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Ab-initio calculations of magnetic behavior in wurtzite $Al_xV_{1-x}N$ compound

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The density functional theory was employed in order to study the structural, electronic, and magnetic properties of the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compound in the wurtzite-type structure. The calculations were executed using the method based on pseudopotential, employed exactly as implemented in Quantum ESPRESSO code. For the description of the electron-electron interaction, generalized gradient approximation (GGA) was used. The analysis of the structural properties shows that the lattice constant increases with the concentration of Al atoms, but the functional relations are not linear. The electronic density studies show that the $Al_{0.25}V_{0.75}N$ and $Al_{0.50}V_{0.50}N$ compounds exhibit a half-metallic behavior, while $Al_{0.75}V_{0.25}N$ is metallic. This compound exhibits a ferromagnetic character with a magnetic moment of 2 μ_β/atom-V. The ground-state ferromagnetic behavior essentially comes from the polarization of the V-3d that crosses the Fermi level. These compounds are good candidates for potential applications in spintronics and as spin injectors.

Key words: Density functional theory (DFT), half-metallic ferromagnetism, structural and electronic properties.

INTRODUCTION

AlN stabilizes in the wurtzite (WZ) structure in bulk form (Nakamura et al., 1997). AlN, as the semiconductor material with the largest band-gap has many superior properties and thus is the best material for constructing devices in the violet region, and it is also used as an electronic packaging material, and is applied to optical disks and lithographic photo masks as well (Jonnard et al., 2004; Carcia et al., 1996; Carcia et al., 1997). Aluminium nitride exhibits stability at high temperatures, considerable thermal conductivity, low thermal expansion, and a high resistance to gases and chemicals (Beheshtian et al., 2012). Also, wurtzite AlN has the largest direct band gap, at 6.1 eV, as well as high acoustic velocity, which distinctly opens up the possibility of fabrication of various optical devices in the ultraviolet wave length region and different surface acoustic wave devices. Recently, Group III semiconductors such as AlN have received great attention because of their possible use as diluted magnetic semiconductors and their potential applications in the field of spintronics. For these applications, ferromagnetism at room temperature is a requirement. In recent years, high-temperature ferromagnetism has been reported by many researchers in several types of transition metal (TM)-doped

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semiconducting nitrides and oxides. Gonzalez et al. (2011) through theoretical studies, predict room-temperature ferromagnetism in p-type Mn-doped GaN (Gonzalez et al., 2011), while Vargas et al. (2015) observed half-metallic ferromagnetism behavior in $Zn_xMn_{1-x}O$ compounds. On the other hand, it has been reported that Sc-, Cr-, Co-, Mn-, Er-, Mg-, Ca- and Cu-doped AlN are ferromagnetic (FM) (Lei et al., 2009; Wu et al., 2007; 2003; Frazier et al., 2003; Yang et al., 2007; Dridi et al., 2011; Wu et al., 2006; Zhang et al., 2008; Huang et al., 2007). But investigations of AlN:V systems are rare, be they theoretical or experimental. For this reason, in this paper the authors present a systematic theoretical study of the structural, electronic and magnetic properties of the $Al_xV_{1-x}N$ compound.

COMPUTATIONAL METHODS

The calculations were carried out within the framework of density functional theory (DFT), as implemented in the Quantum ESPRESSO software package (Giannozzi et al., 2009). The exchange and correlation effects of the electrons were dealt with using the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) (Perdew et al., 1997). Electron–ion interactions were treated using the pseudopotential method (Vanderbilt, 1990; Laasonen et al., 1993). The electron wave functions were expanded into plane waves with a kinetic energy cutoff of 40 Ry. For the charge density, a kinetic energy cutoff of 400 Ry was used. A 6×6×4 Monkhorst-Pack mesh (Monkhorst and Pack, 1976) was used to generate the k-points in the unit cell. The calculations were performed taking into account the spin polarization. Self-consistency was achieved by requiring that the convergence of the total energy be less than 10^{-4} Ry.

To calculate the lattice constant, the minimum volume, the bulk modulus, and the cohesive energy in the wurtzite structure, calculations were fit to the Murnaghan equation of state (Murnaghan, 1944) (Equation 1):

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

Where B_0 is the bulk modulus, its first derivative is B'_0, V_0 is the equilibrium volume of the cell, E_0 represents the ground-state total energy and V is the volume of the unit cell.

RESULTS AND DISCUSSION

Structural properties

To determine the structural properties in the ground state, such as the lattice constant (a_0), equilibrium volume (V_0), bulk modulus (B_0), and total energy (E_0) of the binary compounds AlN and VN and of the three allowed ternary compounds, $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75), 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 in order to find the most favorable magnetic phase of the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compounds. In order to calculate the most favorable AFM structure, the authors using various AFM configuration, for this purpose, the supercells of 1×1×1 (for $Al_{0.50}V_{0.50}N$) and 1×1×2 (for $Al_{0.25}V_{0.75}N$ and $Al_{0.75}V_{0.25}N$) were used to get even numbers of V atom for switching spin state up and down. Figure 1 shows the energy-volume curves for $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compounds in the FM and AFM states. In the ground state, the total energy differences between the FM and AFM states ($\Delta E = E_{FM} - E_{AFM}$) were -0.11, -0.014, and -0.05 eV for x=0.25, 0.50, and 0.75, respectively. In all cases, the FM state was more energetically favorable than the AFM state.

The authors can see that the equilibrium lattice constant a_0 of the binary AlN compound calculated in this paper are in very good agreement with the values reported theoretically and experimentally, since they differ by less than one percent. For the allowed ternary compounds of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75), the structures are obtained by replacing Al atoms with V atoms in the AlN supercell. For x=0.25 and x=0.50, an Al atom is replaced by a V atom in supercells of 8 and 4 atoms, respectively. For x=0.75, three Al atoms are replaced by three V atoms in a supercell of 8 atoms. Figure 2 shows the crystal structure of the allowed ternary compounds, $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75), obtained after the structural relaxation; in all cases, the space group obtained is the tetragonal structure p3 m1 (N° 156).

The authors observe that VN has a larger bulk modulus than the AlN, and the bulk modulus of the $Al_xV_{1-x}N$ compound decreases as the concentration Al increases. However, the values of the bulk moduli of the allowed ternary compounds of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) shown in Table 1 are high, confirming that they are quite rigid, making them good candidates for possible applications in devices operated at high temperature and high power as well as in hard coatings.

Table 1 shows that the equilibrium lattice constant value increases with an increase in the concentration of Al atoms. But the increase in the lattice constant is small, resulted from the minor difference in atomic radius between V (1.34 Å) and Al (1.43 Å). Figure 3 shows the variation of the lattice constant as a function of the Al concentration. It can be observed that the variation in the lattice parameter versus Al composition is nonlinear. A strong deviation from Vegard's law is clearly visible for the equilibrium lattice constants a_0, since there is an upward bowing. This deviation indicates a strong interaction between the ions of V and Al. A similar result was found by Boukra et al. (2010) in their study of

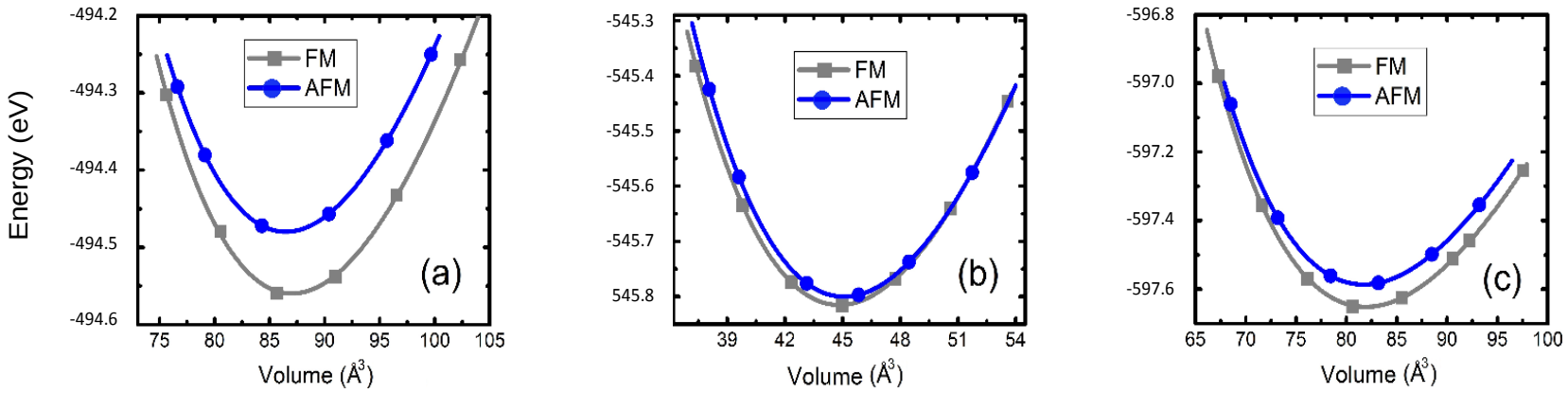

Figure 1. Total energy as a function of volume for (a) $Al_{0.25}V_{0.75}N$, (b) $Al_{0.50}V_{0.50}N$, and (c) $Al_{0.75}V_{0.25}N$ compounds.

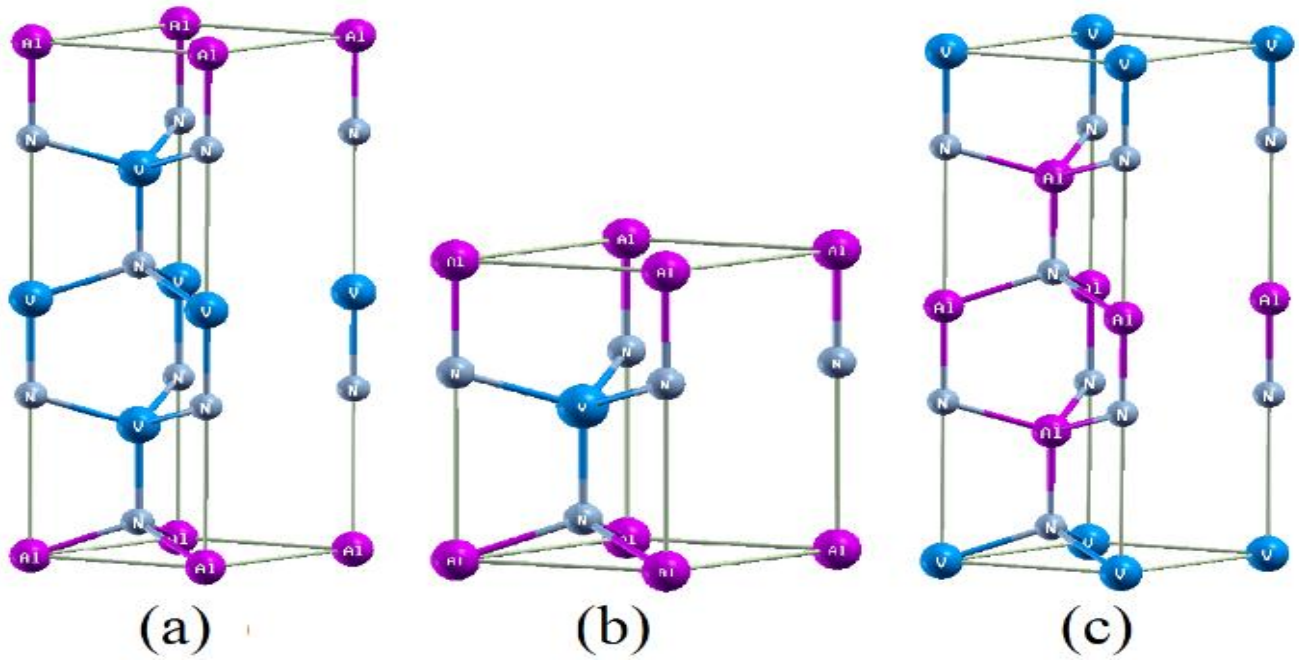

Figure 2. Unit cell of the allowed ternary compounds: (a) $Al_{0.25}V_{0.75}N$, (b) $Al_{0.50}V_{0.50}N$ (c) $Al_{0.75}V_{0.25}N$.

Table 1. Lattice constant (a_0), equilibrium volume (V_0), bulk modulus (B_0), and total energy (E_0) of the binary compounds AlN and VN and of the three allowed ternary compounds, $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75), in the wurtzite structure.

Compound	a_0 (Å)	V_0 (Å^3)	B_0 (GPa)	E_0 (eV)
VN	3.092	44.083	232.564	- 648.837
$Al_{0.25}V_{0.75}N$	3.107	81.917	224.544	- 597.140
$Al_{0.50}V_{0.50}N$	3.118	44.828	209.350	- 545.815
$Al_{0.75}V_{0.25}N$	3.126	87.020	198.170	- 494.559
AlN	3.130	42.217	193.450	- 443.331
Other calculations				
VN	3.10[a]	-	209[a]	-
AlN	3.123[b]	-	192[b]	-
	3.111[c]	-	185[c]	-

a (Gonzalez et al., 2007) theoretical, b (Warner et al., 2002) Theoretical, c (Schulz et al., 1997) Experimental

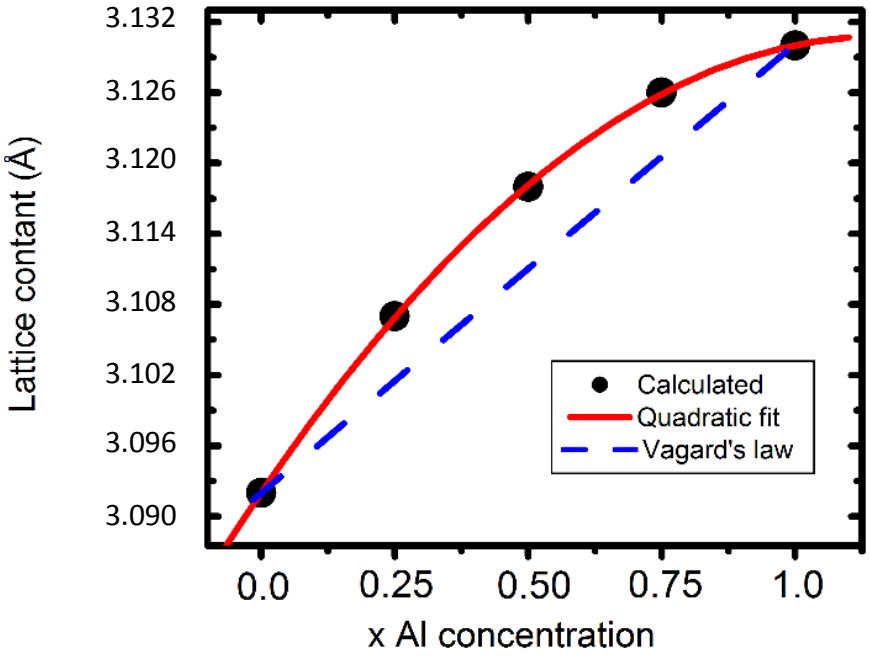

Figure 3. Lattice constant as a function of Al-concentrations.

$Ga_xMn_{1-x}N$ ternary systems using DFT.

In this case, the lattice constant of the $Al_xV_{1-x}N$ (x=0.25, 0.50 and 0.75) ternary compounds seems to obey a quadratic trend. To verify this dependence, the author carried out a fit to a quadratic polynomial and found that the relation between the lattice constant and the concentration x of Al is: $a_{AlxV1-xN}=xa_{AlN}+(1-x)a_{VN}-x(1-x)b$, where a_{AlN} and a_{VN} are shown in Table 1, and b=-0.019 Å.

In order to verify the relative stability of the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compounds with reference to the terminal phases, the author calculated the corresponding formation energy, which is expressed as the difference between the total energy of the ternary $Al_xV_{1-x}N$ phases, $E^{phase}_{Al_xV_{1-x}N}$ and of the references states of wurtzite AlN, $E^{wurtzite}_{AlN}$ and NaCl of VN, E^{NaCl}_{VN} (Zhang and Veprek, 2007; Sheng et al., 2008):

$$E_f = E^{phase}_{Al_xV_{1-x}N} - xE^{wurtzita}_{AlN} - (1-x)E^{NaCl}_{VN}$$

Table 2 shows the energy of formation values of the allowed ternary compounds of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75). The E_0 energies of the binary compounds AlN and

Table 2. Energy of formation of the allowed ternary compounds of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75).

Compound	E_f (eV)
$Al_{0.25}V_{0.75}N$	0.320
$Al_{0.50}V_{0.50}N$	0.270
$Al_{0.75}V_{0.25}N$	0.148

VN in their ground states are negative (Table 1). However, according to the results of Table 2, the value of the energy of formation of each ternary compound is positive; therefore, the $Al_xV_{1-x}N$ compounds (x=0.25, 0.50, and 0.75) are metastable. This finding implies that the compounds cannot grow under equilibrium conditions, and therefore it is necessary to supply energy in order to grow them (Zhang and Veprek, 2007; Sheng et al., 2008). The results obtained for the energy of formation is important, because by knowing these values the growth conditions can be improved in order to enable one to grow good-quality $Al_xV_{1-x}N$ compounds (x=0.25, 0.50, and 0.75).

According to the results of Table 2, the smallest value of the energy of formation corresponds to the $Al_{0.75}V_{0.25}N$ ternary compound; therefore, this is the most energetically stable structure. Additionally, the moderate formation-energy values indicate that the compounds can easily be grown experimentally. The fact that $Al_{0.75}V_{0.25}N$ compound has the lowest formation energy can be understood as follows; the ground state energy of the binary compound VN is smaller than the AlN, due that the VN has more electrons. For this reason, Table 1 shows the ground state energy of the ternary compounds $Al_xV_{1-x}N$ increases with increasing the concentration of Al atoms and therefore the energy of formation of the $Al_{0.75}V_{0.25}N$ ternary compound is the most lowest.

Electronic properties

Figures 4a, b, and c show the total density of states (TDOS) and partial density of states (PDOS) of the orbitals that contribute most near the Fermi level of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compounds, respectively. The TDOS of the allowed ternary compounds $Al_{0.25}V_{0.75}N$ and $Al_{0.50}V_{0.50}N$ (Figures 4a and b) 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 for spin injectors (Vargas et al., 2015). This finding suggests that these ternary compounds can be efficiently used as spin injectors. Figure 4c shows the TDOS of the $Al_{0.75}V_{0.25}N$ compound. It is clear that this ternary compound does not exhibit half-metallicity. Since the valence and conduction bands cross the Fermi level, $Al_{0.75}V_{0.25}N$ has a metallic character.

As seen in Figure 4, for the ternary compounds in the valence band near the Fermi level, the spin-up density (the majority spins) is mainly dominated by the V-3d states, with a small contribution of the N-2p states, which cross the Fermi level. Therefore, the magnetic properties of the ternary compounds essentially come from the polarization of the V-3d orbital.

In order to fully understand the mechanism by which the FM state in the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compound is stabilized; the authors can explain it with the help of the density of states. It can clearly be seen that when the V atom occupies the position of the Al atom in the wurtzite-type supercell, it introduces new states in the energy gap of the AlN semiconductor, resulting in a half-metallic character for $Al_{0.25}V_{0.75}N$ and $Al_{0.50}V_{0.50}N$ and a metallic one for the $Al_{0.75}V_{0.25}N$ compound. The tetrahedral crystal field of the surrounding N ligands splits the fivefold degenerate V-3d states into two-fold degenerate low-energy e_g(d_{z^2} and $d_{x^2-y^2}$) and three-fold degenerate high-energy t_{2g} (d_{xy}, d_{xz} and d_{yz}) states. The electron configuration of the V atom in the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) compounds can be attributed to the V^{3+} (Katayama et al., 2003). Therefore, V atoms have three valence electrons {[Ar]$3d^3$}; two electrons occupy the doubly degenerate e_g states and one electron and two holes the triply degenerate t_{2g} state. Therefore, the major spin states of V-3d are not filled, because although the doubly-degenerate state is completely filled, the triply-degenerate state is only one-third full. As a result, the three electrons produce a total magnetic moment of $2\mu_\beta$/atom-V. This implies that the magnetic moment has a value of μ=2 μ_β for one V atom present in the compounds $Al_{0.50}V_{0.50}N$ and $Al_{0.75}V_{0.25}N$, while μ=6 μ_β for three V atoms in $Al_{0.25}V_{0.75}N$ compound.

Figure 5 shows the band structures of the $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) ternary compounds. For x=0.25 and 0.50 ($Al_{0.25}V_{0.75}N$ and $Al_{0.50}V_{0.50}N$), Figures 5a and b confirm the half-metallic nature of both compounds, while Figure 5c confirms the metallic character of $Al_{0.75}V_{0.25}N$.

In Figure 5, it can seen that the spin-up orientation of the $Al_{0.25}V_{0.75}N$, $Al_{0.50}V_{0.50}N$ and $Al_{0.75}V_{0.25}N$ compounds exhibits dispersed bands above Fermi level; this confirm that the majority spin-up of V-3d is partially filled, and therefore, the fact that there is high polarization of the

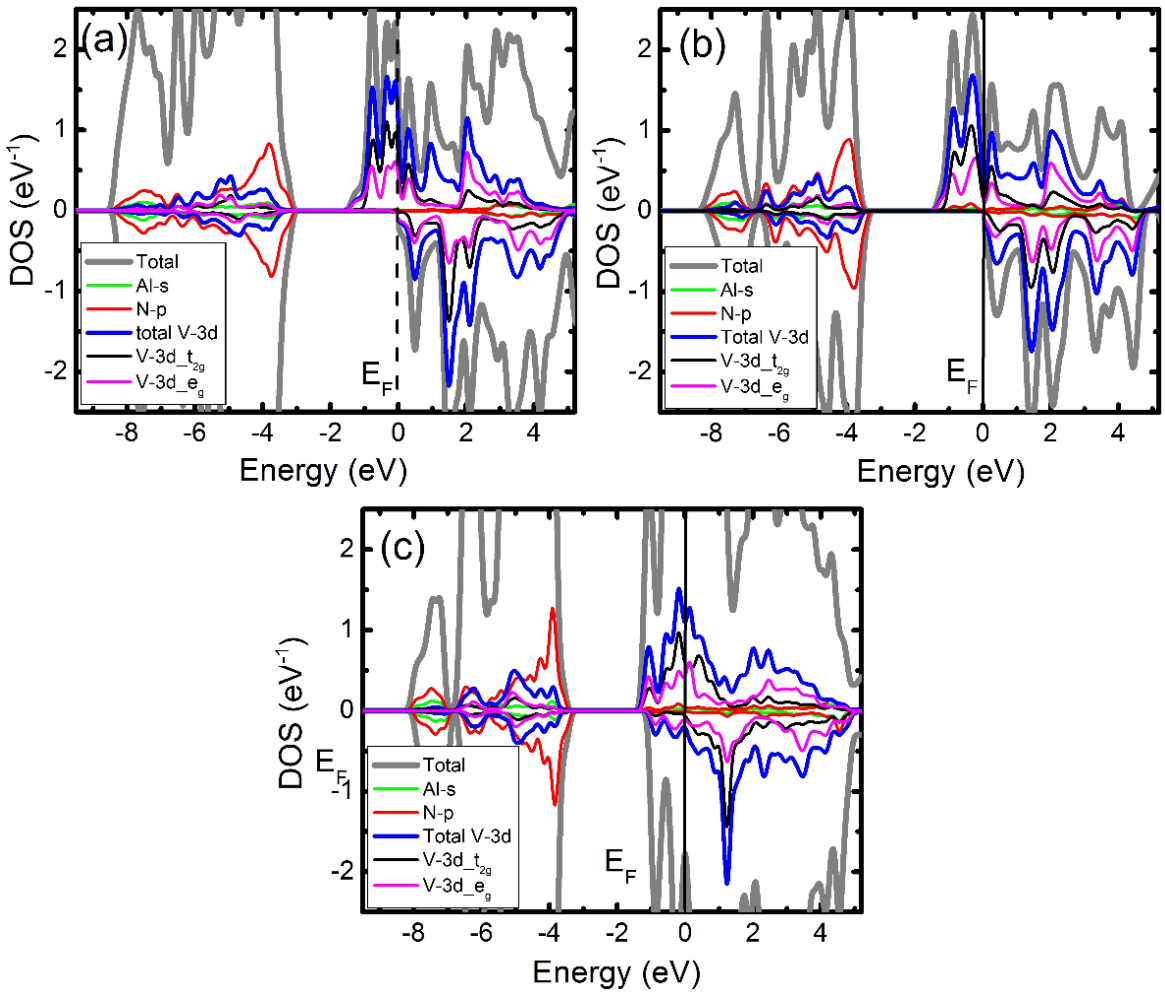

Figure 4. Total and partial density of states of the allowed ternary compounds of $Al_xV_{1-x}N$. (a) x = 0.25 (b) x = 0.50, and (c) x = 0.75.

conduction carriers is confirmed by the fact that the V atoms are coupling ferromagnetically and that there is a high presence of conduction carriers in the majority spin channel. For these reasons, these compounds can be potentially used in spintronics or spin injectors.

Conclusions

The authors report theoretical studies of the structural, electronic, and magnetic properties of $Al_xV_{1-x}N$ compounds, with concentrations of Al atoms x=0.0, 0.25, 0.50, 0.75, and 1.0, by means of first-principles calculations via the pseudopotential method, within the DFT framework and using the GGA approximation. It was found that the lattice constant increases with the concentration x of Al atoms, obeying a quadratic dependence. It was found that the values of the bulk modulus of $Al_xV_{1-x}N$ (x=0.25, 0.50, and 0.75) are high; therefore, these compounds are rigid and are good candidates for application in devices that must function at high temperatures and under high power, and in hard coatings. In addition, it was found that the allowed compounds $Al_{0.25}V_{0.75}N$ and $Al_{0.50}V_{0.50}N$ exhibit a half-metallic behavior with a magnetic moment of 2 μβ/atom-V. The ground-state ferromagnetic behavior essentially comes from the polarization of the V-3d that crosses the Fermi level. These compounds are good candidates for potential applications in spintronics and as spin injectors.

Conflict of Interest

The authors do not declare any conflict of interest.

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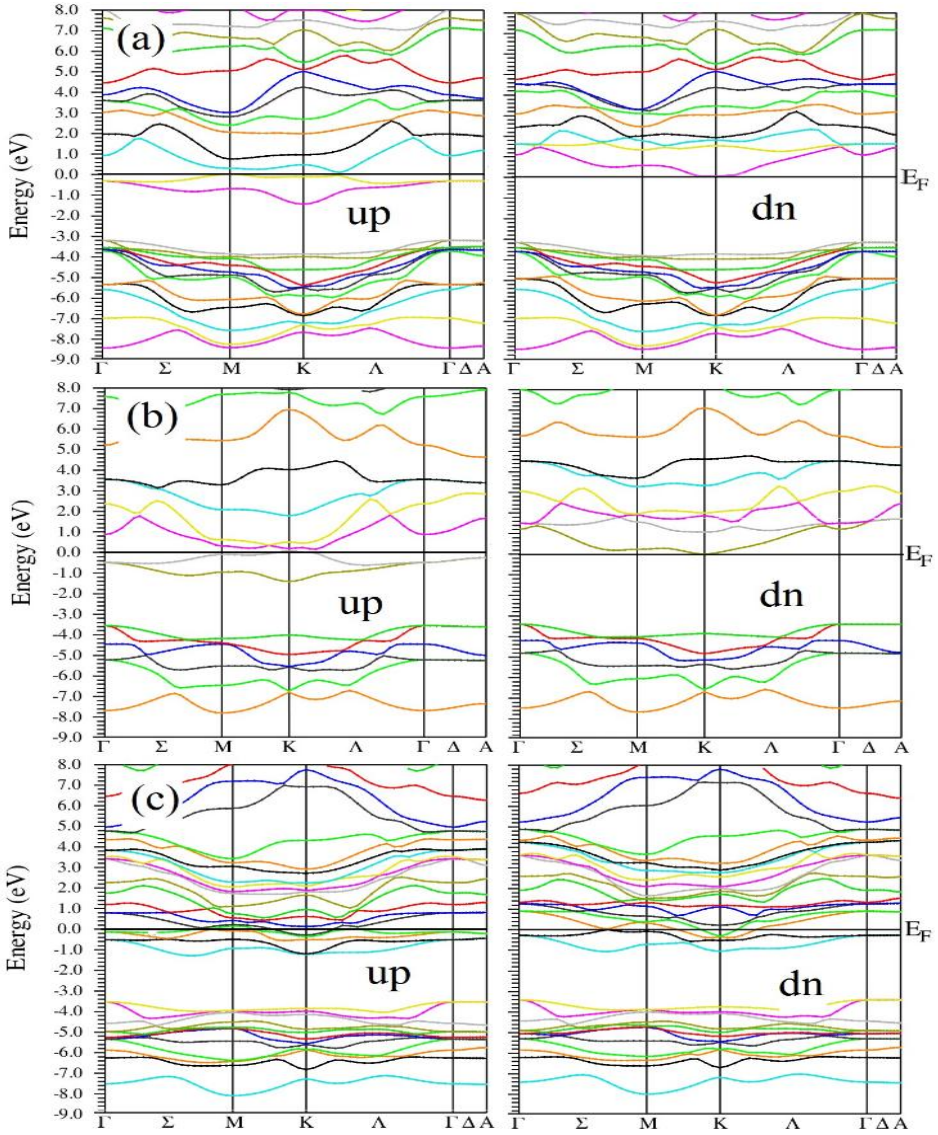

Figure 5. Band structure of allowed ternary compounds of $Al_xV_{1-x}N$. (a) x = 0.25 (b) x = 0.50, and (c) x = 0.75.

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REFERENCES

Beheshtian J, Baei MT, Bagheri Z, Peyghan AA (2012). AlN nanotube as a potential electronic sensor for nitrogen dioxide. Microelectron. J. 43(7):452-455. http://dx.doi:10.1016/j.mejo.2012.04.002

Boukra A, Zaoui A, Ferhat M (2010). Magnetic trends in $Ga_xMn_{1-x}N$, $Al_xMn_{1-x}N$, and $In_xMn_{1-x}N$ ternary systems: A first-principles study. J. Appl. Phys. 108:123904. http://dx.doi.org/10.1063/1.3524049

Carcia PF, French RH, Reilly ML, Lemon MF, Jones DJ (1997). Optical superlattices a strategy for designing phase-shift masks for photolithography at 248 and 193 nm: Application to AlN/CrN. Appl. Phys. Lett. 70:2371. http://dx.10.1063/1.118876

Carcia PF, French RH, Sharp K, Meth JS, Smith BW (1996). Materials screening for attenuating embedded phase-shift photoblanks for DUV and 193-nm photolithography. Proc. SPIE-Int. Soc. Opt. Eng. 2884:255-260. http://dx.doi.org/10.1117/12.262809

Dridi Z, Lazreg A, Bouhafs B (2011). First-principles study of electronic structure and magnetism of cubic $Al_{1-x}Er_xN$ using the LSDA+U approach. J. Magn. Magn. Mater. 323(9):1174-1178. http://dx.doi:10.1016/j.jmmm.2010.12.039

Frazier RM, Stepleton J, Thaler GT, Abernathy CR, Pearton SL, Rairigh R, Kelly J, Hebard AF, Nakarmi ML, Nam KB, Lin JY, Jiang HX, Zavada JM, Wilson RG (2003). Properties of Co-, Cr-, or Mn-implanted AlN. J. Appl. Phys. 94(3):1592. http://dx.10.1063/1.1586987

Giannozzi P, Baroni S, Bonin N (2009). QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. J. Phys. Condens. Matter 21(39):395502. http:dx.doi:10.1088/0953-8984/21/39/395502

Gonzalez N, Majewski JA, Dietl T (2011). Aggregation and magnetism of Cr, Mn, and Fe cations in GaN. Phys. Rev. B 83:184417. http://dx.doi.org/10.1103/PhysRevB.83.184417

González R, López W, Rodríguez J (2007). AB initio studies of the structural and electronics properties of vanadium nitride. J. Ciencia

e Ingeniería Neogranadina 17(1):23-33. http://www.umng.edu.co/web/revistas/revistas-fac.ingenieria/revista-ciencia-e-ingenieria-neogranadina/revista-vol.-17-no.-1

Jonnard P, Capron N, Semond F, Massies J, Martinez-Guerrero E, Mariette H (2004). Electronic structure of wurtzite and zinc-blende AlN. Eur. Phys. J. B 42(3):351-359. http://dx.10.1140/epjb/e2004-00390-7

Katayama H, Sato K (2003). Spin and charge control method of ternary II-VI and III-Vmagnetic semiconductors for spintronics: theory vs. esperiment. J. Phys. Chem. Sol. 64:1447-1452-544. http://dx.10.1016/S0022-3697(03)00126-4

Laasonen K, Pasquarello A, Car R, Lee C, Vanderbilt D (1993). Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. Phys. Rev. B. 47:10142. http://dx.doi.org/10.1103/PhysRevB.47.10142

Lei WW, Liu D, Zhu PW, Chen XH, Zhao Q, Wen GH, Cui QL, Zou GT (2009). Ferromagnetic Sc-doped AlN sixfold-symmetrical hierarchical nanostructures. Appl. Phys. Lett. 95:162501. http://dx.doi.org/10.1063/1.3248257

Monkhorst HJ, Pack JD, (1976). Special points for Brillouin-zone integrations. Phys. Rev. B. 13(12):5188-5192. http://dx.doi.org/10.1103/PhysRevB.13.5188

Murnaghan FD (1944). The compressibility of media under pressure. Proceedings of the National Academy Science U.S.A. 30(9):244-247. http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1078704/

Nakamura S, Senoh M, Nagahama S, Iwasa N, Yamada T, Matsushita T, Sugimoto Y, Kikoyu J (1997). High-Power, Long-Lifetime InGaN Multi-Quantum-Well-Structure Laser Diodes. Jpn. J. Appl. Phys. 36(8B):L1059. http://dx.doi:10.1143/JJAP.36.L1059

Perdew J, Burke K, Ernzerhof M (1997). Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 77(18):3865-3868. http://dx.doi.org/10.1103/PhysRevLett.77.3865

Schulz H, Thieman KH (1977). Crystal structure refinement of AlN and GaN. Solid State Communication 23(11):815-819. http://dx.10.1016/0038-1098(77)90959-0.

Sheng SH, Zhang RF, Veprek S (2008). Phase stabilities and thermal decomposition in the $Zr_{1-x}Al_xN$ system studied by ab initio calculation and thermodynamic modeling. Acta Materialia 56(5):968-976. http://dx.doi.org/10.1016/j.actamat.2007.10.050

Vanderbilt D (1990). Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. Phys. Rev. B. 41:7892(R). http://dx.doi.org/10.1103/PhysRevB.41.7892

Vargas C, Espitia-Rico M, Báez Cruz R (2015). Half-metallic ferromagnetism of $Zn_xMn_{1-x}O$ compounds: A first-principles study. Comput. Condens. Matter 4:1-5. http://dx.doi:10.1016/j.cocom.2015.04.001

Warner JM, Bechstedt F (2002). Properties of strained wurtzite GaN and AlN: Ab initio studies. Phys. Rev. B 66:115202. http://dx.doi.org/10.1103/PhysRevB.66.115202

Wu QY, Huang ZQ, Wu R, Chen LJ (2007). Cu-doped AlN: a dilute magnetic semiconductor free of magnetic cations from first-principles study. J. Phys. Condens. Matter 19(5):056209. http://dx.doi:10.1088/0953-8984/19/5/056209

Wu RQ, Peng GW, Liu L, Feng YP, Huang ZG, Wu QY (2006). Ferromagnetism in Mg-doped AlN from ab initio study. Appl. Phys. Lett. 89:142501. http://dx.doi.org/10.1063/1.2358818

Wu SY, Liu HX, Gu L, Singh RK, Budd L, Schilfgaarde M, McCartney MR, Smith DJ, Newman N (2003). Synthesis, characterization and modeling of high quality ferromagnetic Cr-doped AlN thin films. Appl. Phys. Lett. 82:3047. http://dx.10.1063/1.1570521

Yang Y, Zhao Q, Zhang XZ, Liu ZG, Zou CX, Shen B, Yu DP (2007). Mn-doped AlN nanowires with room temperature ferromagnetic ordering. Appl. Phys. Lett. 90:092118. http://dx.doi.org/10.1063/1.2475276

Zhang RF, Veprek S (2007). Phase stabilities and spinodal decomposition in the $Cr_{1-x}Al_xN$ system studied by ab initio LDA and thermodynamic modeling: Comparison with the $Ti_{1-x}Al_xN$ and TiN/Si_3N_4 systems. Acta Mater. 55(14):4615-4619. http://dx.doi.org/10.1016/j.actamat.2007.04.029

Zhang Y, Liu W, Liang P, Niu HB (2008). Half-metallic ferromagnetism in Ca-doped AlN from first-principles study. Sol. State Commun. 147(7-8):254-257. Http://dx.doi:10.1016/j.ssc.2008.06.008