Electronic and magnetic properties GaN/MnN/GaN and MnN/GaN/MnN interlayers

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Abstract. In this work we execute computational calculations to investigate the structural, electronic and magnetic properties of the GaN/MnN/GaN and MnN/GaN/MnN interlayers. The calculations were carried out by a method based on pseudopotentials, as implemented in the Quantum ESPRESSO code. For the description of the electron-electron interaction, generalized gradient approximation (GGA) was used. The total energy calculation reveal that the GaN/MnN/GaN interlayer is energetically most favourable that the MnN/GaN/MnN. Analysis of the density of states show that the interlayers have metallic behaviour that comes essentially from the hybridization and polarization states Mn-d and N-p cross the Fermi level. The interlayers have magnetic properties with a magnetic moment of $8\mu_B$/cell. Due these properties the superlattices can be potentially used in the field of spintronic.

1. Introduction

MnN has been extensively studied, both theoretically and experimentally, due to its excellent mechanical, physical and chemical properties such as high hardness, high melting point and high resistance to wearing conditions, corrosion and oxidation [1]. On the other hand, GaN is a direct-gap semiconductor that normally crystallizes in wurtzite structure [2]. Due to its excellent properties, GaN has been used in a range of applications like radiation emitting and sensing devices as well as in high-power/high-temperature electronics; moreover, its efficiency in blue, green and yellow LEDs, injection lasers and ultraviolet detectors is truly extraordinary [3-6]. Furthermore, the combination of the semiconductor properties of GaN and the magnetic properties of the transition metal ions is of great current interest because it could be used at applications in diluted magnetic semiconductors (DMS) [7,8]. Such an interest is also placed on various applications in spintronics (e.g. electro-optical switches and spin injectors) [9]. In this work we study the structural and electronics properties of GaN/MnN/GaN and MnN/GaN/MnN interlayers in the wurtzite structure.

2. Computational method

The Calculations were performed within the framework of Density Functional Theory (DFT) such as is implemented in the Quantum ESPRESSO package [10]. The exchange and correlation energies were modelled according to the generalized gradient approximation (GGA) with the Perdew Burke Ernzerhof (PBE) gradient-corrected functional [11]. Electron–ion interactions were treated with the pseudopotential method [12,13]. The electronic wave functions were expanded into plane waves with a kinetic-energy cutoff of 40Ry. For the charge density, a kinetic energy cutoff of 400Ry was used. A 6×6×3 Monkhorst-Pack mesh [14] was used to generate the k-points in the supercell. To calculate the

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lattice constant, the bulk modulus and the total energy of each studied compound, the calculated data are fitted with the Murnaghan equation of state [15]. In other to study the relative stability of GaN/MnN/GaN and MnN/GaN/MnN interlayers the energy of formation was calculated. For the ternary compound, the formation energy is defined as the difference between the total energy of the ternary K=GaN/MnN/GaN (or K=MnN/GaN/MnN) and the total energy of the binary compounds in their ground state MnN-NaCl and GaN-wurtzite, respectively. Therefore, the formation energy is given by Equation (1) [16,17].

$$\Delta E_f = E_K^{wurtzita} - (1-x) E_{MnN}^{NaCl} - x E_{GaN}^{wurtzita} \quad (1)$$

The interlayers were modelled according to special quasirandom structures approach [18] and the disorder aspects was ignored.

3. Results and discussions

3.1. Structural properties

To determine the structural properties in the ground state, such as the lattice constant (a_0), bulk modulus (B_0) and total energy (E_0) of the GaN/MnN/GaN and MnN/GaN/MnN interlayers, in the wurtzite structure, the total energy was calculated as a function of the volume, the results were fit to the Murnaghan equation of state. Figure 1 shows the energy-volume curves for the GaN/MnN/GaN and MnN/GaN/MnN interlayers.

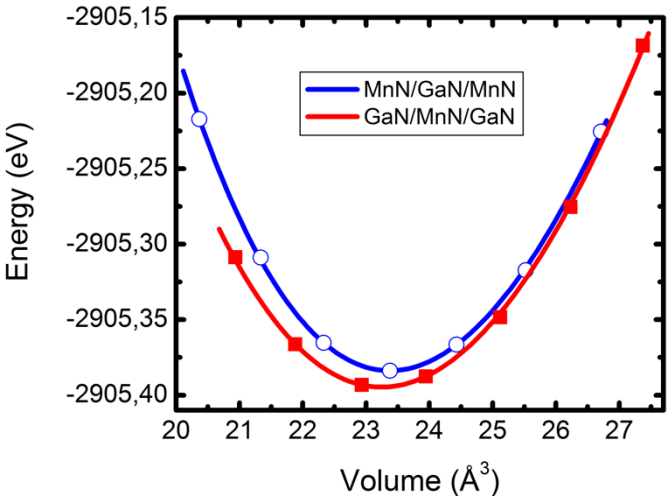

Figure 1. Total energy as a function of the volume of the interlayers.

Table 1. Structural parameters of the interlayers.

Interlayer	a_0 (Å)	c/a	V_0 (Å^3)	B_0 (GPa)	E_0 (eV)	μ (μ_β/cell)	$l_{Ga\text{-}N}$ (Å)	$l_{Mn\text{-}N}$ (Å)
MnN/GaN/MnN	3.194	3.291	46.488	119.67	-2905.394	~8.0	2.887	2.102
MnN/GaN/MnN	3.191	3.321	46.752	120.75	-2905.383	~8.0	2.802	2.098

We observe that the GaN/MnN/GaN interlayer is more energetically favourable that the MnN/GaN/MnN. The calculated values for the lattice constants of the interlayers, the c/a ratio, the equilibrium volume (V_0), the bulk modulus (B_0), the total energy (E_0), the magnetic moment and bond length of the Ga-N and Mn-N (see Figure 2(a)) of the GaN/MnN/GaN and MnN/GaN/MnN interlayers in the wurtzite structure are listed in Table 1. The values of the bulk modules of interlayers are higher, which confirms that they are quite rigid, making them good candidates for possible applications in devices operated at high temperature and high power, as well as hard coatings.

In order to verify the relative stability of the interlayers, we calculated the energy of formation of each interlayer. For this purpose, we calculated the total energy E_0 of the binary compounds GaN and MnN, in their ground states. The values are -3505.20eV and -2307.7eV, respectively. Table 2 shows the values of formation energy ΔE_f calculated using Equation 1.

Table 2. Formation energy.

Superlattice	ΔE_f (eV)
MnN/GaN/MnN	0.906
MnN/GaN/MnN	0.917

In the Table 1 we observed that the total energy of the GaN/MnN/GaN and MnN/GaN/MnN interlayers is negative, in the same way the total energy of the binary compounds MnN and GaN in their ground state is negative, however according to the results of Table 2, the value of the energy of formation of each interlayer is positive. Therefore, GaN/MnN/GaN and MnN/GaN/MnN interlayers are metastable. This means that the interlayer cannot grow under equilibrium conditions, so in order to grow them, it is necessary to supply energy to the system. The Figure 1 confirm that the interlayers are metastable due there are a minimum energy in the corresponding curve. The Figure 2 show the crystal structure of the GaN/MnN/GaN and MnN/GaN/MnN interlayers obtained after structural relaxation. In all cases, the space group obtained is the same, the hexagonal structure whit space group N° 156. It show the bond length Ga-N and Mn-N.

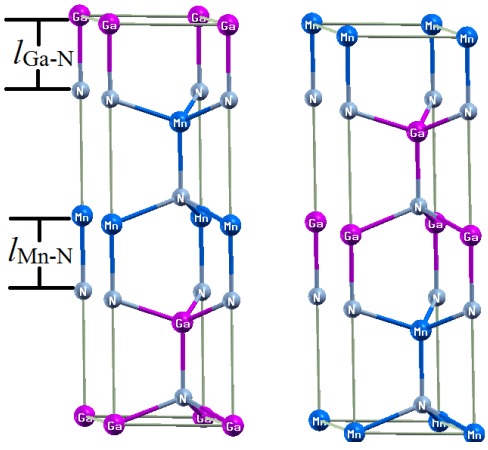

Figure 2. Unit cell of the: (a) GaN/MnN/GaN (b) MnN/GaN/MnN interlayers after structural relaxation. It show the bond length.

3.2. Electronic properties

The Figure 3 shows the total density of states (TDOS) and partial density of states (PDOS) of the orbitals that more contribute near the Fermi level of the interlayer most energetically favourable GaN/MnN/GaN. The interlayer exhibit a metallic behaviour due that of valence orbitals cross the Fermi level. This metallic behaviour it is determined by the states Mn-d in greater proportion and the states N-p in minor proportion. The interlayer has magnetic properties with a total magnetic moment

of $8\mu_\beta$/cell. This value in the magnetic moment value can understood as follows: the magnetic moments of $8\mu_\beta$/cell is due Mn^{3+} configuration, whose electronic configuration Mn^{3+}=:[Ar]$3d^4$; when the Mn atom is in the interlayer, the Mn atom gives three electrons. Then, the Mn atom remain four valence electrons (configuration d^4). These valence electrons couple ferromagnetically, as result the four electrons produce a total magnetic moment of $8\mu_\beta$/cell, as there are two Mn atoms in the supercell (see Figure 2(a)), each Mn atom contribute with $4\mu_\beta$/atom-Mn.

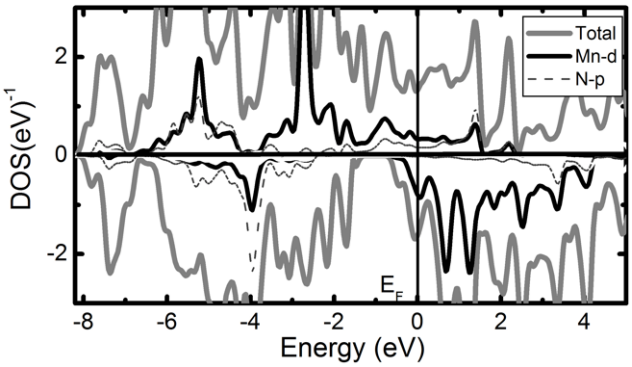

Figure 3. Total and partial density of state of GaN/MnN/GaN.

4. Conclusions

We executed a study of the GaN/MnN/GaN and MnN/GaN/MnN interlayers using the Density Functional Theory DFT in the frame pseudopotential. The total energy calculation reveal that the GaN/MnN/GaN interlayer is energetically most favourable that the MnN/GaN/MnN. The values of the bulk modules of interlayers are higher, which confirms that they are quite rigid, making them good candidates for possible applications in devices operated at high temperature and high power, as well as hard coatings. Analysis of the density of states show that the interlayers have metallic behaviour that comes essentially from the hybridization states Mn-d and N-p cross the Fermi level. The interlayers have magnetic properties with a magnetic moment of $8\mu_\beta$/cell. Due these properties the superlattices can be potentially used in the field of spintronics.

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