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Magnetic behavior in AlxCr1-xN ternary system: a computational calculation

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Abstract

Computational calculations based on density functional theory were used to study the structural, electronic, and magnetic properties of the $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ in the wurtzite phase. The calculations were carried out by means of the pseudopotential method, employing computational Quantum Wien2k package. We found that the variation of the lattice constant with respect to Al concertation follow the Vegard's low. In addition, the density states reveal that three compounds have a metallic ferromagnetic behavior, with a total magnetic moment of total 9.25 μ_β/cell, 3.35 μ_β/cell, and 3.15 μ_β/cell, respectively. This magnetic behavior is mainly dominated by 3d-Cr orbital with a minor contribution of 2p-N orbitals.

Keywords: Density Functional Theory, structural and electronic properties, formation energy.

INTRODUCTIÓN

The aluminum nitride (AlN) is a direct band-gap semiconductor material, among the all group III-nitrides, AlN have the widest band gap in the wurtzite structure ~ 6.2 eV [1]. The AlN has an unusual combination of several exceptional physical and chemical properties such as high thermal conductivity, high electrical resistivity, high melting point, large bulk modulus, mechanical stability, high resistance to corrosion and wear [3-4]. In addition, due to its wide band gap is amply used by semiconductor industry [5] in optoelectronic devices, laser diodes, and optical detectors, micro-electronic devices working in the ultraviolet region and under high temperature conditions [6-10]. Actually, the investigation is focused in the AlN-MT (metal transition) system, due to its potential use as diluted magnetic semiconductor material (DMS), spin injector and other applications in spintronic devices. For these applications is very important the understanding of electronic and magnetic behavior of material. For these reasons in this work we study by means density functional theory calculations, we determine de magnetic behavior of the ternary $Al_xCr_{1-x}N$ compounds (x = 0.25, 050, 0.75) in the wurtzite structure in order to stablish whether $Al_xCr_{1-x}N$ compound is a good DMS.

COMPUTATIONAL METHOD

We performed *ab*-initio calculations using full-potential linearized augmented plane wave (FP-LAPW) method within the framework density functional theory (DFT) [11, 12] as implemented in the Wien2k computational code [13]. The correlation and exchange energies were included with the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [14]. The basis function was expanded up to cutoff parameter of $R_{MT}*K_{max} = 8$ (R_{MT} is the smallest radius of the atomic level within the unit cell and K_{max} is the magnitude of the largest *k* vector of the reciprocal lattice). Brillouin zone integrations were performed with the special k-point method over a 140 Monkhorst-Pack mesh [15]. For the expansion of the potential in the interstitial region between muff-tin spheres, $G_{max} = 12$ was considered. The spherical harmonics for the charge density was expand up to $l_{max} = 10$ inside the atomic spheres. The radii muff-tin of the atoms were 1.6, 1.8, and 2.0 bohr, for N, Al, and Cr respectively. All the calculations were performed with spin polarization. To simulate the ternary wurtzite alloys, we employ 8-atoms supercell for $Al_{0,25}Cr_{0.75}N$ and $Al_{0,75}Cr_{0.25}N$, corresponding to 1x1x2 conventional wurtzite cell, while the $Al_{0,50}Cr_{0.50}N$ we are using the 4-atoms supercell, corresponding to 1x1x1 conventional wurtzite cell, as show fig. 1. 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.

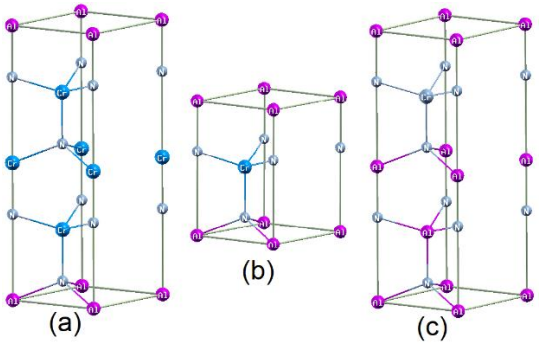

Figure 1. Supercell used for the allowed ternary compounds (a) $Al_{0,25}Cr_{0.75}N$, (b) $Al_{0,50}Cr_{0.50}N$, and (c) $Al_{0,75}Cr_{0.25}N$. Source: Authors

RESULTS AND DISCUSSIONS

Structural properties

To calculate the equilibrium structural parameters such as lattice constant, bulk modullus and total energy of the binary compounds AlN and CrN and the ternary $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds, the values energy-volume obtained after the relaxation process were fitted to the Murnaghan equation of state [16]. The equilibrium parameters are presented in table 1. For the binary AlN and CrN compounds the lattice constant and bulk modullus calculated here are compared with the available data experimental and theoretical.

Table 1. Lattice constant (*a*), ratio c/*a*, and bulk modullus

Compound	*a*(Å)	*c/a*	B_0 (GPa)
AlN	2.120 3.123[a] 3.110[c]	1.610 1.604[b] 1.601[c]	192.15 192.93[b] 185.00[c]
$Al_{0,25}Cr_{0.75}N$	3.1314	3.261	182.45
$Al_{0,50}Cr_{0.50}N$	3.1451	1.636	186.67
$Al_{0.75}Cr_{0.25}N$	3.1591	3.271	189.15
CrN	4.16 4,13[d] 4.08[e] 4,15[f(exp)]	-	308 310[d]

[a] [17] Theoretical reference

[b] [4] Theoretical reference

[c] [18] experimental reference

[d] [19] Theoretical reference

[e] [20] Theoretical reference

[f] [21] experimental reference

We can see in the table 1 the calculated lattice constant and bulk modulus for AlN are in good agreement with obtained from other theoretical and experimental studies, because the maximum discrepancies are ~ 0.32% and ~ 3.86%, respectively. While for CrN the lattice constant (4.16 Å) and bulk modulus (308 GPa) are in excellent agreement with previous theoretically and experimental work, being the maximum discrepancy of ~ 1.9% and ~ 0.65%, respectively. These discrepancies are smaller, which show the reliability of our present calculation.

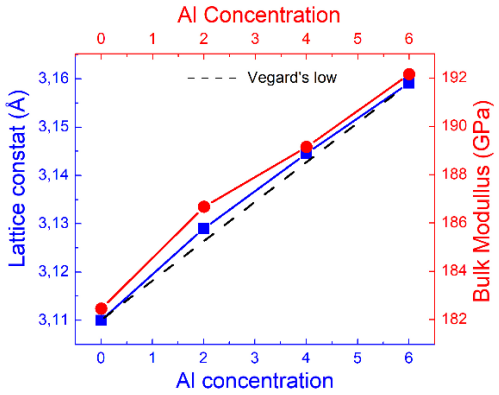

Figure 2. Lattice constant vs concentration (blue) and total bulk modullus vs concentration (red). *Source: Authors*

In the table 1 we note that from the lattice constant 2.120 Å for AlN in the wurtzite structure, the value of the lattice constant of the ternary $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds increases, similarly, the bulk modullus increases with to respect to 192.15 GPa of AlN wurtzite. The fig. 2 show the lattices constant (blue line) and bulk modullus (rede line) versus Al concentration. The increment of the lattice constant occurs because the radius of the Al atom (1.47 Å) is bigger than radius Cr atom (1.27 Å). The variation of the lattice constant follows the Vegard's low, because the dependence the lattices with concertation Al is linear, with a small positive deviation. In the bulk modullus-concentration Al curve (red line in the fig. 2), we can see that bulk modullus of the $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds increases with the concentration Al, this indicate that the $Al_xCr_{1-x}N$ compounds are more rigid, this occurs because the $Nb_xCr_{1-x}N$ compound approaches the pure AlN in the wurtzite structure, which is the ground state of the AlN [4, 17, 18]. In other words, the $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds increase the rigidity when the concentration approaches to pure AlN.

Electronic Properties

To evaluate the total and partial density of states of the pure AlN and $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds the equilibrium lattice constant shown in table 1 were used. The DOS are presented in fig. 3(a)-(d), respectively. The DOS of the pure AlN wurtzite-type is presented in the

fig.3(a). The -AlN have a semiconductor behavior. We calculated a direct band gap of ~ 4.35 eV. This result is in good agreement with other theoretical report, 4.26 eV [22], 4.30 eV [4, 23]; but 4.35 eV calculated here is smaller than of gap energy 6.2 eV reported experimentally [24]. This happens because the GGA approximation underestimates the energy gap in semiconductors. The AlN wurtzite not have magnetism because the spin-up channel is symmetric to spin-down channel. The valence band is dominated by 2p-N and 2p-Al orbital in similar proportion.

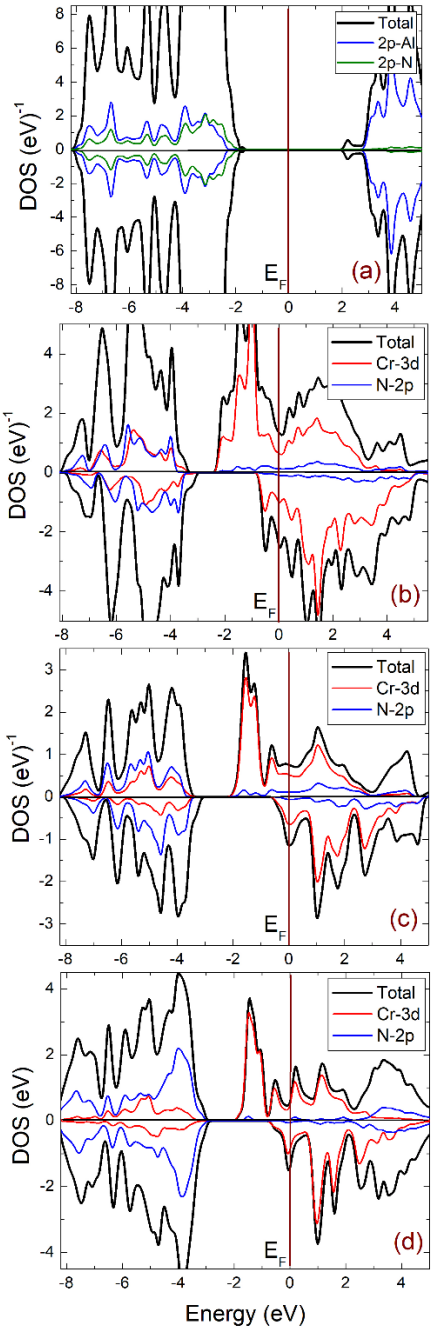

Figure 3. Total and partial DOS of (a) pure AlN, (b) $Al_{0,25}Cr_{0.75}N$, (c) $Al_{0,50}Cr_{0.50}N$, and (d)$Alb_{0.75}Cr_{0.25}N$.
Source: Authors

The DOS of ternary $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds are illustrated in the fig.3(b)-(d), respectively. All ternary compound are metallics. The DOS reveal that due to presence of Cr atom, the ternary compounds acquires magnetic properties because the both spin-up and spin-down channels are nonsymmetric. We can see, in three compounds in valence band just below the Fermi Level the DOS is mainly dominated by 3d-Cr orbital with a minor contribution 2p-N orbital. The values of total magnetic moment of the ternary compounds are 9.25 μ_β/cell, 3.35 μ_β/cell, and 3.15 μ_β/cell, respectively. Where the contribution of the Cr atom in the three compounds is 3.0 μ_β/Cr-atom and the contributions of the nitrogen atoms in the $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ are 0.23 μ_β/cell, 0.31 μ_β/cell, and 0.16 μ_β/cell, respectively. The ferromagnetic properties comes from polarization and hybridization of the 3d-2p states of the Cr and N respectively.

CONCLUSIONS

In summary, we study the structural and electronic properties of ternary $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds in wurtzite structure, using computational calculation in the framework of the density functional theory. For the structural properties, we found that the lattice constant increase with Al concentration following a variation is linear, in accordance with the Vegard's low. The density state calculations reveal that three ternary compounds exhibit a metallic character. The $Al_{0,25}Cr_{0.75}N$, $Al_{0,50}Cr_{0.50}N$, and $Al_{0,75}Cr_{0.25}N$ compounds have ferromagnetic properties with a total 9.25 μ_β/cell, 3.35 μ_β/cell, and 3.15 μ_β/cell, respectively. This ferromagnetic behavior is mainly dominated by 3d-Cr orbital with a minor contribution of 2p-N orbitals.

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REFERENCES

[1] Nakamura S, Senoh M, Nagahama S, Iwasa N, Yamada T, Matsushita T, et al. Jpn J. Appl. Phys. 1997;36:1059.

[2] L.I. Berger, Semiconductor Materials, CRC Press, New York, 1997.

[4] J.F. Murillo G, César Ortega López, Miguel J. Espitia R, Results in Physics 5 (2015) 281–285

[5] U.P. Verma, P.S. Bisht, Solid State Sciences 12 (2010) 665–669

[6] Y.G. Cao, X.L. Chen, J.Y. Li, Y.P. Xu, T. Xu, Q.L. Liu, J.K. Liang, J. Cryst. Growth 213 (2000) 198–202.

[7] N.S. Kanhe, A.B. Nawale, R.L. Gawade, V.G. Puranik, S.V. Bhoraskar, A.K. Das, V.L. Mathe, J. Cryst. Growth 339 (2012) 36–45.

[8] M. Iwata, K. Adachi, S. Furukawa, T. Amakawa, J. Phys. D Appl. Phys. 37 (2004)1041–1047.

[9] O. Ambacher, J. Phys. D Appl. Phys. 31 (1998) 2653–2710.

[10] B. Monemar, J. Mater. Sci. Mater. Electron. 10 (1999) 227–254.

[11] Hohenberg, P., Kohn, W.: Phys. Rev. B 136, 864 (1964)

[12] Kohn, W., Sham, L.J.: Phys. Rev. A 140, 1133 (1965)

[13] P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicka, J. Luitz, Techn. Universitat Wien, Austria, 2001. ISBN 3-9501031-1-2.

[14] J. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple, Physical Review Letter, 77 (1996) 3865.

[15] H. Monkhorst, J. Pack, Special points for Brillouin-zone integrations, Phys Rev B, 13 (1976) 5188.

[16] F.D. Murnaghan, The Compressibility of media under pressure, Proc. Natl. Acad. Sci. U.S.A. 30 (1944) 244–247.

[17] Warner JM, Bechstedt F., Phys. Rev. B 2002; 66:15202.

[18] Schulz H, Thieman KH. Solid State Commun. 1977;23:815.

[19] Zhu Ming and Ke-Hong Wang, Modern Physics Letters B, 29(04):1550009, 2015.

[20] Marco Marin-Suarez and Et al. Leidy L. Alzate-Vargas, Jorge David, Mauricio Arroyave-Franco, Mario E. Vélez, Physica Status Solidi (A) Applications and Materials Science, 215(1):1 (2018).

[21] P. Subramanya Herle, M. S. Hegde, N. Y. Vasathacharya, Sam Philip, M. V. Rama Rao, and T. Sripathi. Journal of Solid State Chemistry, 134(1):120{127, 1997.

[22] Zhao-Yong Jiao, Shu-Hong Ma, Ji-Fei Yang, Solid State Sciences 13 (2011) 331-336.

[23] J. F. Murillo, C. Ortega, M. J. Espitia, Journal of Physics: Conference Series 687 (2016) 012114

[24] Vurgaftman I, Meyer JR, Ram-Mohan LR. J Appl Phys 2001;89:5815