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Short communication

Pressure effects on the electronic and magnetic properties of $Ga_xV_{1-x}N$ compounds: *Ab-initio* study

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ABSTRACT

We report an *ab-initio* study of the pressure effects on the electronic and the magnetic properties of $Ga_xV_{1-x}N$ compounds ($x = 0.25$, 0.50 and 0.75) in wurtzite-derived structures. We use the full-potential linearized augmented plane wave plus local orbitals method (LAPW + lo) within of the spin density functional theory framework. The lattice constant is found to vary linearly with Ga-concentration. The magnetic moment changes for a critical pressure. At $x = 0.75$, a rather abrupt onset of the magnetic moment from 0 to 2 μ_B at P_{cr}~22.8 GPa is observed. For $x = 0.25$ and 0.50 Ga concentrations, the magnetic moment increases gradually when the pressure decreases toward the equilibrium value. We study the transition pressure dependence to a ferromagnetic phase near the onset of magnetic moment for each $Ga_xV_{1-x}N$ compounds. The calculation of the density of states with Ga concentration is carried out considering two spin polarizations. The results reveal that for $x = 0.75$ the compound behaves as a conductor for the spin-up polarization and that the density of states for spin-down polarization is zero at the Fermi level. At this concentration the compound presents a half metallic behavior; therefore this material could be potentially useful as spin injector. At high pressures $P > P_{cr}$ the compounds exhibit a metallic behavior.

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1. Introduction

In recent years, various high performance devices fabricated from III-nitride have generated considerable interest. Gallium nitride (GaN) is one of the wide direct band gap semiconductors, which has a broad range of potential applications for optoelectronic and high power electronic devices. Intensive activities over the recent years have made of the short wave length blue, violet light emitting diodes (LEDs) a commercial reality [1]. Its high thermal conductivity also opens new routes in high-temperature/high-power electronic devices [2,3], as metal-semiconductor field effect transistors (MESFETs), high electron mobility transistors (HEMTs) and heterojunction bipolar transistors (HBTs) [4,5]. Additionally, high Curie temperatures and room-temperature ferromagnetism have been predicted in GaN-doped with transition-metal (MT) elements, which in principle opens the door for room temperature, semiconductor-based spintronic applications [6,7].

The magnetic properties of transitions metal (MT) in GaN regained prominence due to potential application for Dilute Magnetic Semiconductors (DMS) [8,9]. In particular, the 3*d*-MT elements can be expected that substitute Ga-atoms during crystal growth. The knowledge of their associated deep defects is very important to development a new kind of devices such as: electro-optic switches, ultra sensitive magnetic field sensors and quantum–mechanism-based logic for high speed computation [10].

In this paper, we investigate mixed $Ga_xV_{1-x}N$ compounds. As will be shown, the dilution of VN with Ga expands the lattice constant according to Vegard's law as expected. Also Ga incorporation produce the arise of magnetic moment formation. This makes these materials potentially useful as spin injector. In order to model the compounds, simple-ordered model structures (V_3GaN_4, $VGaN_2$, VGa_3N_4) based on supercells of the wurtzite structure were investigated.

2. Computational method

The electronic structure calculations were performed employing the full-potential linearized augmented plane wave method (FP-LAPW) as implemented in the WIEN2k package, which includes the LAPW + lo [11], within of the spin density functional theory (DFT) framework [12,13]. The exchange and correlations electronic energy

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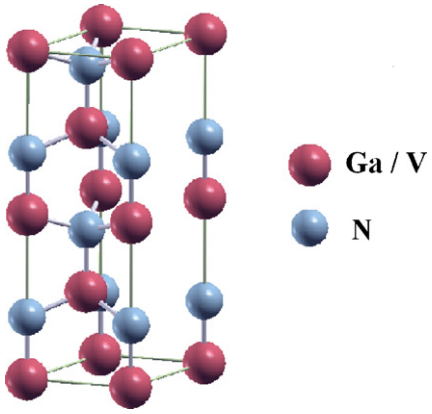

Fig. 1. Unit cell used in our calculation for $Ga_xV_{1-x}N$ compounds in wurtzite-like structure.

were calculated with Generalized Gradient Approximation (GGA) of Perdew et al. [14]. Separation energy between the valence and core states of $-8.0\,Ry$, and the angular momenta up to $l_{max} = 10$, were used. The wave functions in the interstitial region were expanded in plane waves with a cutoff of $K_{max} = 8.0/R_{MT}$ (where R_{MT} is the smallest muffin-tin sphere radii inside the cell). For $Ga_xV_{1-x}N$ compounds muffin-tin radii of 1.80, 1.70 and 1.60 bohr for Ga, V and N atoms were selected respectively. In calculation of the electronic structure, a 50 **k**-points mesh were used in Brillouin irreducible zone generated according to the Monkhorst–Pack scheme [15]. The iteration for self-consistence was continued until the convergence criterium of $1 \times 10^{-4}\,Ry$ was reached.

The $Ga_xV_{1-x}N$ compounds were modeled for $x = 0.25$, 0.50 and 0.75 compositions according to special quasirandom structures approach [16] and the disorder aspects were ignored. For $GaVN_2$ ($x = 0.50$) an hexagonal unit cell with alternating [0 0 0 1] layers of VN and GaN in conventional wurtzite structure was employed. For GaV_3N_4 ($x = 0.25$) and Ga_3VN_4 ($x = 0.75$) an hexagonal unit cell consisting of two wurtzite unit cells piled in the c direction were used [17]. There are eight planes with one Ga (or V) or one N atom in a 1×1configuration, as shown in Fig. 1. In this structure, a V atom replaces to a Ga atom in the unit cell. This atomic substitution (V_{Ga}) has been experimentally observed by Souissi et al. [18] for V-doped GaN samples prepared by metalorganic vapour phase epitaxy technique (MOVPE). On the other hand, the structural internal parameters u_i and c/a ratio were taken from Ref. [19]. The lattice parameters and cohesion energy were found by the fitting the total energy versus volume to the Murnaghan's state equation [20].

3. Results and discussion

Magnetic moment and cohesion energy per unit cell for $Ga_xV_{1-x}N$ compounds are shown in Fig. 2. From minimum point energy of Fig. 2, the equilibrium lattice constant (square points) and the energy (circular points) per unit cell as a function of Ga concentration are presented in Fig. 3. The increase of lattice constant with Ga concentration is due to that Ga-atom is bigger than V-atom. We found a linear dependence according to Vegard's law. Note that the energy also has a linear tendency with the Ga concentration as has been observed in other ternary nitrides [17,21].

As we shown in Fig. 2 for Ga_3VN_4 (triangular points) there is a rather abrupt onset of the magnetic moment from 0 to $2\,\mu_B$ at ~22.8 GPa (3.075 Å). The $GaVN_2$ and GaV_3N_4 compounds presented the same magnetic moment transition but with a slowly pressure dependence. From this figure, we observe the tendency towards magnetism increases as we further decrease the pressure. A similar behavior has been reported by Walter et al. for pure VN in zincblende and rocksalt structures [22].

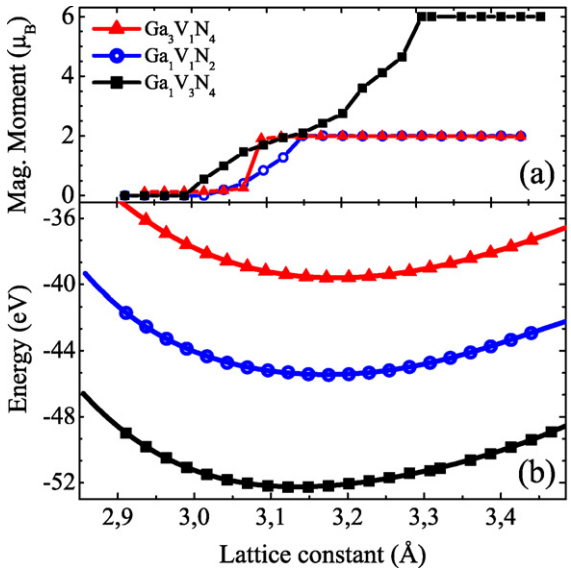

Fig. 2. (a) Magnetic moment and (b) total energy per unit cell as a function of the lattice constant for $Ga_xV_{1-x}N$. In (a) the line is guide to the eye. In (b) the line is a Murnaghan equation of state fit.

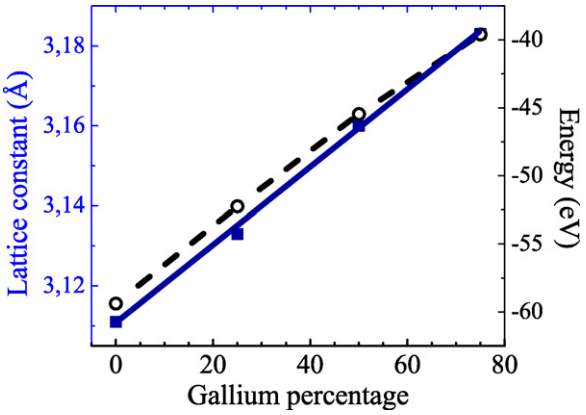

Fig. 3. Equilibrium lattice constant and cohesion energy as function of Ga-concentration in $Ga_xV_{1-x}N$.

We found that in the studied cases, $Ga_xV_{1-x}N$ has a nonzero magnetic moment at the zero pressure. Comparing the total energy of the ferromagnetic (FM) and antiferromagnetic (AFM) configurations for $x = 0.25$ and 0.50 compounds at the equilibrium volume, the FM is found to be lower in energy and is the predicted to be preferred state. Such as has been found by Katayama-Yoshida and Sato for diluted concentrations of V atoms in the GaN semiconductor [23].

In Table 1 we show a summary of the structural and magnetic results for $Ga_xV_{1-x}N$ compounds. We give the equilibrium lattice constant (a_o), critical pressure at which the magnetic moment appears (P_{cr}), saturation value of the magnetic moment per unit cell

Table 1
Structural and magnetic properties of $Ga_xV_{1-x}N$ compounds.

	a_o (Å)	P_{cr} (GPa)	μ (μ_B)	P_F(%)
Ga_3VN_4	3.184	22.8	2.00	100
$GaVN_2$	3.167	24.8	2.00	78.8
GaV_3N_4	3.139	26.7	6.00	31.8

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