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Effective field theory and Ab-initio calculation of p-type (Ga, Fe)N within LDA and SIC approximation

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ABSTRACT

Based on first-principles spin-density functional calculations, using the Korringa–Kohn–Rostoker method combined with the coherent potential approximation, we investigated the half-metallic ferromagnetic behavior of (Ga, Fe)N co-doped with carbon within the self-interaction-corrected local density approximation. Mechanism of hybridization and interaction between magnetic ions in p-type (Ga, Fe)N is investigated. Stability energy of ferromagnetic and disorder local moment states was calculated for different carbon concentration. The local density and the self-interaction-corrected approximations have been used to explain the strong ferromagnetic interaction observed and the mechanism that stabilizes this state. The transition temperature to the ferromagnetic state has been calculated within the effective field theory, with a Honmura–Kaneyoshi differential operator technique.

1. Introduction

Diluted magnetic semiconductors (DMS) have been extensively studied due to their future applications in silicon technology; the ferromagnetism in DMS was observed in Mn-doped GaAs [1], but not at room temperature. These materials exhibit also half metal behavior (i.e., metals in one spin direction and insulator in other spin direction). The search for developing dilute magnetic semiconductors (DMSs) with high Curie temperature (T_C) and half metal behavior has been the subject of interest for a new generation of spintronics [2]. Studies of III–V diluted magnetic semiconductor were focused on (Ga, Mn)As [1] and (Ga, Mn)N as promising materials for spintronics applications [3,4]. Experimentally and numerically few results are known for the case of (Ga,Fe)N. The magnetic properties of p-type (Ga, Fe) N compound show a ferromagnetic state at room temperature [5–7]. Numerically Sato and Katyama-Yoshida [8], had made a calculation based on KKR–CPA method for randomly substituted Fe impurities in GaN and found a spin-glass state for any concentration of Fe in $Ga_{1-x}Fe_xN$. Recently, we showed using Ab-intio calculation that without additional holes doping to $Ga_{0.95}Fe_{0.05}N$, the Fermi level separates a completely filled majority spin-band from a completely empty minority-spin-band resulting in a spin-glass state and we showed that the co-doping by carbon or by acceptor defect like Ga vacancies atoms can change the ground state from no-metallic anti-ferromagnetic state to half-metallic ferromagnetic state [9,10].

The aim of this paper is to study the effect of LDA Self-Interaction-Corrected (SIC) on the magnetic properties of $Ga_{0.05}Fe_{0.05}N_{1-x}C_x$. A mechanism of exchange interaction between magnetic ions in p-type Fe-doped GaN for different Carbon concentration. The observed half-metallic ferromagnetic state results from the hybridization of *d*-states of Fe and *p*-state of C at Fermi energy, E_f. Using the effective field theory, with a Honmura–Kaneyoshi differential operator technique, the transition temperature to the ferromagnetic state was calculated and compared with Curie temperature computed from Ab-initio calculation.

2. Calculation method

The electronic structures are calculated by using the Korringa–Kohn–Rostoker (KKR) method combined with coherent potential approximation (CPA). The KKR–CPA method is one of the most efficient band structure calculation methods for treat disorder systems like DMS. Akai and Dederichs have developed the KKR–CPA method to treat transition metal alloys [11] and InAs-based DMS [12]. For LDA approximation we use a Vosko, Wilk and Nusair (VWN) functional [13], which predicts a band gap of 2.72 eV or bulk GaN (Fig. 1). In order to implement the self-interaction correction,

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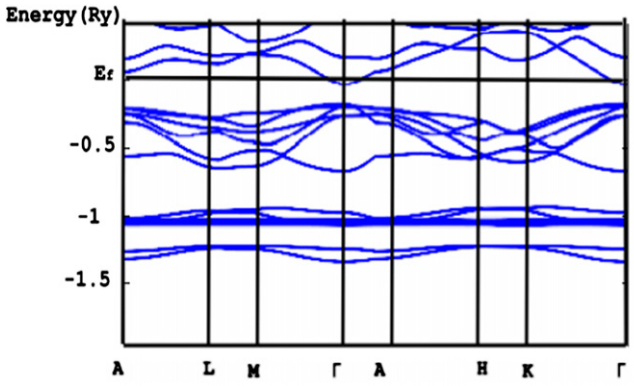

Fig. 1. Band structure calculation of GaN.

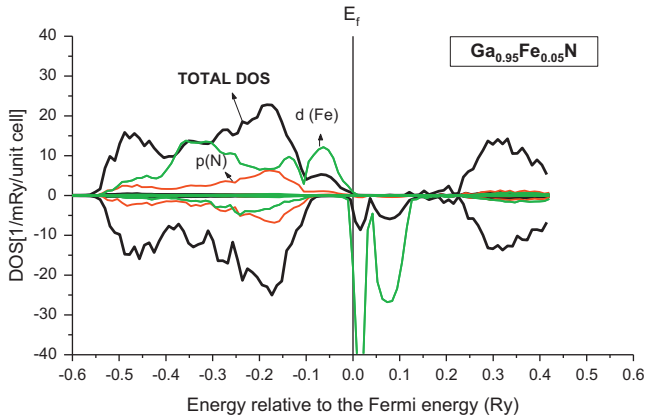

Fig. 2. Total and local density of states of a $Ga_{0.95}Fe_{0.05}N$ within LDA approximation.

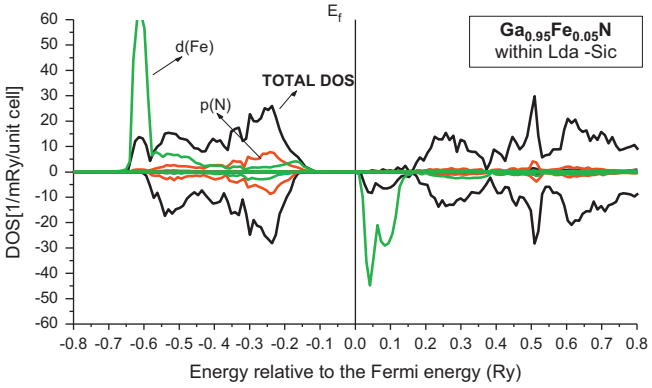

Fig. 3. Total and local density of states of a $Ga_{0.95}Fe_{0.05}N$ within SIC approximation.

we use the SIC approximation [14–16] which is considered as an extension of LDA, in the sense that the Kohn–Sham wave function is projected onto a set of localized orbital basis. The SIC approximation differentiates, for each orbital, the energy gain due to hybridization of the orbital with the valence band and the energy gain upon localization of the orbital. In the present work, the SIC approach has been implemented within the muffin–tin spheres as the basis set in KKR–CPA code.

LDA is always very poor for the impurity doped wide band gap semiconductors, M. Toyoda et al. showed that SIC-LDA calculation is good for the impurity do-doped wide band gap semiconductors GaN [15] or ZnO [16]

GaN have the wurtzite crystal structure, and their lattice constants are $a=3.180$ Å and $c=5.166$ Å, the internal coordinate u for the GaN wurzite structure is $u=0.377$ Å [10]. A fraction of Ga atoms were replaced by magnetic impurities randomly. The form of the crystal potential is approximated by a muffin–tin potential, and the wave functions in the respective muffin–tin spheres were expanded in real harmonics up to $l=2$, where l is the angular momentum quantum number defined at each site. We use higher K-points up to 425 in the irreducible part of the first Brillouin zone. In the present calculations, we used the KKR–CPA code MACHIKANEYAMA2002v09 package produced by Akai [17].

3. Results and discussion

Figs. 2 and 3 show the total and partial densities of states (DOS) for $Ga_{0.95}Fe_{0.05}N$ with LDA and SIC approximation respectively, where both majority-and minority-spin components display a band gap, which indicates that the introduction of Fe impurities does not destroy the semiconducting nature of these materials for LDA and SIC approximation. For $Ga_{0.95}Fe_{0.05}N$ the d-Fe states do not contribute to the half-metallic behavior for LDA and SIC approximation. Fig. 4 shows the band structures for spin-up and spin-down of $Ga_{0.95}Fe_{0.05}N$ within LDA and SIC approximation, in comparison with pure GaN Fig. 1, the band structures of $Ga_{0.95}Fe_{0.05}N$ changed a lot with SIC approximation compared with LDA approximation. The band gap become smaller than that of pure GaN for LDA approximation, and larger than GaN with SIC approximation, and d-Fe level is more localized in valence band compared to LDA approximation. The magnetism in the GaN-based DMSs under carrier doping treatment is investigated. Figs. 5 and 6 show the total and local density of states of $Ga_{0.95}Fe_{0.05}N_{1-x}C_x$ systems for $x=0.02$; 0.04; 0.06 and $x=0.10$ for LDA and SIC approximation. As the hole concentration increases, by the substitution of N with C, the ferromagnetic state is stabilized. Fig. 5 shows that for LDA approximation, the Fermi energy passes through the spin-up density of states and causes a delocalization of Fe d-electrons, the global energy minimum is now obtained in the Fe^{3+}state because the 3d state of Fe is partially filled. We can distinct overlap between Fe-3d and N-2p states in the spin-up bands which leads to significant DOS at the Fermi energy and hence to the half-metallic character of C co-doped $Ga_{0.95}Fe_{0.05}N$ system.

In this case holes coming from p-state of Carbon are itinerant in keeping with their d-character due to the large hybridization of the C-p states with the Fe-3d states. For this, kinetic energy is higher, so efficiently that the ferromagnetic state is stabilized by d–d RKKY exchange mechanism. For SIC approximation according to the band structure calculations (Fig. 6), due to the hole states, the majority spin-band is partially filled for p-state of Carbon atom, while, for d state of Fe atoms, it is more localized in valence band. By LDA and SIC approximation with C-doped there are carriers to mediate the long range ferromagnetic interaction. There are no contributions to the DOS from the spin-down band. The system thus behaves as a half-metallic system. We can distinct overlap between Fe-3d and C-2p states in the spin-up bands which leads to significant DOS at the Fermi energy for LDA approximation but for SIC approximation the majority spin-band is only partially filled for p-state of Carbon atom. Fig. 7 shows the mean field Curie temperature of $Ga_{0.95}Fe_{0.05}N_{1-x}C_x$ systems for $x=0.02$; 0.04; 0.06 and $x=0.10$ evaluated in the LDA and in the SIC approximations. Due to the self-interaction correction, the Fe majority d-states are shifted to lower energies, while the resonance at the Fermi level is diminished and dominated by p-state of carbon and nitrogen atoms an exchange splitting become more large for SIC approximation compared to LDA approximation. This increases the importance of ferromagnetic interaction and augmented Curie temperature for higher carriers concentration. For