

Ab initio calculations of half-metallic ferromagnetism in $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices

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Abstract. We employed density functional theory (DFT) in order to study the electronic and magnetic properties of $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices, in the wurtzite structure. The calculations were carried out using the pseudopotential method, employed exactly as implemented in Quantum Espresso code. For the description of the electron-electron interaction, generalized gradient approximation (GGA) was used. We found that the superlattices exhibit a half-metallic ferromagnetic behaviour and all the superlattices have magnetic properties with a magnetic moment of $2\mu_B/\text{cell}$. Analysis of the density of states show that ferromagnetic behaviour of the superlattices can be explained by the strong hybridization between states V-d and N-p crossing of the Fermi level. Due these properties the superlattices can be potentially used in the field of spintronics or spin injectors.

1. Introduction

At the present time the understanding of magnetic behaviour of system with reduced dimensionality is one of the most important challenges in condensed matter physics, due the prospect of using the spin y developing devices in the field of spintronics. Spintronic devices use both the electrical charge and the spin of electrons to improve considerably the functionality of devices designed with conventional semiconductors [1–5]. For this reason, current research in spintronics is focused in the study of magnetic behaviour of new materials, for example, magnetic ordering of dopants in semiconductors, the magnetic properties of alloys formed by semiconductors with other compounds. Due potential applications in diluted magnetic semiconductors with high-temperature ferromagnetism, spin injectors, in magnetic memories or ultrahigh-density hard disks. Of particular interest are alloys with semiconductor having a half-metallic behaviour and have magnetic properties. This new materials one of the two spin channels is metallic and the other is semiconducting, leading to 100% spin polarization in the ground state at the Fermi level and can thus be used as spin injectors for magnetic random access memories or in other spin-dependent devices. This fact shows that it is worthwhile to carry out theoretical studies of $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices that will provide information on the structural, electronic, and magnetic properties of these superlattices and enable the design of new devices that will contribute to the development of current semiconductor technology.

2. Computational method

The calculations are performed within the DFT framework using the Quantum Espresso package [6]. The correlation and exchange effects of the electrons are treated using the generalized gradient



approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [7]. Electron-ion interactions were treated with the pseudopotential method [8,9]. The electron 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 6×6×4 Monkhorst-Pack mesh [10] was used to generate the k-points in the unit cell.

The calculations are performed taking into account the spin polarization due to the presence of the V atom. To calculate the lattice constant, the bulk modulus and the total energy of each studied superlattice, the calculated data are fitted with the Murnaghan equation of state, equation (1).

$$E(V) = E_0 + \frac{B_0 V}{B'_0} \left[\left(\frac{V_0}{V} \right)^{\frac{B'_0}{B'_0 - 1}} + 1 \right] - \frac{B_0 V_0}{B'_0 - 1} \quad (1)$$

Where B_0 is the bulk modulus and its first derivative is B'_0 , V_0 is the equilibrium volume of the cell, and E_0 is the total energy. The $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices were modeled according to special quasirandom structures approach [11] and the disorder aspects were ignored. The $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattice a hexagonal unit cell with alternating [0001] layers of (AlN, GaN and InN) and VN in conventional wurtzite structure was employed, as show the Figure 1. Where a and c are the lattice constants, u denotes the dimensionless parameter of the internal structure and the positions of the atoms are: for V or M (0,0,0), (1/3,2/3,1/2) and N (0,0, u), (1/3,2/3, $u+1/2$).

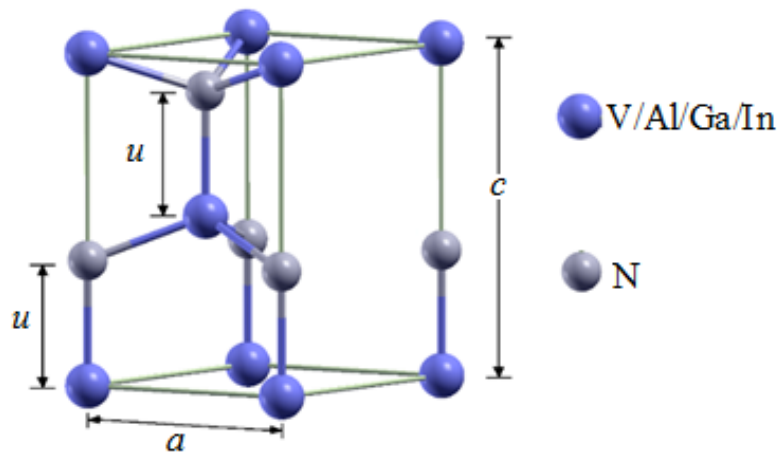


Figure 1. Unit cell $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices.

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 $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices, 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, Equation (1). Additionally, the total energy variation was calculated as a function of the volume of the ferromagnetic (FM) and antiferromagnetic (AFM) phases to find the most favourable magnetic phase of the superlattices. Figure 2 shows the energy-volume curves for $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices in the FM and AFM states.

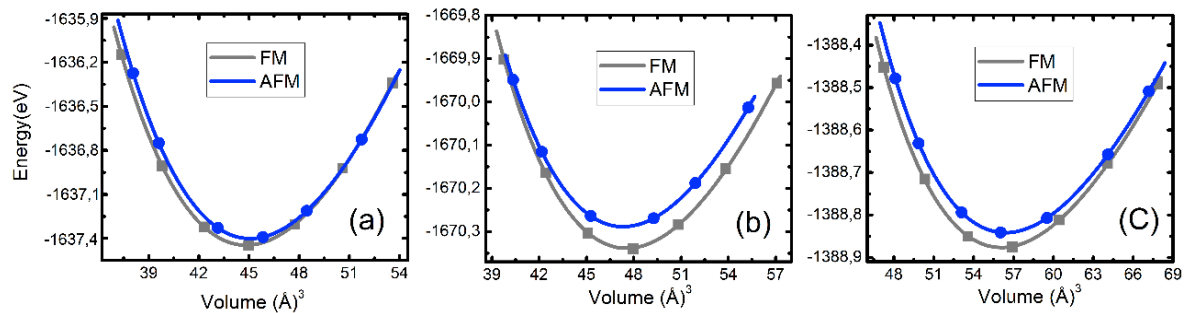


Figure 2. Total energy as a function of the volume of the superlattices (a) $(\text{VN})_1/(\text{AlN})_1$, (b) $(\text{VN})_1/(\text{GaN})_1$ (c) $(\text{VN})_1/(\text{InN})_1$ in the FM and AFM states.

In the ground state, the total energy differences between the FM and AFM states ($E = E_{\text{AFM}} - E_{\text{FM}}$) were -0.029, -0.051 and -0.043 eV for $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$, respectively. In the three cases, the FM state is more energetically favourable than the AFM state. Our results and other selected theoretical results are provided in Table 1.

Table 1. Structural parameters lattice constant (a_0), bulk modulus (B_0) and total energy (E_0) of the superlattices.

Superlattice	a_0 (Å)	c/a	V_0 (Å ³)	B_0 (GPa)	E_0 (eV)	μ (μ_B)
$(\text{VN})_1/(\text{AlN})_1$	3.171	1.628	44.82	174.87	-1637.44	~ 2.0
$(\text{VN})_1/(\text{GaN})_1$	3.227 3.267 ^a	1.631	47.41	176.07	-1670.33	~ 2.0
$(\text{VN})_1/(\text{InN})_1$	3.406	1.636	56.10	165.20	-1388.87	~ 2.0

^aTheoretical reference [12].

The calculated lattice constant for $(\text{VN})_1/(\text{GaN})_1$ accord well with theoretical value reported, since it differs by less than one percent. The values of the bulk modules of the superlattices 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. On the other hand, despite the difference in the crystalline structure between $(\text{VN})_1$ NaCl and $(\text{AlN})_1$, $(\text{GaN})_1$, $(\text{InN})_1$ wurtzite, joining of the layers of the VN with AlN, GaN and InN to form a superlattice had not change the AlN, GaN and InN wurtzite structure, as seen in Table 1 in the value of the c/a ratio of the superlattices, which are very close to the value ideal of the c/a (1.63) of AlN, GaN and InN in the wurtzite structure.

3.2. Electronic properties

Figure 3 shows the total and partial spin-polarized density of states of the $(\text{VN})_1/(\text{AlN})_1$, $(\text{VN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ superlattices. The Figure 3 shows that they are half-metallic and ferromagnetic; this result occurs because in the valence band close to the Fermi level, the majority spins (spin-up) are metallic, and the minority spins (spin-down) are semiconductors. These compounds have a spin polarization of 100% of the conduction carriers in the ground state, which is a requirement of the spin injectors [5].

This finding suggests that these ternary compounds can be efficiently used as spin injectors. Figure 3 shows that in the valence band near the Fermi level, the spin-up density (the majority spins) is mainly dominated by the V-3d states and, to a lesser extent, by the N-2p states, which cross the Fermi level. The magnetic properties comes essentially of the vanadium atom and is attributed at V^{3+} configuration, because the V atom is the superlattice gives three electrons, the V atom remain two

valence electrons (The electronic configurations $V^{3+}=[Ar]3d^2$). This valence electrons couple ferromagnetically, as result the two electrons produce a total magnetic moment of $2\mu_B/\text{atom-V}$.

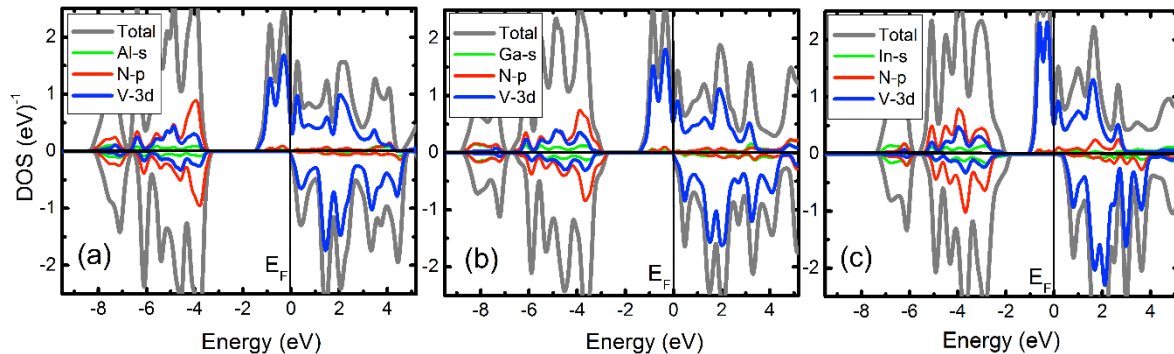


Figure 3. Total and partial density of state of (a) $(VN)_1/(AlN)_1$, (b) $(VN)_1/(GaN)_1$, (c) $(VN)_1/(InN)_1$ superlattices.

4. Conclusions

We reported first principles calculations to determine the structural, electronic, and magnetic $(VN)_1/(AlN)_1$, $(VN)_1/(GaN)_1$ and $(VN)_1/(InN)_1$ superlattices. The calculated values of the bulk modules are quite high; therefore, the superlattices are quite rigid, which makes them attractive for potential applications at high temperatures and for hard coatings. On the basis of the density of states, we found that the superlattices exhibit a half metallic behaviour, due to the orbital V- and N-p that cross the Fermi level. Finally, we found that $(VN)_1/(AlN)_1$, $(VN)_1/(GaN)_1$ and $(VN)_1/(InN)_1$ superlattices exhibit magnetic properties with magnetic moment $2\mu_B$. These properties show that superlattices are good candidates for possible applications in diluted magnetic semiconductors; spin injectors, and other spintronics applications.

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