interaction between electrons were taken into account with the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [23]. For the expansion of the electronic function in plane waves, we used values of kinetic energy cutoff and charge density of 40 Ry. Brillouin zone integrations were performed with the special k-point method over a 6×6×12 Monkhorst-Pack mesh [24] for a unit cell. To simulate AlN and GaN in the zincblende structure, we constructed a $2a$ x $2b$ x $1c$ supercell with 32 atoms. In the concentrations $AlC_{0.0625}N_{0.9375}$ and $GaC_{0.0625}N_{0.9375}$, one N atom were replaced by one C atom, in the supercell. For the pure AlN compound and the $AlC_{0.0625}N_{0.9375}$ and $AlC_{0.125}N_{0.875}$ concentrations, a relax-type calculation was carried out in which all atoms in the supercell moved in the three directions. All calculations were carried out with spin polarization, and the optimization process ended when the forces became smaller than 10^{-4} eV/Å. The convergence threshold for self-consistent field iteration was 10^{-5} eV.

RESULTS AND DISCUSSIONS

Structural properties

Table 1. Lattice constant and bulk modulus in zincblende phase

Compound	a_0 (Å)	B_0 (GPa)
AlN	4.3815	206.52
	4.3800[a]	212.70[b]
	4.3790[c]	211.78[d]
	4.3700[e]	202.00[e]
GaN	4.533	175.75
	4.552f	175.32f
	4.590[g]	-
$AlC_{0.0625}N_{0.9375}$	4.3800	204.00
$GaC_{0.0625}N_{0.9375}$	4.5430	171.73

[a] Theoretical Reference [25]

[b] Theoretical Reference [26]

[c] Theoretical Reference [27]

[d] Theoretical Reference [28]

[e] Experimental Reference [29]

[f] Theoretical reference [30]

[g] Theoretical reference [31].

To calculate the equilibrium lattice constant and bulk modullus of AlN, GaN, $AlC_{0.0625}N_{0.9375}$, and $GaC_{0.0625}N_{0.9375}$ compounds we performed a minimization process using the vc-relax calculation. The equilibrium parameters calculated are shown in table 1 and are compared with available data reported experimental and theoretically for other authors.

We can see in the table 1 for binary AlN and GaN compounds the calculated lattice constant and bulk modullus are in good agreement with reported from other theoretical and experimental investigation. For AlN the maximum discrepancies with to respect lattices constant and bulk modullus calculated here are ~ 0.26% and ~ 2.90%, respectively. While for GaN the lattice constant (4.533 Å) and bulk modulus (175.75 GPa) are in excellent agreement with previous theoretically and experimental work, being the maximum discrepancy of ~ 1.24% and ~ 0.25%, respectively. These discrepancies are smaller, which show the reliability of our present calculation.

For the $AlC_{0.0625}N_{0.9375}$, and $GaC_{0.0625}N_{0.9375}$ compounds, we note that lattice constant of the ternary compounds (4.38 Å) and (4.543 Å) change slightly with to respect the lattices constant of binary AlN and GaN compounds (4.3825 Å) and (4.533 Å), respectively. This happens because the atomic radius of C (0.914 Å) is very near to atomic radius N (0.92 Å). On the other hand, we observe that $AlC_{0.0625}N_{0.9375}$, and $GaC_{0.0625}N_{0.9375}$ preserve their hardness, because the bulk modullus are very close to the AlN and GaN compounds.

Electronic Properties

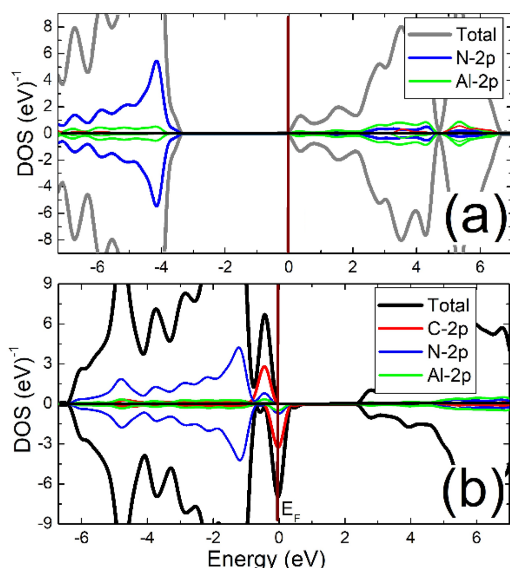

Figure 1. Total and partial density of state, (a) AlN pure and (b) $AlC_{0.0625}N_{0.9375}$. Source: Authors

To calculate the density of states (DOS) of the AlN, $AlC_{0.0625}N_{0.9375}$, GaN, and $GaC_{0.0625}N_{0.9375}$ we used the equilibrium parameters listed in table 1. The DOS of AlN and $AlC_{0.0625}N_{0.9375}$ are shown in fig. 1(a)-(b), respectively. The DOS of GaN and $GaC_{0.0625}N_{0.9375}$ are illustrated in the figure 2(a)-(b) respectively.

We can see that pure AlN-zincblende is a semiconductor material. This behavior is mainly dominated by 2p-N and 2p-Al states, and the calculated value of the energy band gap is 3.37 eV, which is very close to previous theoretical results of 3.38 eV [32], 3.40 eV [33], and 3.36 eV [34].

In the figure 1(b) we can see when one C atom occupy the positions of the N atoms, the compounds have a half-metallic character, because only the spin channel (spin down) crosses the Fermi level. The DOS of the $AlC_{0.0625}N_{0.9375}$ compound shows that the spin density is mainly situated around the C atom, with a small contribution from the first- and second-neighboring Al and N atoms, respectively. For this reason, near the Fermi level the main contribution to the total DOS comes from the 2p-C orbital, with a minor contribution from the 2p-N and 2p-Al orbitals. The hybridization and the polarization between 2p-C, 2p-N, and 2p-Al generate a finite magnetic moment for the $AlC_{0.0625}N_{0.9375}$ compound, with values of 1.0 μ_β/cell. The values of the magnetic moment are integers; this confirm the half-metallic character of the compounds. due to these properties the compound has potential applications as spin injectors and other applications in spintronics.

The figure 2(a) show the DOS of the GaN-zincblende compound. The GaN have a semiconductor behavior. The calculated a direct band gap was 1.78eV, the magnitude of this gap agrees well with values reported theoretically [30]. The figure 2(b) show the DOS of $GaC_{0.0625}N_{0.9375}$, we note when one C atom occupy the positions of the N atoms, the new compound has a metallic character, this behavior is produced by hybridization between 2p-C and 2p-N states. The $GaC_{0.0625}N_{0.9375}$ compound not have magnetic properties, this is confirmed by the DOS because the majority spin is symmetric with de minority spin

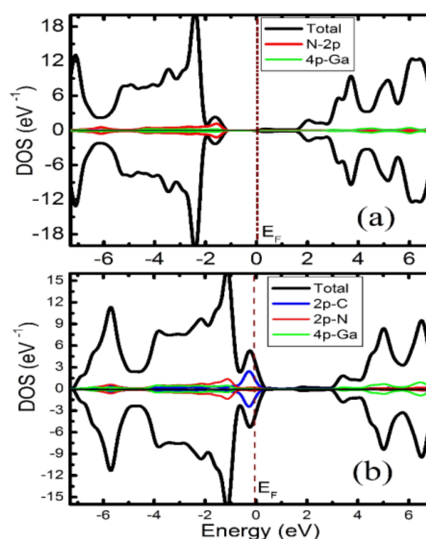

Figure 3. Total and partial density of state, (a) GaN and (b) $GaC_{0.0625}N_{0.9375}$. Source: Authors.

CONCLUSIONS

In summary, we executed first-principles calculations for study the substitution effects of the carbon by nitrogen atom on the structural and electronic properties of AlN and GaN. We found that the $AlC_{0.0625}N_{0.9375}$ and $GaC_{0.0625}N_{0.9375}$ compounds preserve their rigidity because has bulk modullus very near to the binary AlN and GaN compounds. additionally, the DOS show when the carbon atom occupy the positions of the N atoms, The AlN and GaN compounds losses the semiconductors behavior. The $AlC_{0.0625}N_{0.9375}$ acquire a half-metallic character with a magnetic moment of 1.0 μ_{β}/cell and $GaC_{0.0625}N_{0.9375}$ compound has a metallic behavior without magnetic properties.

ACKNOWLEDGEMENTS

The authors are very grateful to the Investigations center of the Universidad Distrital Francisco José de Caldas for its financial support

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