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Calculation of the electronic and magnetic properties of VN/AlN/VN superlattice in the NaCl and wurtzite phases

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Abstract

We report results of first-principles total energy calculations within pseudopotential method with the generalized gradient approximations, to study the electronic and magnetic properties of VN/AlN/VN superlattice in the cubic (NaCl) and hexagonal (wurtzite) structures. The band structure and density states show that after relaxation process in NaCl phase the superlattice has a metallic behavior with a magnetic moment of 2.66 μ_β/cell. While in the wurtzite phase the superlattice has a half-metallic ferromagnetic character with a magnetic moment of 4.0 μ_β/cell. Hence, in wurtzite structure the superlattice is good candidate for potential applications in spintronic and as spin injectors.

Keywords: Density Functional Theory, electronic and magnetic properties, superlattice.

INTRODUCTIÓN

The transition metal nitrides, such as vanadium nitride (VN) has been studied extensively due to its excellent physical properties, as high rigidity, high resistance to wear and corrosion. The VN has been used as hard coating in cutting tools; the VN crystalizes in the cubic phase sodium chloride (NaCl) [1-6]. On the other hand, aluminum nitride AlN is direct band gap semiconductor material, this compound has very applications fields, such as optical devices, laser diodes, spintronics, injector spins and diluted magnetic semiconductors [6-12]. Actually, the theoretical and experimental studies there is a big interest in the study of the superlattices of the metal transition with semiconductor material, in order to improve the structural, electronic, and magnetic properties and get a new material with superior physical and chemical properties. In such way that, the superlattices have a better performance and a greater number of applications that the VN and AlN compound. In this paper we investigated the electronic and magnetic properties of the VN/AlN/VN superlattice in the NaCl and wurtzite phase, because these are respective ground state of the VN and AlN, respectively.

COMPUTATIONAL METHOD

In the framework of the density functional theory [13, 14] within pseudopotential method [15, 16] and using the Quantum ESPRESSO computational code [17], computational calculation was performed. The correlation and exchange interaction between electrons were included with the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [18]. 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 8x8x4 Monkhorst-Pack mesh [19] for a unit cell. To simulate VN/AlN/VN superlattice, we intercalated one VN layer and one AlN layer along the direction [001] for the NaCl and [0001] for wurtzite structure. For the binary VN and AlN compounds and VN/AlN/VN superlattice, we carry out a vc-relax-type calculation was performed. In this calculation all atoms in the supercell moved in the three directions. All calculations were carried out with spin polarization, in order to determine the presence of magnetic properties in the superlattice. 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

All the equilibrium structural parameter was calculated carry out the minimization process. For this, we performed a ve-relax calculation, in which the atoms of the supercell move in three directions and the same time the lattice constants the supercell are varying. First, we calculated the lattice constant and bulk modullus of the binary VN and AlN compounds, these calculated values were compared with data reported theoretical and experimentally. For AlN compound in the wurtzite structure, the values of the lattice constant and bulk modullus are 3.120 Å and 192.150 GPa, respectively. These values are in good agreement with other values 3.123 Å and 192.920 GPa reported theoretically [1, 2] and 3.110 Å and 185.00 GPa informed experimentally [3]. On the other hand, for VN compound we found 4.10 Å and 228 GPa by lattice constant and bulk modullus respectively. These results are in excellent agreement with the reported theoretical and experimental [4-6].

Now, we reported the main structural equilibrium parameter for the VN/AlN/VN superlattice. The lattice constant and bulk modullus of the superlattice in the NaCl structure are 2.989 Å

and 264.424 GPa, respectively. For the wurtzite phase the lattices constant is 3.142 Å and bulk modullus is 263.842 GPa. We note that in two structures (NaCl and wurtzite) the superlattice have more rigidity that the VN and AlN compounds, because have a larger bulk modullus than binary compounds. Hence, there is a improve in the structural properties in the new material.

Electronic Properties

The band structure and density states (DOS) along high symmetry path was calculated used the equilibrium lattice constant 2.989 Å for NaCl structure and 3.142 Å for wurtzite phase. Band structure of the superlattice in the NaCl phase is presented in figure 1. It is known that the AlN is a semiconductor material, the band structure show that due to the junction of the AlN monolayer with the VN monolayer, the AlN loses its semiconductor properties, the VN/AlN/VN superlattice have a metallic behavior. Because both the spin up and spin down cross the zero of the energy (the Fermi Level).

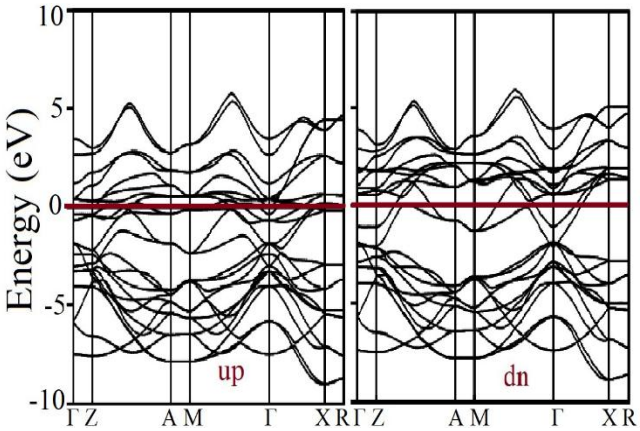

Figure 1. Band structure of VN/AlN/VN superlattice in the NaCl structure. Source: Authors.

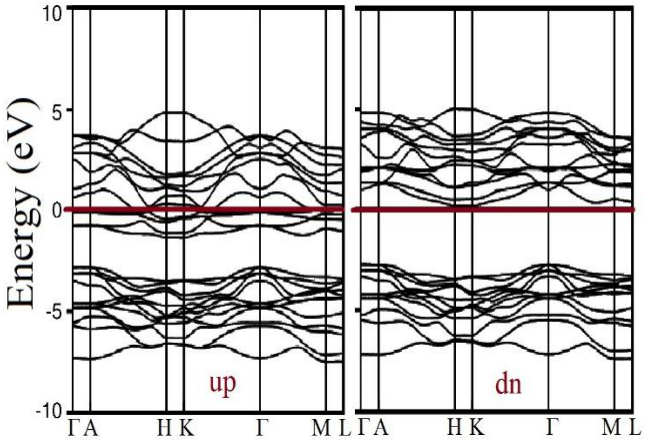

Figure 2. Band structure of VN/AlN/VN superlattice in the wurtzite structure. Source: Authors

The band structure of the superlattice in the wurtzite structure is show in the figure 2

In the wurtzite structure the AlN losses the semiconductor behavior once again. the VN/AlN/VN superlattice have a half-metallic behavior, because the spin up are metallic and spin down are semiconductors. In other words, the spin up channel cross the zero of the energy and spin down has a gap of 2.5 eV. In order to, determine the electronic orbitals that contribute to the behaviors in the two structures studied, we calculated the DOS.

The figure 3(a)-(b) show the DOS of the VN/AlN/VN superlattice in the NaCl and wurtzite phases, respectively.

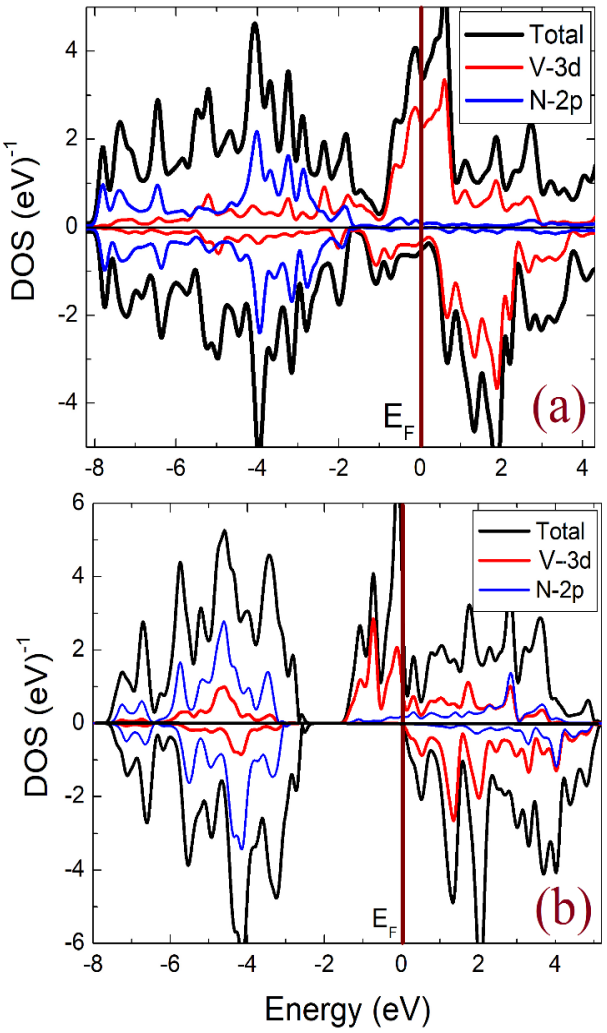

Figure 3. Total and partial density state of the VN/AlN/VN superlattice. (a) NaCl and (b) wurtzite structure. Source: Authors

The figure 3(a) show the total and partial DOS of the superlattice in the NaCl structure. The DOS confirm again that the superlattice have a metallic character. Additionally, we can see that the superlattice has a magnetic properties, because spin up channel is not symmetric with the spin down channel. The

superlattice has a magnetic moment of 2.66 μ_β/cell. On the other hand, the figure 3(b) show the DOS of the superlattice in the wurtzite structure. The DOS confirm once again that the superlattice have half-metallic character in the wurtzite structure. Being the spin up metallic and spin down semiconductor. The superlattice have magnetic properties with a value of magnetic moment of 4.0 μ_β/cell. The magnetic moment of the superlattice in the wurtzite structure is integer, this confirms for the last time that the superlattice in wurtzite structure is half-metallic. This magnetic property is first requirement for the superlattice to make good candidate for potential applications in spintronic and as spin injectors.

In the two structures studied here, the magnetic properties in the superlattice comes from the hybridization and polarization between metallic V-3d states and nonmetallic N-2p orbitals. The strong hybridization between V-3d and N-2p states, results in strong covalent bonding p-d, which is responsible of the high hardness of the VN/AlN/VN superlattice. Finally. We can see that the magnetic properties are mainly dominated by V-3d orbital with a minor contribution of N-2p orbitals.

CONCLUSIONS

In this paper, we calculated the structural, electronic and magnetic properties of VN/AlN/VN superlattice in the NaCl and wurtzite structures, using pseudopotential method within density functional theory. We found that the superlattice is more rigid than the VN and AlN compounds. because has a larger bulk modullus than binary compounds. Therefore, the superlattice could have a better performance as a hard coating. The band structure and density states calculation shows that, in the NaCl structure the superlattice has a metallic behavior with a magnetic moment of 2.66 μ_β/cell, while in the wurtzite structure the superlattice have a half-metallic ferromagnetic character, with a magnetic moment of 4.0 μ_β/cell. The magnetic properties come from the hybridization and polarization between of metallic V-3d states and nonmetallic N-2p orbitals. In the structure wurtzite, the superlattice to make good candidate for potential applications in spintronic, as spin injectors and other application in the diluted magnetic semiconductor field.

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