International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 18 (2018) pp. 13859-13863

Different Behavior Ferromagnetic of Ti-doped AlN and GaN in Cubic Phase

Luis C. Sánchez P[1], Cesar Ortega López[1], Miguel J. Espitia R[2]

[1]*Grupo de Materiales y Sistemas Complejos GAMASCO, Universidad de Córdoba, Montería, Colombia.*

[2]*Grupo GEFEM, Universidad Distrital Francisco José de Caldas, Bogotá, Colombia.*

Abstract

In this paper we carry out computational calculations using pseudopotential method within density functional theory and employing computational Quantum ESPRESO package, for study the magnetic behavior of $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ compounds in zincblende phase. The density states calculation show that the two compounds have a ferromagnetic behavior, being the $Al_{0.9375}Ti_{0.0625}N$ metallic with a magnetic moment of 0.85 μ_β/cell, while the $Ga_{0.9375}Ti_{0.0625}N$ is half-metallic with a magnetic moment of 1.0 μ_β/cell. The magnetic properties come from of the hybridization and polarization of 3d-Ti and 2p-N orbitals. Being of main contribution of 3d-Ti states.

Keywords: DFT calculations, electronic and magnetic properties.

INTRODUCTIÓN

The group III nitrides semiconductors such as aluminum nitride (AlN) and gallium nitride (GaN) has been studied in the last few decades. These investigations are motivated by application in laser diodes, in high-voltage [1], optoelectronic devices, photo-detectors [2-4], high-temperature microwave applications [5, 6], and micro-electronic devices working in the ultraviolet region [7-10]. Under normal temperature and pressure conditions AlN and GaN crystallize in the wurtzite structure However, depending of the substrate and the growth conditions, zincblende phase can be obtained [11, 12]. Recently, AlN and GaN in cubic zincblende phase has been grown by different experimental techniques, such as solid-state reaction [13], molecular beam epitaxy MBE [14], the vapor–liquid–solid (VLS) route [15], and reactive pulsed laser deposition [16], while GaN has been grown by means of metalorganic chemical vapor deposition [17, 18] and molecular bean epitaxy (MBE) [19-22]. Though it is expected that AlN and GaN cubic zincblende phase applications will be similar to those developed for AlN and GaN wurtzite, many researchers have found several advantages of the zincblende over the wurtzite structure [23–25], because the zincblende phase of AlN and GaN doesn't have a polarized internal electric field [26], due to its high crystallographic symmetry. The absence of an internal electric field in AlN and GaN zincblende improves its electronic properties, because of higher carrier mobility, higher drift velocities, and better doping efficiencies [23–25]. At the same time, there are additional advantages for group-III semiconductors in the cubic phase; for example, in GaN zincblende its was found that there is a reduction in the radiative radiation time by two orders of magnitude compared to GaN wurtzite [27]. Actually, several theoretical investigations [28–37] and experimental studies [38–47] have found that AlN and GaN doped with transition metals (TM) [48–50] turned out to be a good diluted magnetic semiconductor for use in spintronics devices. All these studies of TM-doped AlN and GaN were made in the wurtzite structure, in spite of the fact that AlN and GaN cubic zincblende phase has been grown and many advantages of AlN and GaN in cubic phase with respect to AlN and GaN wurtzite phase have been reported, the theoretical or experimental studies of Ti doped AlN and GaN cubic zincblende phase are scares. For this reason, in this paper we did detailed study of electronic and magnetic properties of $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ in cubic zincblende phase.

COMPUTATIONAL METHOD

In this paper calculations were performed using the Quantum ESPRESSO computational code [51] based in the pseudopotential method [52, 53] within density functional theory (DFT) [54, 55]. The correlation and exchange effects between electrons the correlation and exchange interaction between electrons were included with the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [56]. For the expansion of the electronic function in plane waves, we used a value of kinetic energy cutoff of 40 Ry. Brillouin zone integrations were performed with the special k-point method over a 6×6×12 Monkhorst-Pack mesh [57] for a unit cell. To simulate AlN and GaN ´pure in the zincblende structure, we constructed a *2a* x *2b* x *1c* supercell with 32 atoms (fig. 1). For the concentration $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$, one of the Al (and Ga) atom was replaced with one Ti atom in the supercell. For the pure AlN and GaN compound, and $Al_{0.0625}Ti_{0.9375}N$ and $Ga_{0.0625}Ti_{0.9375}N$ concentrations, were performed a relax type calculation in which all atoms in the supercell move in the three directions. All calculations were carried out with spin polarization and 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.

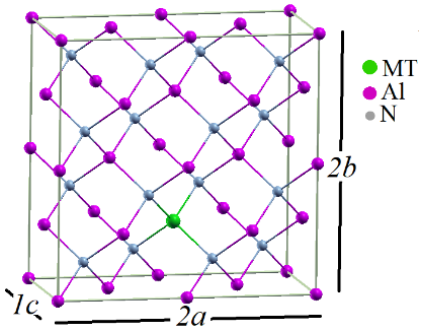

Figure 1. Conventional unit cell of pristine AlN and GaN in the zincblende structure. Source: Authors

RESULTS AND DISCUSSIONS

Structural properties

The lattice constant and bulk modullus of the AlN, GaN, $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ in zincblende structure, were determinate fitting the calculated energy-volume values to the Murnaghan equation of state [58]. Additionally, for the $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ compounds we determined the character magnetic, namely ferromagnetic (FM) and antiferromagnetic (AFM) phase was calculated, several AFM configurations with different spin orientations were calculated until obtaining the energetically most stable structure. The figure 2 show the energy vs volume curves for the ternary compounds in the FM and AFM magnetic phases.

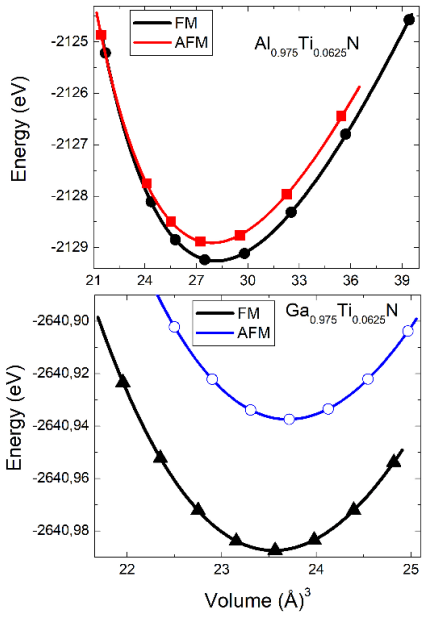

Figure 2. Total energy vs volume curves for $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ in zincblende structure. The points are the calculated values and the continuous curve is the fit. Source: Authors

The main equilibrium parameters of AlN, GaN, $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$. are listed in table 1 along with available data reported experimental and theoretically for other authors.

The values of lattice constant and bulk modullus for AlN and GaN compounds calculated in this work, are in good agreement with reported from other theoretical and experimental investigation. Being the maximum discrepancies of ~ 1.22% and ~ 5.82% for GaN; while for AlN the discrepancies are ~ 0.26% and ~ 2.90%, for lattice constant and bulk modullus respectively. These discrepancies are smaller, which show the reliability of our present calculation

Table 1. Lattice constant (a) and bulk modullus for AlN, GaN, $Al_{0.9375}Ti_{0.0625}N$, and $Ga_{0.9375}Ti_{0.0625}N$.

Compound	a(Å)	B_0 (GPa)
Pristine-AlN	4.3815	206.52
	4.3800[a]	212.70[b]
	4.3790[c]	211.78[d]
	4.3700[e]	202.00[e]
Pristine-GaN	4.556	201.75
	4.590[f]	206.90[g]
	4.500[h]	190[h]
$Al_{0.0625}Ti_{0.9375}N$	4.3886	186.98
$Ga_{0.0625}V_{0.9375}N$	4.5220	196.94

[a] Theoretical [5]

[b] Theoretical [59]

[c] Theoretical [60]

[d] Theoretical [61]

[e] Experimental [62]

[f] Theoretical [63]

[g] Theoretical [64]

[h] Experimental [65]

We observe that the lattice constant of the $Al_{0.9375}Ti_{0.0625}N$ is smaller than the lattice constant of $Ga_{0.9375}Ti_{0.0625}N$, this happen because the atomic radius of the Al is smaller than of the Ga. atom Additionally, as we can see in the figure 1, the two $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ compounds the FM phase es most favorable, the difference of energy between AFM and FM phase $\Delta E = E_{AFM} - E_{FM}$ are: 321 mV and 655 mV, respectively. Hence, he ground state of $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ zincblende is ferromagnetic.

Electronic Properties

To evaluate the electronic and magnetic properties, we calculated the spin-polarized density of states (DOS) along the symmetry path of $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ in the zincblende structure. The DOS were calculated with the equilibrium lattice constant show in table 1. The DOS of the two compounds are illustrated in the figure 3(a)-(b), respectively. Where we have chosen the Fermi Level as zero of energy.

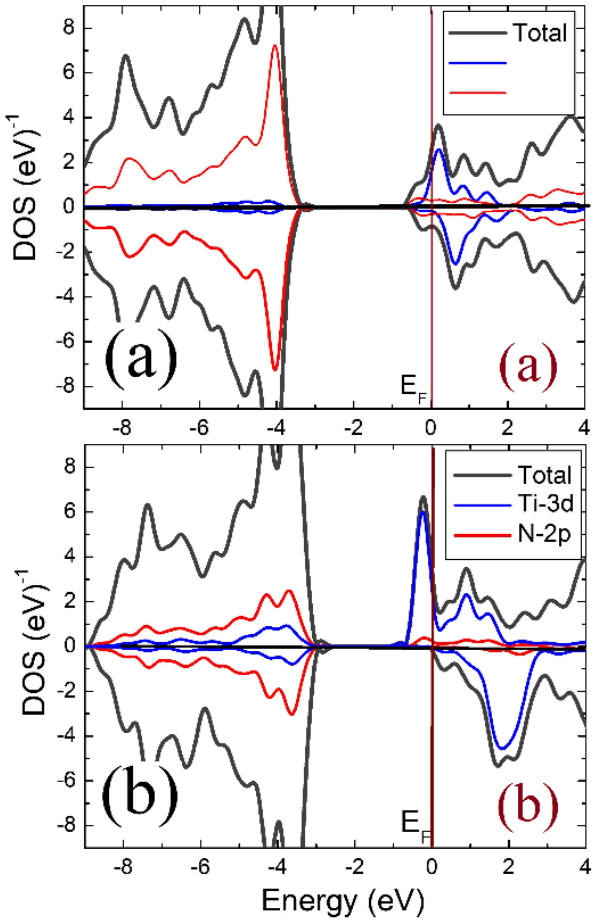

Figure 3. Total and partial density of states of (a) $Al_{0.9375}Ti_{0.0625}N$, (b) $G_{0.9375}Ti_{0.0625}N$ compounds. Source: Authors.

The DOS for $Al_{0.9375}Ti_{0.0625}N$ shows a metallic behavior, because the two spin channels cross the fermi level, while the DOS of $G_{0.9375}Ti_{0.0625}N$ compound reveals a half-metallic character, with the spin down being semiconducting and the spin up being metallic. For $G_{0.9375}Ti_{0.0625}N$ due to the spin up orientation's being partially filled, there are sufficient states behaving like free holes. Consequently, these compounds have 100% spin polarization of the conduction carriers and satisfy this requirement for use as spin injectors.

We can see in the figure 3 the DOS of the two compounds shows that the spin density is mainly situated around the Ti atom, with a minimum contribution from the first-neighboring N atoms. For this reason, near the Fermi level the main contribution to the total DOS comes from the 3d-Ti orbital, with a minimum contribution from the 2p-N orbital. The hybridization and the polarization between 3d-Ti and 2p-N generate magnetic effects in $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ compounds with a finite magnetic moment, with values of 0.85 μ_β, 1.0 μ_β per cell, respectively. We note that the magnetic moment value of $Ga_{0.0625}Ti_{0.9375}N$ is integer, this prove again their half-metallic ferromagnetic behavior.

CONCLUSIONS

In summary, we studied electronic and magnetic properties of $Al_{0.9375}Ti_{0.0625}N$ and $Ga_{0.9375}Ti_{0.0625}N$ compounds zincblende structure, using computational calculation within of density functional theory. We found that the two compounds have ferromagnetic behavior, but $Al_{0.9375}Ti_{0.0625}N$ compound have metallic character with a magnetic moment of 0.85 μ_β/cell, while the $Ga_{0.9375}Ti_{0.0625}N$ compound has half-metallic behavior with a magnetic moment of 1.0 μ_β/cell. The magnetic properties come from hybridization and polarization between metallic states 3d-Ti and nonmetallic states 2p-N. Due to the half-metallic ferromagnetic character of $Ga_{0.9375}Ti_{0.0625}N$ is a good candidate for application in the diluted magnetic semiconductor field.

ACKNOWLEDGEMENTS

The authors are very grateful to the Investigations Center (CIUC) of the Universidad Córdoba for its financial support.

REFERENCES

[1] Arbouche O, Belgoumène B, Soudini B, Driz M 2009 Computational Materials Science 47 432

[2] Kimura T and Hashizume T 2009 Journal of Applied Physics 105 014503

[3] Ito H and Ishibashi T 1991 J. Appl. Phys. 30 994

[6] Tang H, Webb J.B, Bardwell J.A, Raymond S, Salzman J and Uzan S.S 2001 Appl. Phys. Lett. 78 757.

[4] Nakamura S 1997 Solid State Commun. 102 237

[5] Nakamura S, Senoh M, Iwasa N and Nagahama S.-I 1995 Applied Physics Letters 67 1868

[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] Vaudo R.P, Xu X.P, Salant A, Malcarne J and Brandes G.R 2003 Phys. Status Solidi 200 18

[12] E.-A. Choi, J. Kang, K.J. Chang, Phys. Rev. B 74 (2006) 245218

[13] I. Petrov, E. Mojab, R.C. Powell, J.E. Greene, Appl. Phys. Lett. 60 (1992) 2491

[14] Schupp T, Lischka K., D. J. As, 2010 Journal of Crystal Growth 312 1500

[15] R. Thapa, B. Saha, K.K. Chattopadhyay, Journal of Alloys and Compounds 475 (2009) 373–

[16] Satoshi Mohri, Tsuyoshi Yoshitake, Takeshi Hara, Kunihito Nagayama, Diamond & Related Materials 17 (2008) 1796–1799

[17] H. Vilchis, V.M.Sánchez-R. lectrical behavior of Mg doped cubic GaN on c-GaN structure. Materials Sciencein Semiconductor Processing 37 (2015) 68–72

[18] H. Vilchis, V.M. Sanchez-R., A. Escobosa. Cubic GaN layers grown by metalorganic chemical vapor deposition on GaN templates obtained by nitridation of GaAs. Thin Solid Films 520 (2012) 5191–5194

[19] S.V. Novikov, N.M. Stanton, R.P. Campion, C.T. Foxon, A.J. Kent. Free-standing zinc-blende (cubic) GaN layers and substrates. Journal of Crystal Growth 310 (2008) 3964– 3967

[20] D.J. As, E. Tschumak, H. Pöttgen, O. Kasdorf, J.W. Gerlach, H. Karl, K. Lischka. Carbon doping of non-polar cubic GaN by CBr4

[21] E. Martinez-Guerrero E. Bellet-Amalric, L. Martinet, G. Feuillet, B. Daudin, H. Mariette, P. Holliger, C. Dubois, C. Bru-Chevallier, P. Aboughe Nze, T. Chassagne, G. Ferro, Y. Monteil. Structural properties of undoped and doped cubic GaN grown on SiC.001. JOURNAL OF APPLIED PHYSICS VOLUME 91, NUMBER 8 2002

[22] Fumiyoshi Takano, Hironori Ofuchi, JeungWoo Lee, Koki Takitac, Hiro Akinaga. Growth and characterization of Mn-doped cubic-GaN. Physica B 376–377 (2006) 658–662

[23] H. Ismail, E. Belloti, K.F. Brennan, J. Kolnik, R. Wang, P.P. Ruden, J. Appl. Phys. 81 (1997) 7827.

[24] O. Ambacher, J. Majewski, C. Miskys, A. Link, M Hermann, M. Eickhoff, M. Stutzmann, F. Bernardini, V. Fiorentini, V. Tilak, B. Schaff, L.F. Eastman, J. Phys.: Condens. Matter 14 (2002) 3399.

[25] C. Mietze, M. Landmann, E. Rauls, H. Machhadani, S. Sakr, M. Tchernycheva, F.H. Julien, W.G. Schmidt, K. Lischka, D.J. As, Phys. Rev. B 83 (2011) 195301.

[26] D.J. As, Microelectron. J. 40 (2009) 204.

[27] J. Simon, N.T .Pelekanos, C. Adelmann, E. Martinez-Guerrero, R.Andre´ , B. Daudin, Le Si Dang, H. Mariette, Phys. Rev. B 68 (2003) 035312.

[28] W.W. Lei, D. Liu, P.W. Zhu, X.H. Chen, Q. Zhao, G.H. Wen, Q.L. Cui, G.T. Zou, Applied Physics Letters 95 (2009) 162501.

[29] Yao G, Fan G, Xing H, Zheng S, Ma J, Zhang Y and He L 2013 Journal of Magnetism and Magnetic Materials 331 117

[30] Dinh V and Katayama-Yoshida H 2005 ferromagnetism and curie temperature of Vanadium-doped nitrides, Journal of Electron Microscopy 54 (Supplement 1) i61

[31] Espitia M, Díaz J., Castillo L, International Journal of Physical Science 2016 11 11

[32] Q.Y. Wu, Z.Q. Huang, R. Wu, L.J. Chen, Journal of Physics: Condensed Matter 19 (2007) 056209

[33] R. Q. Wu, G. W. Peng, L. Liu , and Y. P. Feng, Z. G. Huang, Q. Y. Wu, Applied Physics Letters **89**, 142501 (2006)

[34] Miguel J. Espitia R, John H. Díaz, César Ortega López, International Journal of Physical Sciences (10)17 (2015): 520-527.

[35] Miguel J.Espitia R, Jonh H. Díaz, Luis Eduardo Castillo, International Journal of Physical Sciences (1)1 (2016) 11-18.

[36] M.J. Espitia Rico, J. H. Díaz F, C. Ortega López, Journal of Physics: Conference Series 687 (2016) 012069

[37] J.H. Díaz F, M.J. Espitia R, J.A. Rodríguez Martínez, Journal of Physics: Conference Series 743 (2016) 012004

[38] R.M. Frazier, J. Stapleton, G.T. Thaler, C.R. Abernathy, S.J. Pearton, R. Rairigh, J. Kelly, A.F. Hebard, M.L. Nakarmi, K.B. Nam, J.Y. Lin, H.X. Jiang, J.M. Zavada, R.G. Wilson, J. Appl. Phys. 94 (2003) 1592.

[39] S.Y. Wu, H.X. Liu, L. Gu, R.K. Singh, L. Budd, M. van Schilfgaarde, M.R. McCartney, D.J. Smith, N. Newman, Applied Physics Letters 82 (2003) 3047.

[40] R.M. Frazier, J. Stepleton, G.T. Thaler, C.R. Abernathy, S.L. Pearton, R. Rairigh, J. Kelly, A.F. Hebard, M.L. Nakarmi, K.B. Nam, J.Y. Lin, H.X. Jiang, J.M. Zavada, R.G. Wilson, Journal of Applied Physics 94 (2003) 1592

[41] D. Kumar, J. Antifakos, M.G. Blamire, Z.H. Barber, Appl. Phys. Lett. 84 (2004) 5004.

[42] Wistrela E, Bittner A, Schneider M Reissner M and Schmid U 2017Jornal of Applied Physics 121 115302.

[43] D. Pan, J. K. Jian, A. Ablat, J. Li, Y. F. Sun, and R. Wu, J. Appl. Phys. 112, 053911 (2012).

[44] Y. Yang, Q. Zhao, X.Z. Zhang, Z.G. Liu, C.X. Zou, B. Shen, D.P. Yu, Applied Physics Letters 90 (2007) 092118

[45] Pearton, Appl. Phys. Lett. 83, 1758 (2003).

[46] K.Y. Ko, Z.H. Barber, M.G. Blamire, J. Appl. Phys. 100 (2006) 083905.

[47] J. T. Luo, Y. Z. Li, X. Y. Kang, F. Zeng, F. Pan, P. Fan, Z. Jiang, and Y. Wang, J. Alloys Compd. 586, 469 (2014).

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

[49] Kai Li, Xiaobo Du, Yu Yan, Hongxia Wang, Qing Zhan, Hanmin Jin, Physics Letters A 374 (2010) 3671–3675

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

[51] P. Giannozzi, S. Baroni, N. J. Bonin, a modular and open-source software project for quantum simulations of materials, Condens. Matter, 21 (2009) 395502.

[52] Vanderbilt D, Soft self-consistent pseudopotentials in a generalized eigenvalue formalism, Phys. Rev. B, 41 (1990) 7892.

[53] K. Laasonen, A. Pasquarello, R. Car, C. Lee, D. Vanderbilt, Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials, Phys Rev B, 47 (1993) 10142.

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

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

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

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

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

[59] A.E. Merad, M.B. Kanoun, J. Cibert, H. Aourag, G. Merad, Materials Chemistry and Physics 82 (2003) 471–477

[60] S. Goumri-Said, M.B. Kanoun, A.E. Merad, G. Merad, H. Aourag, Chem. Phys. 302 (2004) 135

[61] M.B. Kanoun, A.E. Merad, G. Merad, J. Cibert, H. Aourag, Solid-State Electronics 48 (2004) 1601–1606

[62] C. Stampfl, C.G. Van de Walle, Phys. Rev. B 59 (1999) 5521.

[63] V.I. Gavrilenko, R.Q. Wu, Phys. Rev. B 61 (2000) 2632

[64] S. Saib, N. Bouarissa, Physica B 387 (2007) 377–382.

[65] I. Petrov, E. Mojab, R.C. Powell, J.E. Greene, Appl. Phys. Lett. 60 (1992) 2491