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THE MAGNETIC CHARACTERISTICS AND ELECTRONIC CONFIGURATION OF GAN COMPOUND MODIFIED BY INDIVIDUAL IMPURITIES (Fe AND Ni)

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ABSTRACT. The Korringa–Kohn–Rostoker (KKR) method coupled with the coherent potential approximation (CPA) is employed to examine the magnetic characteristics and electronic configuration of GaN that has been infused with individual impurities (Fe and Ni). The partial and total DOS of all systems were determined. Our investigation focuses on assessing the impact of varying doping concentrations on the band gap and total energies. To comprehensively explore this subject, we analyze and interpret the magnetic moment of GaN substances across a range of doping concentrations.

KEY WORDS: Electronic structure, Magnetic proprieties, Band gap, KKR method, CPA approximation, GaN compounds

INTRODUCTION

Diluted magnetic semiconductors (DMSs) have piqued considerable interest in industrial electronics, primarily because of their potential applications in spintronic devices [1]. Among the wide range of semiconductor compounds utilized in modern electronics, group III nitrides, particularly GaN, are noteworthy. The GaN structure boasts a relatively large direct band gap, low electron affinity, piezoelectricity, mechanical strength, and high thermal conductivity [2], rendering it an excellent material platform for improved performance characteristics in opto-electronic device applications. Additionally, ongoing scientific research is aimed at comprehending the fundamental electronic structure and magnetic properties of the nitrides, with the ultimate goal of enhancing crystalline quality through various methods [3].

In addition, doping GaN with magnetic impurities provides additional flexibility for spin-based electronic applications, such as magnetic random-access memory and quantum computing [4]. Several experimental studies have reported on the magnetic properties of GaN [5-9]. Moreover, Sato and Katayama-Yoshida's recent theoretical work predicted diverse magnetic properties for GaN, which incorporate varying concentrations of Cr, Co, and V based on a local spin-density approximation that assumes Ga atoms are randomly substituted with the magnetic atoms [10].

Ab initio couplings enable us to anticipate the presence of a canted phase and offer insights into experimental observations for diluted magnetic semiconductors, such as GaMnAs [11]. The electronic structure of $Ga_{1-x}Mn_xAs$, a bulk diluted magnetic semiconductor, is thoroughly investigated in by Gray *et al.* [12]. Additionally, Turek *et al.* [13], Zhu *et al.* [14], and Valedbagi *et al.* [15] explore the optical conductivity, density of states, Fermi energy, and inverse participation ratio under varying impurity concentrations. Meanwhile, Diet *et al.* [16] scrutinizes the ferromagnetic phases of Co spins at low temperatures utilizing the Zener model.

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The objective of this paper is to investigate the magnetic characteristics and electronic configuration of GaN doped with (Ni and Fe) through implementation of the KKR method coupled with the coherent potential approximation (CPA) [17]. The study presents the calculation of partial and total densities of state (DOS) of GaN material, along with the evaluation of band gap and magnetic moment for diverse levels of dilution concentrations.

CALCULATION METHOD

The KKR method, coupled with the coherent potential approximation (CPA) devised by Akai and Dederichs for analyzing transition metal alloys [22], including the Vosko, Wilk, and Nusair (VWN) [23], was employed in this study. The KKR-CPA method was specifically implemented for the DMS analysis. For this purpose, the KKR-CPA code MACHIKANEYAMA2002v08 package, developed by Akai [22], was utilized in the calculations.

In this study, the crystal potential was modeled using a muffin tin potential approximation. The wave functions were then expanded in real harmonics within their corresponding muffin tin spheres. The calculations were conducted using 1000 K points in the irreducible portion of the first Brillouin zone. GaN possesses a Wurtzite crystal structure, with its parameters defined as follows: a = 3.180 Å, c = 5.1897 Å, and an internal coordinate of u = 0.376 [24]; and a = 3.60 Å, c = 5.74 Å, with an internal coordinate of u = 0.377 [20].

RESULTS AND DISCUSSION

Now it would be useful to study the magnetic properties and the electronic structure of GaN materials doped with single impurities (Fe and Ni) using KKR method combined with the coherent potential approximation [17] (CPA). In the first part, we illustrate the DOS of GaN materials by VWN method as plot in Figure 1. It is found that the band gap is in good agreement with the experiment results. In the second part, we examine the effect of the dilution concentrations (Fe and Ni) on the GaN materials. In Figure 2, we illustrate the density of states (DOS) of GaN for different doping concentrations of Fe. From these figures, it is shown that the Fermi energy level, the total density of states of spin-up and spin-down, for $x < 0.21$, are clearly symmetrical which reveals the presence of magnetism in the diluted systems. On the other hand, we plot in Figure 3 the corresponding density of states (DOS) of the GaN doped with Ni. It should be note that the spin-down of 3d M-states are situated in the conduction band of the GaN materials doped with Fe. Contrariwise, in the GaN materials doped with Ni the spin-down of 3d M-states are situated in the valance band. However, for $x > 0.21$, the magnetic order disappears in favor of a small gap energy.

Furthermore, we illustrate in Figure 4 the band gap of GaN materials as a function of x-concentrations doped with Fe and Ni. It is found that the band gap of GaN materials doped with the Fe and Ni decreases when increasing the concentration doping values. Finally, the total and partial magnetic moments of GaN doping of Fe and Ni are obtained in Table 1 and Table 2, respectively. Finally, we plot in Figure 5 the behavior of the total energy as function of the parameters c/a. This figure showed that the minimum of total energy corresponding to c/a = 1.75.

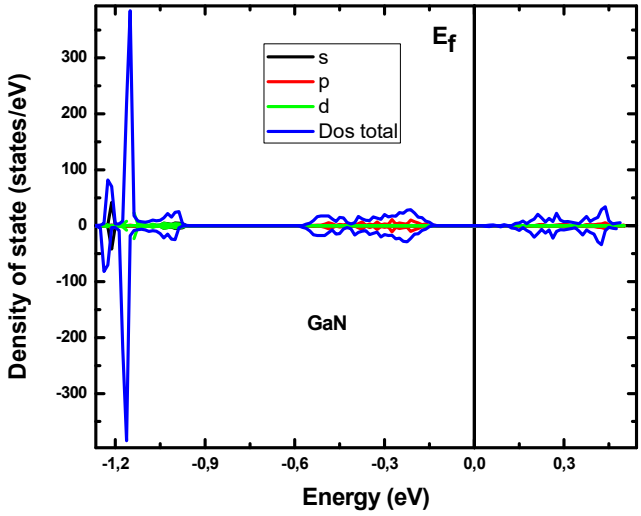

Figure 1. T o t a l and local density of state for the GaN.

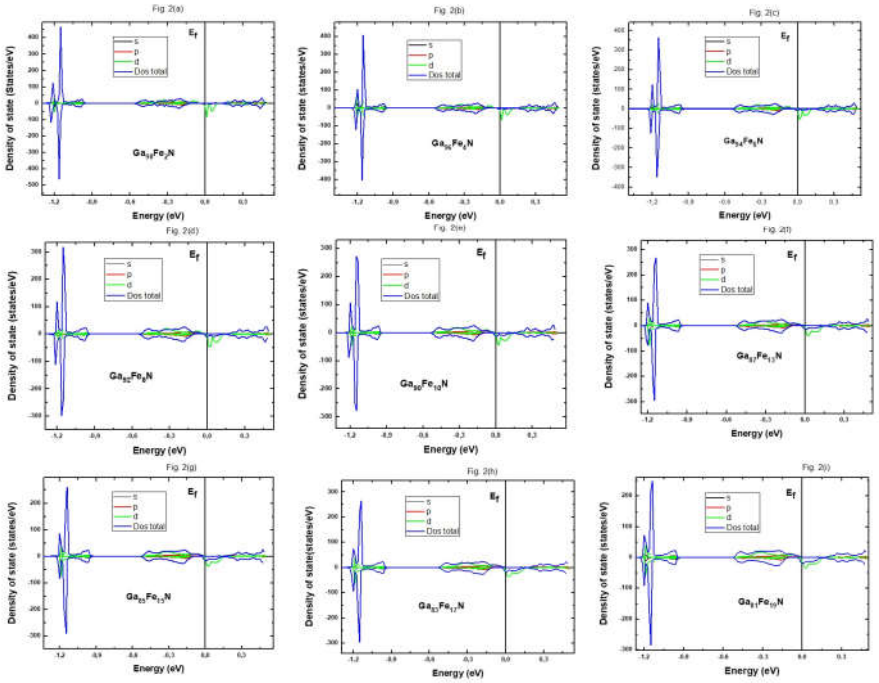

Figure 2. Total and local DOS of $Ga_{1-x}Fe_xN$ for different values of diluted concentrations x: 0.02, 0.04, 0.06, 0.08, 0.10, 0.13, 0.15, 0.17, 0.19 and 0.21.

Table 1. Total and partial magnetic moment of GaN doping by iron Fe materials for different values of concentrations.

$Ga_{1-x}Fe_xN$	M (Ga) $10^{-3}\mu_B$	M (Fe) μ_B	M (N) μ_B	Total magnetic moment μ_B
$Ga_{98}Fe_2N$	0.99	3.55189	0.01185	3.56473
$Ga_{96}Fe_4N$	1.97	3.58022	0.02413	3.60632
$Ga_{94}Fe_6N$	3.00	3.59141	0.03633	3.63074
$Ga_{92}Fe_8N$	3.96	3.60112	0.04844	3.65352
$Ga_{90}Fe_{10}N$	5.02	3.61797	0.06129	3.68428
$Ga_{87}Fe_{13}N$	6.53	3.62095	0.07866	3.70614
$Ga_{85}Fe_{15}N$	7.45	3.61102	0.08881	3.70728
$Ga_{83}Fe_{17}N$	8.47	3.61583	0.10039	3.72469
$Ga_{81}Fe_{19}N$	9.44	3.58423	0.10734	3.70101
$Ga_{79}Fe_{21}N$	10.46	3.58334	0.11783	3.71163

Table 2. Total and partial magnetic moment of GaN doping by nickel Ni materials for different values of concentrations.

$Ga_{1-x}Ni_xN$	M (Ga) $10^{-3}\mu_B$	M (Ni) μ_B	M (N) μ_B	Total magnetic moment μ_B
$Ga_{98}Ni_2N$	0.53	1.65397	0.01363	1.66813
$Ga_{96}Ni_4N$	1.07	1.67027	0.02878	1.70012
$Ga_{94}Ni_6N$	-1.53	-1.61597	-0.04138	1.65888
$Ga_{92}Ni_8N$	1.89	1.55634	0.05137	1.60960
$Ga_{90}Ni_{10}N$	-2.29	-1.49543	-0.05963	1.55735
$Ga_{87}Ni_{13}N$	3.33	1.23373	0.04707	1.28413
$Ga_{85}Ni_{15}N$	2.76	1.23732	0.06560	1.30568
$Ga_{83}Ni_{17}N$	3.21	1.19285	0.07004	1.26610
$Ga_{81}Ni_{19}N$	3.53	1.07629	0.06786	1.14768
$Ga_{79}Ni_{21}N$	3.50	0.94613	0.06316	1.01279

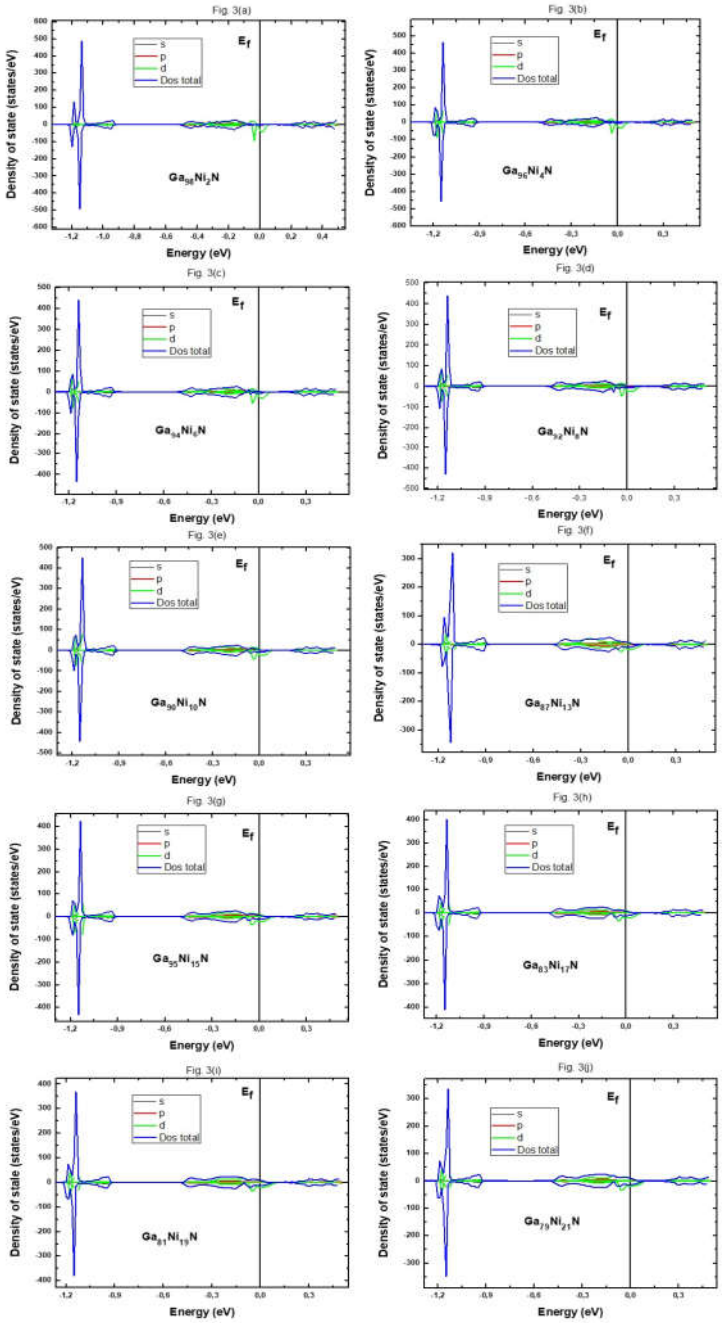

Figure 3. Total and local DOS of $Ga_{1-x}Ni_xN$ for different values of diluted concentrations x: 0.02, 0.04, 0.06, 0.08, 0.10, 0.13, 0.15, 0.17, 0.19 and 0.21.

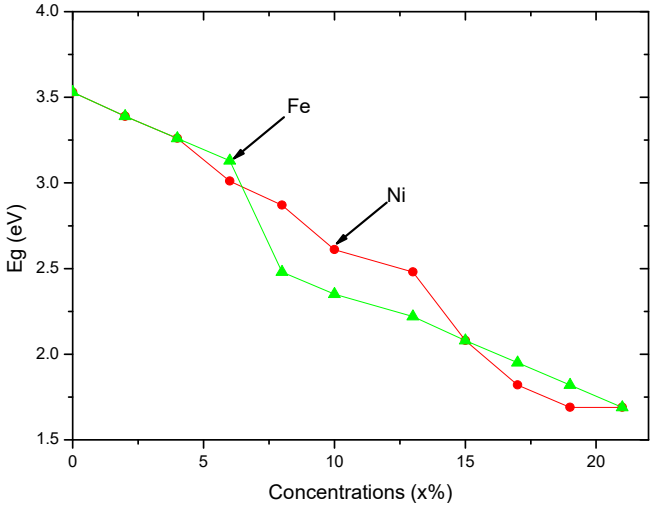

Figure 4. Band gap as a function with doped Ni and Fe in GaN with different percent.

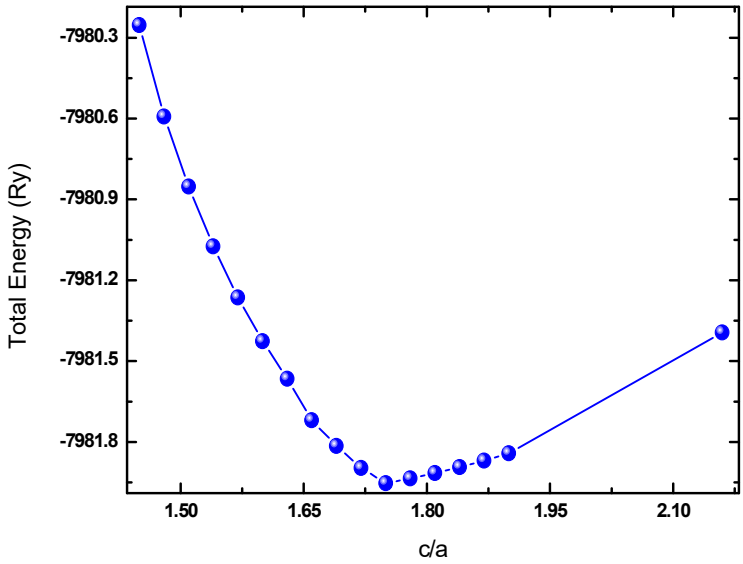

Figure 5. Total energy as a function of the parameter's c/a.

CONCLUSION

This study examines the magnetic properties and electronic structure of GaN materials doped with single impurities Fe and Ni, utilizing the KKR method and coherent potential approximation (CPA). The investigation includes analysis of partial and total density of states across the entire

system. Furthermore, we explore the impact of doping concentrations on the band gap. Lastly, we determine the magnetic moment of each atom for various doping concentrations.

REFERENCES

1. Qi, S.; Jiang, F.; Fan, J.; Wu, H.; Zhang, S.B.; Gehring, G.A.; Zhang, Z.; Xu, X. Spin polarization in GaN-based diluted magnetic semiconductors. *Phys. Rev. B* **2011**, 84, 205204.
2. Zuo, X.; Yoon, S.-D.; Yang, A.; Duan, W.-H.; Vittoria, C.; Harris, V.G. Ferromagnetism in GaN thin films. *J. Appl. Phys.* **2009**, 105, 07C508.
3. Lourenço, M.B.; Carvalho, M.D.; Fonseca, P.; Gasche, T.; Evans, G.; Godinho, M.; Cruz, M. M. Magnetic properties of transition-metal-doped GaN. *J. Alloys Compd.* **2014**, 612, 176-184.
4. Dietl, T.; Ohno, H.; Matsukura, F.; Cibert, J.; Ferrand, D. Zener model description of ferromagnetism in zinc-blende magnetic semiconductors. *Science* **200**0, 287, 1019-1022.
5. Pearton, S.J.; Overberg, M.E.; Thaler, G.T.; Abernathy, C.R.; Kim, J.; Ren, F.; Theodoropoulou, N.; Hebard, A.F.; Daniel Park, Y.; Room temperature ferromagnetism in GaMnN and GaMnP. *Physica Status Solidi (a)* **2003**, 195, 222-227.
6. Chen, P.P.; Makino, H.; Kim, J.J.; Yao, T. Magnetic behavior of GaN thin films. *J. Cryst. Growth* **2003**, 251, 331-336.
7. Overberg, M.E.; Abernathy, C.R.; Pearton, S.J.; Theodoropoulou, N.A.; McCarthy, K.T.; Hebard, A.F. Magnetic properties of GaMnN. *Appl. Phys. Lett.* **2001**, 79, 3128-3130.
8. Kuwabara, S.; Kondo, T.; Chikyow, T.; Ahmet, P.; Munekata, H. Structural and magnetic properties of GaN films. *Jpn. Appl. Phys. Lett. Part 2* **2001**, 40, L724; Rkhioui, N.; Tahiri, N.; El Bounagui, O. Magnetic properties of GaN. *J. Supercond. Nov. Magn.* **2016**, doi: 10.1007/s10948-016-3687-8.
9. Jin, H.; Dai, Y.; Huang, B.; Whangbo, M.H. Exchange interactions and ferromagnetism in GaN. *Appl. Phys. Lett.* **2009**, 94, 162505.
10. Sato, K.; Katayama-Yoshida, H. Stability of ferromagnetism in p-type GaN. *Jpn. Appl. Phys. Part 2* **2001**, 40, L485.
11. Bouzerar, G.; Bouzerar, R.; Cépas, O. Magnetic properties of GaN. *Phys. Rev. B* **2007**, 76, 144419.
12. Gray, A.X.; Minár, J.; Ueda, S.; Stone, P.R.; Yamashita, Y.; Fujii, J.; Braun, J.; Plucinski, L.; Schneider, C.M.; Panaccione, G.; Ebert, H.; Dubon, O.D.; Kobayashi, K.; Fadley, C.S. Electronic structure of GaN. *Nat. Mater.* **2012**, 11, 957-962.
13. Turek, M.; Siewert, J.; Fabian, J. Theoretical study of GaN. *Phys. Rev. B* **2008**, 78, 085211.
14. Zhu, L.; Luo, H. Magnetic properties of transition-metal-doped GaN. *J. Alloys Compd.* **2016**, 685, 619-632.
15. Valedbagi, S.; Mohammad Elahi, S.; Abolhassani, M. R.; Fathalian, A.; Esfandiard, A. Optical properties of GaN films. *Optical Mater.* **2015**, 47, 44-50; Rkhioui, A.; Masrour, R.; Hlil, E. K.; Bahmad, L.; Hamedoun, M.; Benyoussef, A. Structural and magnetic properties of GaN. *J. Supercond. Nov. Magn.* **2013**, 26, 3419-3428.
16. Dietl, T.; Ohno, H.; Matsukura, F.; Cibert, J.; Ferrand, D. Zener model description of ferromagnetism in zinc-blende magnetic semiconductors. *Science* **2000**, 287, 1019-1022.
17. Akai, H. Ferromagnetism and electronic structure of GaN. *J. Phys. Condens. Matter* **1989**, 1, 8045-8052.
18. Santos, J.P.T.; Marques, M.; Teles, L.K.; Ferreira, L.G. Antiferromagnetism with spin polarization of GaN-based diluted magnetic semiconductors. *Phys. Rev. B* **2010**, 81, 115209.
19. Abd El-Lateef, H.M.; Elkanzi, N.A.A.; Alsirhania, A.M.; Alali, I.K.; Alkorbi, F.; Ryad, R.M.; Saber, E.S.A.; Ali, A.M. Nickel oxide nanoparticles as sustainable catalysts for efficient synthesis and anti-microbial evaluation of 2-amino-4H-pyran derivatives. *Bull. Chem. Soc. Ethiop.* **2024**, 38, 657-670.

20. Das, S.N.; Biswal, S.K.; Behera, A.; Belbsir, H.; El-Hami, K.; Mohapatra, R.K. Experimental and rheological modelling on the stabilization of iron ore slurry using a biosurfactant extracted from *Aloe barbadensis* Miller. *Bull. Chem. Soc. Ethiop.* **2024**, 38, 615-629.
21. El-Habeeb, A.A.; Refat, M.S. Enoxacin fluoroquinolone antibacterial agent complexes with Pt(IV), Ru(III) and Ir(III) ions: Synthesis, spectroscopic, physicochemical characterizations and biological studies. *Bull. Chem. Soc. Ethiop.* **2024**, 38, 685-699.
22. Vosko, S.H.; Wilk, L.; Nusair, M. Accurate spin-dependent electron liquid correlation energies for local spin density calculations: a critical analysis. *Can. J. Phys.* **1980**, 58, 1200-1211.
23. Qian, G.-R.; Dong, X.; Zhou, X.-F.; Tian, Y.; Oganov, A.R.; Wang, H.-T. Novel low-energy boron framework allotropes predicted within density functional theory. *Comput. Phys. Commun.* **2013**, 184, 2111-2118.
24. Strite, S.; Chandrasekhar, D.; Smith, D.J.; Sarie, J.; Chen, H.; Teraguchi, N.; Morkoc, H. Growth and characterization of GaN. *J. Cryst. Growth* **1993**, 127, 204-214.