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Determination by means computational calculations the phase stability and structural properties of VN/AlN/VN compound

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Abstract

In this work we performed computational calculations using pseudopotential method within density functional theory and employing computational Quantum ESPRESO code, for study phase stability and the structural properties of the VN/AlN/VN interlayer. The calculations were carry out in the rock-salt (NaCl), cesium chloride (CsCl), nickel arsenide (NiAs), wurtzite and zincblende structures. We found that the most stable phase is the wurtzite because have the formation energy lowest, with a value of 0.997 eV/cell. In addition, at high pressure we predict a transition phase from wurtzite to NaCl, with a transition pressure of 6.7 GPa. We found that the bulk modullus of the interlayer is higher that bulk modullus of the AlN and VN compounds.

Keywords: DFT calculations, interlayer, structural and electronic properties, formation energy.

INTRODUCTIÓN

The aluminum nitride (AlN) is a semiconductor material of the group III-nitride, have a direct band gap of 6.1 eV [1, 2]. The AlN has superior physical properties, such as high melting point, high electrical resistivity, high thermal conductivity, mechanical stability, high resistance to corrosion and wear [3-4]. Additionally, due to its wide band gap has been used successfully by semiconductor industry [5], for example in laser diodes, optoelectronic devices, optical detectors, and micro-electronic devices working in the ultraviolet region [6-10]. Under normal condition the AlN crystallizes in the wurtzite structure. However, depending on the substrate and the growth conditions, NaCl phase can be formed. On the other hand, the vanadium nitride (VN) is a metallic material that crystalizes in NaCl structure [11]. Actually, there is very interest in the investigation of new materials for photon detector application. In particular, constructed with AlN y metal transition nitrides; some superconducting tunnel junctions has been successfully obtained. As the NbN/AlN/NbN it was grown by means magnetron sputtering technique [12] and recently, Nakayama *et al* [13] grown the TiN/AlN/TiN junction. In this paper, we did a study of structural properties of VN/AlN/VN interlayer, we determine de phase relative and calculated the formation energy.

COMPUTATIONAL METHOD

We performed first-principles calculations using pseudopotential [14, 15] method within the framework density functional theory (DFT) [16, 17] as implemented in the Quantum ESPRESSO computational code [18]. The correlation and exchange energies were included with the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [19]. For the expansion of the electronic function in plane waves, we used values of kinetic energy cutoff and charge density of 40 Ry and 400 Ry, respectively. Brillouin zone integrations were performed with the special k-point method using Monkhorst-Pack mesh method [20] for a unit cell. To simulate the VN/AlN/VN interlayer in the five phases, we intercalate two layers of AlN between two VN layers in the direction [001]. 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

The lattice constant, ratio c/a, bulk modullus, and total energy of the VN/AlN/VN interlayer in the CsCl, NaCl, NiAs, wurtzite and zincblende structures, were determinate fitting the calculated energy-volume values to the Murnaghan equation of state [21]. The figure 1 show the energy vs volume curves of the five structures considered in this paper.

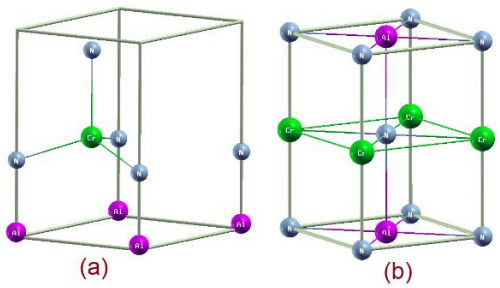

Figure 1. Total energy vs volume curves for CsCl, NaCl, NiAs, wurtzite, and zincblende structures. The points are the calculated values and the continuous curve is the fit. Source: Authors

As we can see in the figure 1, all structures studied in this paper are stable o metastable, because there is an energy local minimum in each energy-volume curve. We note that the wurtzite structure is the enterically most favorable, because it has the minimum energy value lowest. In addition, the curve of the wurtzite structure intersects with the NaCl phase of smallest equilibrium volume, because the lattices constant of the NaCl phase are smaller than those of wurtzite structure. Therefore, to high pressure there is a transition phase from wurtzite to NaCl phase. In order to determine the transition pressure value, the Gibbs free energy $G = E + PV - TS$ [22] was used. Since the calculations are made in the ground state ($T = 0°$ K), the term $TS = 0$, the Gibbs free energy reduces to $G = H = E + PV$, where H is the enthalpy, E is total energy, P is the pressure, and V in the volume. We used this equation for all structures considered in this investigation. The figure 2 illustrate the enthalpy vs pressure curves for wurtzite and NaCl phases. We observe that VN/AlN/VN interlayer will change from wurtzite structure to NaCl phase at a transition pressure of P_T = 6.7 GPa. Before transition pressure ($P < P_T$) the phase most stability correspond to wurtzite structure because have the lowest values of enthalpy, while after transition pressure ($P > P_T$), the most phase stability is NaCl structure because minor enthalpy.

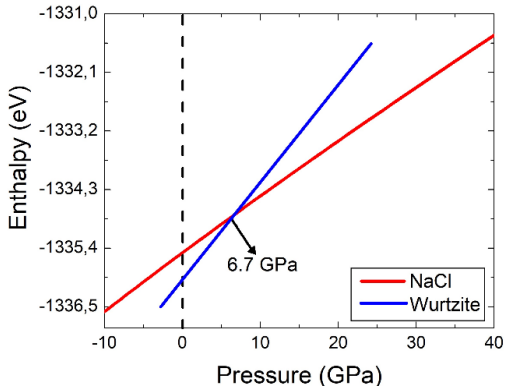

Figure 2. Enthalpy vs pressure for interlayer in the wurtzite (blue line) and NaCl (red line) phases. Source: Authors

The equilibrium parameters of the binary AlN and VN in the ground state, wurtzite and NaCl respectively, are listed in table 1 and are compared with available data reported experimental and theoretically for other authors.

Table 1: Lattice constant (a), ratio *c/a,* bulk modullus, and total energy in the ground state wurtzite and NaCl for AlN and VN, respectively.

	a_0 (Å)	c/a	B_0 (GPa)	E_0 (eV)
AlN	3.120 3.123[a] 3.110[c]	1.610 1.604[b] 1.601[c]	192.15 192.93[b] 185.00[c]	-1765.32
VN	4.10 4.06[c] 4.14[e]	-	228 233[d]	-2409.48

[a] [23] Theoretical reference [b] [24] Theoretical reference

[c] [25] experimental reference [c] [26] Theoretical reference

[d] [27] experimental reference [e] [28] experimental reference

We can see in the table 1 the vales of lattice constant and bulk modullus for VN and AlN compounds calculated here, are in good agreement with reported from other theoretical and experimental researchs. For VN the maximum discrepancies are ~ 0.97% and ~ 2.15%, respectively. While for AlN the lattice constant (3.12 Å) and bulk modulus (192.150 GPa) are in excellent agreement with previous theoretically and experimental work, being the maximum discrepancy of ~ 0.321% and ~ 3.90%, respectively. These discrepancies are smaller, which show the reliability of our present calculation.

Table 2. are listed lattice constant, c/a ratio, equilibrium volume, bulk modulus, and total energy of the VN/GaN/VN interlayer.

Table 2: Lattice constant, c/a ratio, equilibrium volume, bulk modulus, and total energy, of the VN/AlN/VN interlayer

Phase	a_0 (Å)	c/a	B_0 (GPa)	E_0 (eV)
CsCl	2.585	-	263.694	-1333.656
NaCl	2.989	$\sqrt{2}$	264.424	-1335.486
NiAs	2.809	1.810	260.794	-1335.278
Wurtzite	3.142	1.628	263.842	-1335.480
Zincblende	4.443	-	265.468	-1335.267

In the table 2, verify again that the most favorable phase for interlayer is the wurtzite structure, because has the minor value of the total energy. The wurtzite phase is most favorable than NaCl by an energy difference of 187 meV. In addition, we note that the bulk modullus of the interlayer (with an average value 263.644 GPa) is larger than the bulk modullus of AlN (192.15 GPa) and VN (228 GPa). We observe that in the five phases the value of the bulk modullus of the interlayer VN/AlN/VN is approximately the same (263.644 GPa in average), this happen because the bulk modullus is an intrinsic property of materials and does not depend on its size.

Finally, in order to check the energy stability of the multilayer we calculated the formation energy, which is defined as the difference between the total energy of the VN/AlN/VN interlayer, and the total energy of the binary compounds in their ground states, that is, VN in NaCl and AlN in wurtzite (E_{VN}^{NaCl} and $E_{AlN}^{Wurtzite}$, respectively); therefore, the energy of formation is given by [29-31]:

$$E_f = E_{VN/AlN/VN} - (1-x)E_{VN}^{NaCl} - xE_{AlN}^{Wurtzite} \quad (1)$$

In this case, the interlayer has two VN layers and two AlN layers, there is a concentration is 50-50, therefore, $x = 0.50$. The calculated values of formation for the interlayer in the five structures considered in this work a listed in the table 3.

Table 3: Formation energy

Compound	phase	E_f (eV)
VN/GaN/VN	CsCl	3.008
	NaCl	1.178
	NiAs	1.386
	Wurtzite	0.977
	Zincblende	1.397

The formation energy confirm again that wurtzite phase is the most favorable for the interlayer because has the formation energy value (0.977 eV) most lowest, being the CsCl the phase less favorable because has the highest formation energy with a value of 3.008 eV. The formation energy in the wurtzite phase is positive, hence is metastable, this finding implies that the interlayer cannot grow under equilibrium conditions, and therefore, it is necessary to supply energy to grow it. The moderate value 0.977 eV indicate that can be grown easily.

CONCLUSIONS

In summary, we studied the phase relative and structural properties of VN/AlN/VN interlayer in the CsCl, NaCl, NiAs, wurtzite, and zincblende structures, using computational calculation within of density functional theory. We found that the wurtzite is the most favorable crystallization phase with a formation energy of 0.977 eV/cell, the bulk modullus of the interlayer is high, most higher that the bulk modullus of the binary VN and AlN compounds, this indicate that the multilayer is quite rigid and could be used as hard coating.

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