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2008 J. Phys.: Condens. Matter 20 295221

(http://iopscience.iop.org/0953-8984/20/29/295221)

J. Phys.: Condens. Matter **20** (2008) 295221 (7pp) doi:10.1088/0953-8984/20/29/295221

Electronic and magnetic structures of 4f in $Ga_{1-x}Gd_xN$

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Received 3 March 2008, in final form 10 May 2008
Published 1 July 2008
Online at stacks.iop.org/JPhysCM/20/295221

Abstract

Electronic structures and magnetic properties of Gd-doped GaN have been investigated within the framework of density functional theory. First, the density of states and band structure of GdN (terminal compound of $Ga_{1-x}Gd_xN$) are presented. Second, the wurtzite type GaN:Gd magnetic semiconductors are studied by changing the Gd content. Magnetic stability, net spin exchange splitting and correlation of 4f electrons are analyzed, comparing them to the GaN:TM cases. Finally, the magnetic moment in Gd-doped GaN is calculated. Changing the Gd concentration hardly influences the magnetic moment of the system. Analyzing the $x = 0.03\,125$ case, we find that the polarized magnetic moment of N by Gd atoms is very small, only about 0.01 μ_B and the polarization of N away from Gd can be ignored. Both long range spin polarization of the GaN matrix by the Gd atoms and the obvious magnetic moment change with Gd content are not found in our work. This study provides a further understanding of electronic and magnetic structures for $Ga_{1-x}Gd_xN$.

1. Introduction

The rare-earth (RE) elements play an important role in many functional materials and exhibit rich physical properties. The type of material doped by RE metals has attracted more and more attention. Why? It is because 4f orbitals are more localized in RE metals so that the direct coupling between the 4f ions is weak, and 4f RE elements can have larger magnetic moments than the 3d transition metals (TMs). Thus, different electronic structures and novel magnetic properties are possibly observed. It is significant to study these materials containing RE elements.

GaN, with the wide direct bandgap, strong bonding, high thermo-conductivity and chemo-stability, is regarded as one of the most promising semiconductors. In particular, the dilute magnetic semiconductor (DMS) on GaN has been extensively investigated because of its potential applications in spintronic devices. Most of the materials that have been studied are semiconductors doped with the partially filled 3d TMs. The hole-mediated ferromagnetic feature at room temperature [1–3] and high T_c behavior [4] of the 3d TM-doped GaN have been well recognized. However, the high T_c behavior in the wide gap semiconductor type material is often destroyed due to the formation of precipitates [4] or compensated by n-type carriers [5]. Recently, GaN doped by the partially filled 4f RE atoms overcomes this defect and exhibits high T_c [6–10]. Furthermore, ferromagnetism has already been found in $Ga_{1-x}Gd_xN$, with T_c above 400 K [7, 11–13]. This shows that the electronic and magnetic structures in the GaN:RE system are intriguing.

On the other hand, electronic structures and magnetic properties of 4f materials are attractive too in types of rare-earth nitrides [14, 15] and Gd pnictides [16]. Hund's second rule is obeyed in all RE nitrides except for EuN and YbN, where a cubic symmetry solution has lower energy. In these cases, the divalent solution is also in competition with the trivalent solution. The symmetry breaking in most cases lowers the total energy and is essential to remove f states from the Fermi level in some cases being two electrons or holes away from a closed or half-filled shell. The spin magnetic moments are nearly integer, defined by the number of filled 4f states. The orbital magnetic moment is of comparable magnitude to the spin moment except for GdN (where the orbital moment is zero). An effective zero moment is observed in SmN, as spin and orbital moment are of nearly equal magnitude but in the opposite direction. For Gd pnictides, there is a small overlap between the conduction band at the X point and the valence band at the Γ point in the majority-spin energy band.

A small gap opens in the spin-minority energy band of GdP and GdAs, which are thus half-metallic. This spin-minority gap closes in semimetallic GdSb and GdBi. While GdN is found to be ferromagnetic, the other Gd pnictides are found to be antiferromagnetic, with ordering along [111]. These theoretical results indicate that these materials have a broad range of electronic and magnetic properties. At the same time, the study of these rare-earth nitrides and Gd pnictides enhances research interest in the GaN:RE system, too.

In particular, Dhar *et al* found a colossal magnetic moment as high as 4000 μ_B on average per Gd atom in the 400–700 nm thick GaN layer with a Gd concentration ranging from 7×10^{15} to 2×10^{19} cm^{-3} [7]. For this interesting phenomenon, Dhar *et al* suggested that the colossal magnetic moment arises from the long range polarization of Gd. From theoretical calculations, Dalpian *et al* examined the electronic structures of GaN doped by Gd in the zinc-blende type (z-type) and gave a possible explanation that the electron-induced stabilization leads to strong ferromagnetism in $Ga_{1-x}Gd_xN$ [17]. Despite the partial success in the research on f-electron material, the semiconductor material doped with RE elements has not been well understood. To get a better understanding of the nature of magnetic coupling in these RE-doped systems, electronic structures and magnetic properties of GaN:Gd in the wurtzite type (w-type) structure including the hypothetical w-GdN are investigated in detail by performing total energy and band structure calculations. Compared to the reported z-type GaN:Gd and GaN:TM cases, the results on GaN doped with Gd in the w-type structure are stressed.

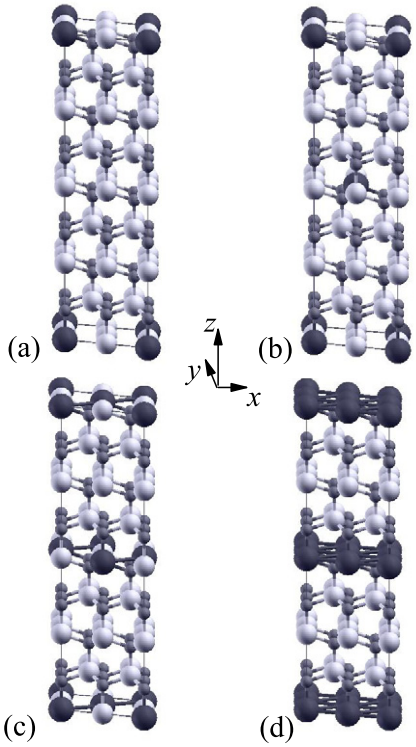

Figure 1. Gd atomic positions in the $2\times2\times4$ supercell of several doping models: (a) $x = 0.03\,125$, (b) $x = 0.0625$, (c) $x = 0.125$ and (d) $x = 0.25$. Large black, small black and large light spheres represent the Gd, N and Ga atoms, respectively.

2. Details of calculations

All electronic structural calculations have been performed in the framework of density functional theory (DFT) with the exchange–correlation functional being treated as the local spin density approximations (LSDA) in the form of Ceperly and Alder by Perdew and Wang [18]. The Kohn–Sham equations are solved using the highly accurate all-electron full-potential linear augmented plane-wave plus local orbital (FP-LAPW + lo) method [19, 20] as implemented in the WIEN2k code [21]. This method makes no shape approximation for the potential or the electron density. Within the FP-LAPW + lo calculation, the muffin-tin (MT) radii are 2.0, 1.4 and 2.2 au for Ga, N and Gd, respectively. We set $R_{MT}K_{MAX} = 7.0$ (R_{MT} is the smallest MT spherical radius present in the system and K_{MAX} is the truncation of the modulus of the reciprocal lattice vector) and $G_{MAX} = 14$ (G_{MAX} is used to truncate the plane-wave expansion of the potential and density in the interstitial region). The Ga-$3p^6 3d^{10}$, N-$2s^2$ and Gd-$5s^2 5p^6$ are treated as semicore states and the Ga-$4s^2 4p^1$, N-$2p^3$ and Gd-$4f^7 5d^1 6s^2$ are valence states.

The unit cell parameters [22] of the w-type GaN are selected as $a = 3.189$ Å and $c = 5.185$ Å, and the $2\times2\times4$ supercell is adopted in this calculation. $Ga_{1-x}Gd_xN$, $x = 0.0$, $0.03\,125$, 0.0625, 0.125, 0.25 and 1.0, are selected to simulate doping situations by changing the number of Gd atoms. Figures 1(a)–(d) show the Gd atomic positions in the $2\times2\times4$ supercell for $x = 0.03\,125$, 0.0625, 0.125 and 0.25, respectively. In this calculation, the spin orientations align along the ⟨001⟩ direction. The Brillouin-zone integrations are performed using $4\times4\times1$ Monkhorst–Pack special k points [23] for the w-type structure. Considering the balance of computational cost and precision, we inspect the variations of electronic and magnetic properties by changing the Gd–N bond length instead of optimization and relaxation.

3. Results and discussions

GaN and GdN, two terminal compounds of $Ga_{1-x}Gd_xN$, are supposed to have the same structure as the w-type. We firstly analyze their electronic structures. It is well known that GaN is a wide direct bandgap semiconductor. For GdN, our calculation demonstrates that it is an indirect bandgap semiconductor with the gap smaller than that of GaN, which is also different from GdN in the rocksalt structure where the semimetallic characteristic is observed [15]. Figure 2 exhibits the total and partial density of states (DOS) of z-GdN and w-GdN. It is found that 4f electrons form the local peak near the Fermi level. The 4f states are completely occupied in majority-spin (spin up), while they are empty in minority-spin (spin down), due to the half-filled 4f band in Gd. For w-GdN, a large number of occupied 4f states are mainly located around 2.5 eV below the Fermi level, and an almost equal number of unoccupied 4f states are localized around 2.2 eV above the Fermi level. From figure 2(b), the ionic characteristic is

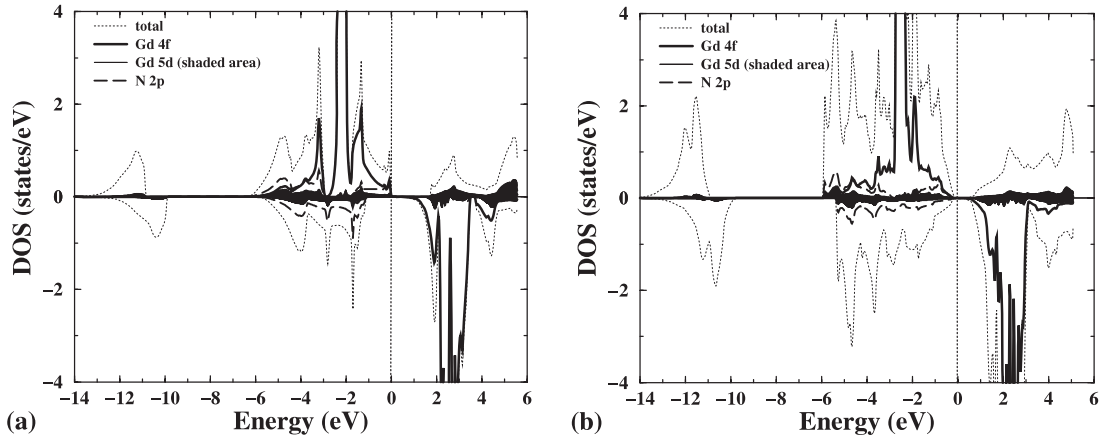

Figure 2. Total and partial DOS of GdN: (a) zinc-blende, (b) wurtzite.

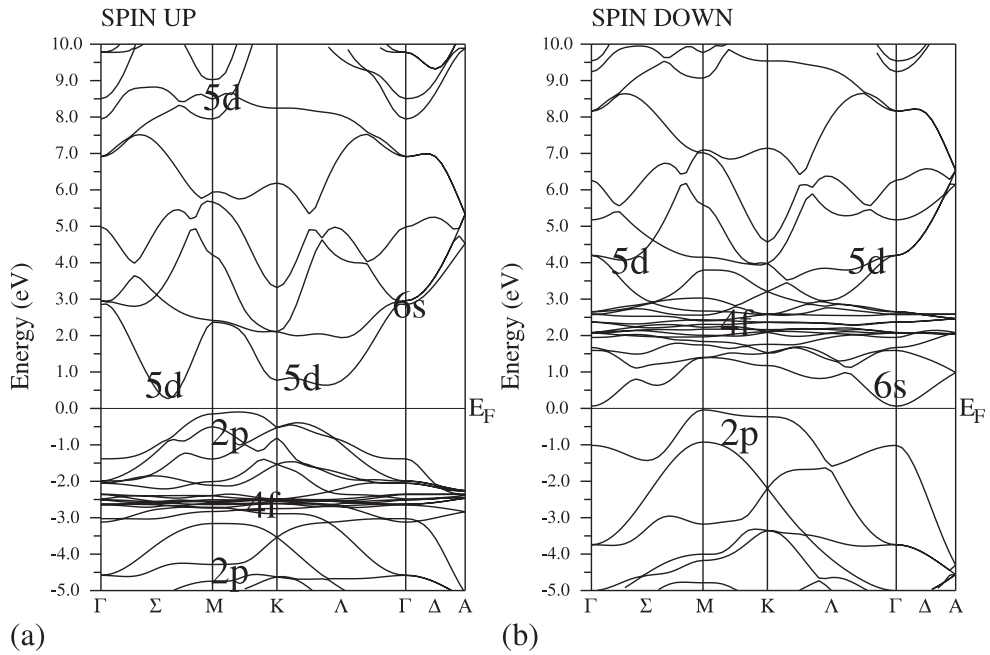

Figure 3. The calculated band structures of GdN in the w-type: (a) spin up, (b) spin down.

dominant, and the weak covalence interaction exists between Gd and N by the hybridization of Gd 5d and N 2p.

As a comparison, we refer to [17] and define the net spin exchange splitting (majority-spin maximum (minimum) subtracting minority-spin maximum (minimum) in valence bands (VBs) (or conduction bands (CBs))), $\Delta\varepsilon$, to investigate the spin splitting of electronic states induced by RE metals. For w-GdN, the net spin exchange splitting is $\Delta\varepsilon \sim -0.05$ eV in valence states and $\Delta\varepsilon \sim -0.25$ eV in conduction states. For z-GdN, the $\Delta\varepsilon$ in both valence and conduction states is about -1.0 eV. It is found that the complicated splitting of 4f orbitals and a smaller $\Delta\varepsilon$ value are present in w-GdN. Hence, the gaps of majority-spin and minority-spin channels in z-GdN are correspondingly larger than those in w-GdN. In addition, the net spin exchange splitting in w-GdN is close to MnN, but the positive $\Delta\varepsilon$ is obtained in MnN [24].

The band structure along highly symmetrical k-point (Γ (0,0,0), M (1/2, 0, 0), K (1/3, 1/3, 0), A (0, 0, 1/2)) directions also reveals the electronic characteristics of 4f in w-GdN, as shown in figure 3. For the majority-spin channel, the VBs maximum is between the M and K point, and the CBs minimum is between the Γ and M point. For the minority-spin channel, the VBs maximum is at the M point and the CBs minimum is at the Γ point. Thus, an indirect bandgap is observed in this system, especially the visible gap in the majority-spin band. Analyzing the characteristic band, in the majority-spin VBs, Gd 4f bands are in the midst of N 2p bands, which indicates that the coupling interaction between 4f and 2p orbitals exists in the same symmetrical direction. The majority-spin CBs are composed of Gd 5d bands and a small number of Gd 6s. In the minority-spin channel, the VBs mainly result from N 2p and a little Gd 5d, while the CBs are made up of Gd 6s, 5d and 4f bands. Gd 6s and 5d bands are separated by the Gd 4f band, which means that the interaction of s–d electrons is forbidden. But the spatial wavefunctional coupling interaction between Gd 4f and 6s as well as Gd 4f and 5d electrons is

Table 1. The net spin exchange splitting $\Delta\varepsilon$ (eV) in valence bands (VBs) and conduction bands (CBs) of $Ga_{1-x}Gd_xN$.

	x				
	0.03 125	0.0625	0.125	0.25	1.0
$\Delta\varepsilon$ (VBs)	−0.26	−0.22	−0.08	−1.0	−0.05
$\Delta\varepsilon$ (CBs)	−0.05	−0.11	−0.30	−0.71	−0.25

Table 2. Spin magnetic moment of Gd and N in $Ga_{1-x}Gd_xN$ with the w-type and the z-type, as $x = 1.0, 0.25, 0.125, 0.0625, 0.03\,125$, in units of μ_B.

		x				
		1.0	0.25	0.125	0.0625	0.03215
w-type	N	−0.027	−0.016	−0.017	−0.011	−0.010
	Gd	6.758	6.735	6.730	6.737	6.730
z-type	N	−0.012	−0.003	−0.010	−0.010	−0.011
	Gd	6.750	6.738	6.716	6.722	6.730

allowed in the same symmetrical direction. In addition, it is also noted that the splitting of the 4f band is more complex in the w-type GdN. Under the tetrahedral crystal field, the 4f orbitals are split into t_1, t_2 and a_1 states [17] corresponding to three obvious 4f DOS peaks in figure 2(a). While under the hexahedral environment, the splitting of 4f orbitals becomes complicated, more subbands of 4f appear in figure 3.

Regarding stability, the GaN is more stabilized in the w-type structure while the GdN is stable in the z-type structure. For GdN, the total energy of w-type is 0.3 eV per unit cell higher than that of z-type.

Furthermore, to investigate the w-GaN magnetic semiconductor doped with Gd, we analyze these $x = 0.03\,125, 0.0625, 0.125$ and 0.25 situations in $Ga_{1-x}Gd_xN$. The calculational models are shown in figure 1. Figure 4 shows their total density of states including the 4f projected density of states of a Gd atom. It is very clear that the Fermi level is always at the maximum position of the VBs with the change of Gd content. These systems are still semiconductors: however, the bandgap gradually becomes smaller with the increase of Gd content. Different from GaN:Gd, the GaN doped by TMs usually exhibits semimetallic or metallic characteristics, such as GaN:Fe [25] and GaN:Mn [26] where the Fermi level crosses the minority-spin or majority-spin band, respectively. Calculating the net spin exchange splitting, negative values are obtained in these doping systems, as shown in table 1. The net spin exchange splitting in CBs is less than that in the corresponding VBs in most cases, which is opposite to the Gd-doped GaN in the z-type. At the same time, the absolute value of $\Delta\varepsilon$ is smaller than that of GaN doped by TMs, because these f–s, f–p and f–d couplings in GaN:Gd are often weaker than those d–s, d–p hybridizations in GaN:TM. Thus, more Gd atoms in GaN only slightly enhances the magnetic coupling interaction between Gd atoms through the N atom. This is demonstrated by the spin magnetic moments of Gd and N atoms presented in table 2 for several Gd doping cases. It is found that the absolute magnetic moment increases with x, but the change is very small.

It is also well known that the 3d electronic correlation effect is very important in those cases doped with TMs, in particular the half-filled 3d band in Mn is the same as the half-filled 4f band in Gd. Therefore, the LDA + U (U is the on-site Coulomb energy) type calculation [27] is often adopted to analyze the correlation of local electrons. The U correction can lead to more exact results. Under most situations, the U can push off occupied and unoccupied states, which results in a bandgap and a strong bonding interaction and makes the system more stable. In this work, we have already performed the LSDA + U (U = 8.0 eV for Gd 4f) calculation including the spin–orbital coupling effect for $Ga_{1-x}Gd_xN$, $x = 0.0625$. As a result, it is found that the shape and energy position of electronic states are unchanged except for a very small variation in the calculated numerical values. The reason is that Gd has a $4f^7 5d^1 6s^2$ valence configuration and LSDA + U does not change the f electronic occupation in this system. This similar phenomenon is also observed in the previous calculation with the z-type structure [17]. In other words, the correlation effect of 4f electrons is not strong in this GaN:Gd system. The LSDA exchange correlation formation can give sufficient and reliable results.

From the analysis above, the 4f orbitals are more localized compared to 3d orbitals, and their splitting is also more complicated in the crystal field. The electronic energy level of 4f is lower than that of 3d in these doped GaN cases. Consequently, a weak coupling interaction exists between 4f and s (p, d) states. But the correlation feature of 4f electrons in this $Ga_{1-x}Gd_xN$ is invisible. Checking the influence of crystal distortion, the calculation is performed by changing the Gd–N bond length to discuss the variation of electronic structures. The result presents a small difference due to the variation in the Gd environment, but it is very slight because 4f electrons are localized at the deeper energy level.

The w-$Ga_{1-x}Gd_xN$ is stabilized at the antiferrimagnetic phase, which is different from those experimental results [7, 11–13]. In comparison, the z-$Ga_{1-x}Gd_xN$ [17] is also stable at the antiferrimagnetic phase while the stabilized ferrimagnetic phase is usually obtained in the GaN:TM system. In addition, the energy difference between ferrimagnetic and antiferrimagnetic phases becomes smaller in GaN:Gd, compared with that in GaN:Fe and GaN:Mn systems. It is also found that the system is more stable when the distance between Gd atoms is much smaller at certain doping concentrations. The total energy is about 11 meV lower for the nearest neighbor of Gd atoms, compared to the next-nearest neighbor situation. This situation is the opposite to some cases of GaN doped by TMs, as well as other doped compounds, such as impurities in Bi_2O_3 [28]. Moreover, the next-nearest neighbor antiferrimagnetic coupling is the most stable configuration in ZnO:Mn [29].

Another interesting aspect is the magnetism induced by 4f electrons in $Ga_{1-x}Gd_xN$. As mentioned above, a colossal magnetic moment in the GaN thin film with very low impurity concentration has been found by Dhar *et al* recently [7]. It is explained that the colossal magnetic moment results from the polarization of the surrounding non-magnetic N atoms by Gd, and this kind of polarization is long range ordering. We consequently perform a calculation to investigate the magnetic moment in the $Ga_{1-x}Gd_xN$ system. It is found that the total magnetic moment of the unit cell is close to integer,

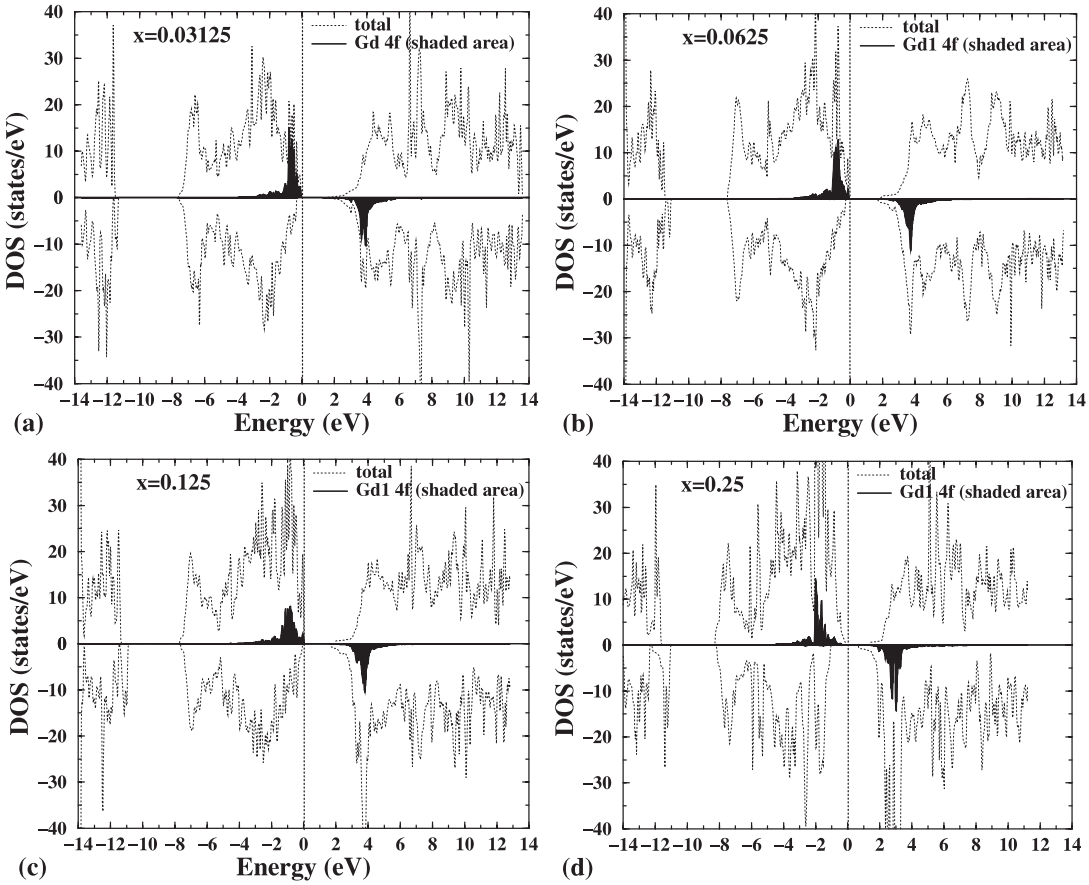

Figure 4. Total DOS of $Ga_{1-x}Gd_xN$ in the w-type, $x = 0.03\,125$, 0.0625, 0.125 and 0.25, including the 4f partial DOS of a Gd atom (shaded area).

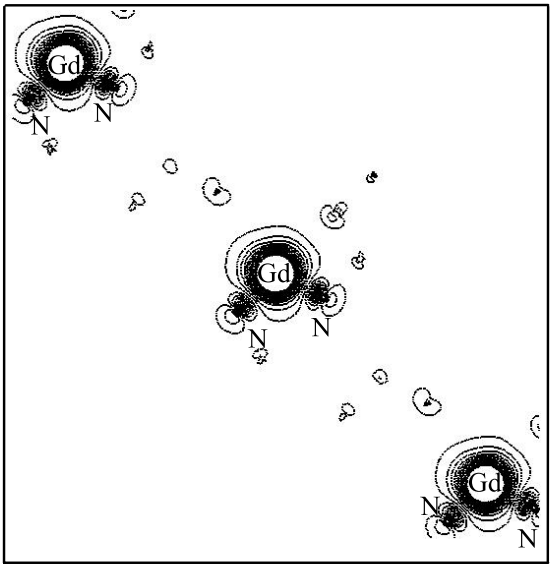

Figure 5. The calculated spin density contour on the (110) plane of $Ga_{1-x}Gd_xN$ in the w-type, as $x = 0.03\,125$.

almost 7.0 μ_B per Gd atom. The spin moment and orbital moment of Gd are on average 6.73 and 0.14 μ_B, respectively. The orbital moment of 0.14 μ_B is unexpected. Indeed, the theoretical value from Hund's rule should be zero. The possible reason is that the crystal distortion results in the incomplete degeneration of 4f orbitals under the crystal field, while the crystal distortion is just ignored in this calculation. The sum of spin and orbital moment is less than the 8.4 μ_B of free Gd^{3+}. However, the total magnetic moment mainly results from the contribution of 4f, especially its spin magnetic moment. The N atoms polarized by the nearest-neighbor Gd provide very small negative magnetic moments, only about -0.01 μ_B. The spin density contour on the (110) plane is shown in figure 5 for $Ga_{1-x}Gd_xN$ as $x = 0.03\,125$, which reflects the polarization of N atoms induced by Gd. We find that the N atoms are visibly polarized by the surrounding Gd atom, but this range of polarization of Gd is very short. Thus, the extent of polarization becomes very weak when far away from the Gd atom. Even though the N atom is the nearest neighbor of Gd, the polarized magnetic moment is only about 0.01 μ_B in the opposite magnetic moment direction. Thus, it is impossible to obtain any colossal magnetic moment in this GaN doped with Gd system. When we vary the doping concentration, table 2 confirms that the magnetic moment is almost unchanged.

In addition, further investigating the extension of polarization of Gd, we put Gd atoms close to the N atoms for the case $Ga_{1-x}Gd_xN$ as $x = 0.03\,125$. The results show that the magnetic moment of Gd decreases, to about 5.8–6.5

μ_B, although the polarized magnetic moment of N becomes slightly larger in the latter calculated situation. This calculation indicates that the small crystal distortion is not an important factor influencing the total magnetic moment in this system. The large variation of magnetic moment is not easily obtained.

From the above result, our calculated magnetic moment is far less than the experimental one reported by Dhar *et al*. By analyzing, we suggest two possible reasons as follows: the obvious contrast of impurity concentration and the difference between film and bulk of this system. On the one hand, the doping concentration in this calculation is about 10^3–10^6 times higher than the experimental one, and the impurities are homogeneously doped in our calculated system. Thus high impurity concentration will result in a small distance of two nearest-neighbor Gd atoms. As mentioned by Dhar *et al*, the polarization of the GaN matrix by Gd atoms can be described as a rigid sphere of influence around each Gd atom and this polarization is long ranged. Then those rigid spheres polarized by Gd will overlap under higher Gd concentration. Thus, the polarizations from surrounding Gd atoms will be a standoff in the overlap region. As a result, only N atoms near Gd exhibit polarized magnetic moments. From the perspective of effective polarization, the polarization is still short ranged. In contrast, with the doping concentration in the experiment, the large distance of Gd atoms possibly leads to an actual long range polarization and the large summation of polarized magnetic moments which is far larger than that of the Gd atom itself. Considering the limit of computational conditions, it is impossible to perform a calculation with so low a doping concentration of the experiment. Therefore, the large difference of concentration perhaps brings about this discrepancy, though we have tried our best to realize lower doping concentrations using a bigger supercell of the $2 \times 2 \times 4$ cell. On the other hand, it is in the Gd-doped GaN thin film that the colossal magnetic moment is observed, while the system considered in our calculation is of bulk phase character. Compared with the bulk material, the stress, strain and inhomogeneous doping probably result in the change of magnetic structures in the ultrathin film with the external magnetic field [30]. From previous research, the giant magnetic moment is just found in this kind of magnetic thin film, such as Fe and Co on or in a Cs film [31], Co-doped $SnO_{2-\delta}$ [32] thin film and Co-doped ZnO film [33]. Hence, neither the large magnetic moment change nor the long range polarization is observed in this Gd-doped GaN bulk material with the current impurity concentration range. However, our investigation advances our understanding of electronic and magnetic properties in the Gd-doped GaN bulk system.

4. Conclusions

The electronic and magnetic structures of the Gd-doped GaN have been studied within DFT. For w-GdN, the more complicated 4f electronic states and the small net spin exchange splitting are presented, compared to the z-GdN. The GaN is much more stabilized in the w-type structure, while the GdN is much more stabilized in the z-type structure. For $Ga_{1-x}Gd_xN$, the stabilized antiferrimagnetic phase and a more stabilized state induced by localized impurities are obtained in this work, which is different from GaN:TM and other doping cases. The coupling interactions between 4f and p (s, d) are weaker than those between 3d and s (p) electrons in GaN:TM. As a general conclusion, the GaN doped with Gd is always a semiconductor in the probed impurity concentration range. Furthermore, no increasing trend of magnetic moment is observed due to the short range polarization of Gd in this bulk material. The total magnetic moment of the unit cell is close to an integer and mainly arises from the spin contribution of 4f electrons, while the N magnetic moment polarized by Gd is ignorable. Even though changing the Gd–N bond length, the total magnetic moment has an invisible variation, which means that the Gd–N bond length and the small crystal distortion are not important factors leading to the large magnetic moment. Thus, our study improves our further understanding on the electronic characteristics and magnetic properties induced by 4f in the GaN:Gd system.

Acknowledgments

This work was supported by the National Science Foundation of China under grant nos. 10504036 and 90503005, the Special Funds for Major State Basic Research Project of China (973) under grant no. 2005CB623603, the Knowledge Innovation Program of the Chinese Academy of Sciences, and the Director Grants of CASHIPS. Part of the calculations were performed at the Center for Computational Science of CASHIPS and the Shanghai Supercomputer Center.

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