Effect of Gd doping on the magnetism and work function of $Fe_{1-x}Gd_x$/Fe (001)*

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(Received 3 August 2013; revised manuscript received 23 October 2013; published online 25 March 2014)

The magnetism and work function Φ of $Fe_{1-x}Gd_x$/Fe (001) films have been investigated using first-principles methods based on the density functional theory. The calculated results reveal that Gd doping on the Fe (001) surface would greatly affect the geometrical structure of the system. The restruction of the surface atoms leads to the transition of magnetic coupling between Gd and Fe atoms from ferromagnetic (FM) for $0.5 \leq x \leq 0.75$ to antiferromagnetic (AFM) for $x = 1.0$. For $Fe_{1-x}Gd_x$/Fe (001) ($x = 0.25, 0.5, 0.75, 1.0$), the charge transfer from Gd to Fe leads to a positive dipole formed on the surface, which is responsible for the decrease of the work function. Moreover, it is found that the magnetic moments of Fe and Gd on the surface layer can be strongly influenced by Gd doping. The changes of the work function and magnetism for $Fe_{1-x}Gd_x$/Fe (001) can be explained by the electron transfer, the magnetic coupling interaction between Gd and Fe atoms, and the complex surface restruction. Our work strongly suggests that the doping of the metal with a low work function is a promising way for modulating the work function of the magnetic metal gate.

Keywords: first-principles method, doping, magnetism, work function

PACS: 63.20.dk, 75.70.–i, 65.40.gh, 75.50.Bb **DOI:** 10.1088/1674-1056/23/5/056301

1. Introduction

Magnetic tunnel junctions have become important components appearing in magnetic random-access memory, the read heads of magnetic disks, and semiconductor-based spin devices. Inserting a tunnel barrier has become a key method to achieve the spin injection. However, spin injection into Si is still elusive because the Schottky barrier formation leads to a huge conductivity mismatch of the ferromagnetic (FM) tunnel contact and Si,[1] which is detrimental to spin transport and spin injection. Moreover, it cannot be solved by adjusting the tunnel barrier thickness.[2,3] An accepted route to overcome the electrical mismatch and prevent interfacial chemical reactions is to employ the tunneling of spins through an oxide barrier such as Al_2O_3.[4] Min *et al.* presented a radically different approach for spin-tunneling resistance control using low-work-function ferromagnet Gd ($\Phi = 3.1$ eV) inserted at the FM/tunnel barrier interface.[5] It was found that in this way, the resistance–area (RA) product of FM/Al_2O_3/Si contacts can be tuned over eight orders of magnitude, while simultaneously maintaining a reasonable tunnel spin polarization. It was also suggested that the lowering effective work function of the FM by inserting Gd is related to the structure and the magnetism at the Fe/Gd interface. Recently, the effect of a ferromagnetic Gd marker layer on the effective work function of Fe in a Fe/Gd/Al_2O_3/Si stack has been systematically investigated.[6] When the Gd marker thickness was changed from 0 nm to 2.7 nm, the measured effective work function of Fe at the Fe/Gd/Al_2O_3 interface was reduced from 4.5 eV to 3.7 eV. Moreover, from ^{57}Fe conversion electron Mossbauer spectroscopy, a certain degree of Fe–Gd mixing at the interface was observed. It was also suggested that, with increasing Gd interlayer thicknesses, the lowering effective work function of Fe is related to the changes of the structure and magnetism in the Fe/Gd interface. The work function can be tuned by several methods. For example, the alloying modulation of the work functions for binary alloys has been studied in experiments and theories.[7–11] Xu *et al.* have revealed that the surface alloy composition and the surface orientation can affect the work functions of MoTa and NiPt systems in a distinctive fashion.[10,11] Also, Park *et al.* have found that the submonolayer of an overlying metal can significantly affect the work functions of NiAl and PtAl systems.[12] However, up to now, the impact of Gd doping on the work function of the $Fe_{1-x}Gd_x$/Fe surface has not been studied well. In this paper, based on first principles calculation, we investigate the effect of Gd doping on the magnetism and work function of $Fe_{1-x}Gd_x$/Fe (001). The calculated results reveal that the geometrical structure of Fe(001) can be greatly affected by Gd doping. The surface restruction of atoms leads to the transition of magnetic coupling between Gd atoms from ferromagnetic for $0.5 \leq x \leq 0.75$ to antiferromagnetic (AFM) for $x = 1.0$. Moreover, the work function of $Fe_{1-x}Gd_x$/Fe (001) can be reduced by Gd doping, and the modulated range reaches 1.12 eV (from 3.86 eV to 2.74 eV).

*Project supported by the National Natural Science Foundation of China (Grant No. 11004039) and the National Basic Research Program of China (Grant No. 2011CBA00200).

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2. Method

The work functions of the $Fe_{1-x}Gd_x$/Fe (001) surfaces were calculated using a first principles method based on the density-functional theory (DFT).[13] All calculations were carried out using the Vienna *ab initio* simulation package, employing the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof for the exchange–correlation function.[10,14–22] As Gd is a typical heavy metal, the spin-orbit coupling should be considered. The moderate correlation of 3d electrons and the strong correlation of f electrons in Gd require adding an on-site Coulomb interaction U. In the GGA+U method,[23] the parameters U and J represent the on-site Coulomb interaction energy (Hubbard U) and the atomic-orbital intra-exchange energy (Hund's coupling parameter), respectively. In the calculation, the optimal values of $U_{\rm eff}$ were determined by comparing the calculated magnetic moments with the experimental and other calculated values.[24–26] Finally, the values of $U_{\rm eff}$ for Fe and Gd were chosen as 0.2 eV and 6.9 eV, respectively. All $Fe_{1-x}Gd_x$/Fe (001) surfaces were modeled by a nine-layer Gd/Fe slab with a (2×2) unit cell. The supercell contained 36 atoms, where there were 4 atoms in each layer, and the periodic boundary conditions were applied with 15 Å of a vacuum between the slabs. Brillouin-zone integrations had been performed via the Methfessel–Paxton technique[27] on a $5\times5\times1$ k mesh. A cutoff energy of 300 eV was used for the plane-wave expansion of the electron wave function. These parameters ensured a convergence better than 1 meV for the total energy. The atomic coordinates in the supercell were fully relaxed using the conjugate-gradient algorithm[28] until the maximum Hellmann Feynman force on a single atom was less than 0.02 eV/Å. After relaxation, the work functions were calculated as the differences between the electrostatic potential in the middle of the vacuum region and the metal Fermi energy.[29]

Our convergence test indicated that a slab consisting of a minimum of four metal layers is required. Subsequent calculations of the work functions of the $Fe_{1-x}Gd_x$/Fe (001) surfaces were performed using slabs of nine layers and a 2×2 surface unit cell with the four bottom layers being frozen. In order to verify our computational approach, we calculated the lattice constants and magnetic moments M of bulk Fe and Gd, the magnetic moments of the topmost layer atoms $M_{\rm sur}$, and the work functions Φ for Fe(001) and Gd(001). The calculated results and the corresponding experimental data are listed in Table 1. From the Table, it is found clearly that the calculated lattice constants, magnetic moments, and work functions are consistent with those in experiments and other calculated data from Refs. [30]–[39]. Moreover, our calculated work function of 3.86 eV is slightly less than the experimental value of 4.24 eV, which should be attributed to the strained effect in real films.[35]

Table 1. Lattice constants and magnetic moments M for bulk Fe and Gd (in GGA and GGA+U); magnetic moments of the topmost layer atoms $M_{\rm sur}$ and the work functions Φ for Fe (001) and Gd(001).

	Lattice constant/Å			$M/\mu_{\rm B}$			$M_{\rm sur}/\mu_{\rm B}$		Φ/eV		
	this work	other calculation	Expt.	this work		Expt.	this work	other	this work	other	Expt.
				GGA	GGA+U		GGA+U	calculation		calculation	
Fe	2.830	2.830[a]	2,703[b]	2.07	2.20	2.20[c]	2.98	2.98[d]	3.86	3.86[e]	4.24[f]
Gd	$a=3.636$, $c=5.783$		$a=3.622$, $c=5.74$[g]	7.50	7.63	7.63[h]	7.73	7.77[i]	2.9		3.1[j]

[a] Ref. [30]; [b] Ref. [31], experimental lattice constant is extrapolated to $T=0$ K; [c] Ref. [32]; [d] Ref. [33]; [e] Ref. [34]; [f] Ref. [35]; [g] Ref. [36]; [h] Ref. [37]; [i] Ref. [38]; [j] Ref. [39]

3. Results and discussion

To investigate the effect of Gd doping on the work function and magnetism of $Fe_{1-x}Gd_x$/Fe(001), different compositions of the surface layer for the $Fe_{1-x}Gd_x$/Fe (001) system were constructed by varying the ratio of the four Gd and Fe atoms. Four doping contents with $x=0.25$, 0.50, 0.75, 1.00 were considered. The calculated results indicated that, the Gd doping hardly influences the x and y positions of Gd and Fe atoms. In the x–y plane, the lattice constants for $x=0.00$, 0.25, 0.50, 0.75, 1.00 stay as (2.830±0.001) Å. However, the Gd doping has a great effect on their z positions. Figures 1(a)–1(e) show the side views of the atom arrangements for $Fe_{1-x}Gd_x$/Fe (001) films with $x=0.00$, 0.25, 0.50, 0.75, 1.00, respectively. For $x=0.25$, the Gd atom is higher than the other three Fe atoms on the surface layer. For $x=0.50$, both catercorner Gd atoms move outward away from the surface, and the remaining two Fe atoms are lower than the Gd atoms. For $x=0.75$, both catercorner Gd atoms move outward away from the surface, and both the remaining Fe and Gd atoms stay lower. For $x=1.00$, four Gd atoms all move outward away from the surface, while both catercorner Gd atoms are higher than the remaining ones. Especially, for $x\leq0.75$, the coupling between Gd and Fe atoms is ferromagnetic. However, for $x=1.00$, there exists antiferromagnetic coupling between Gd and Fe atoms, which is similar to the antiferromagnetic coupling between Mn and Fe for the Mn/Fe (001) film.[30] These

results should be due to the changes of the atom arrangements aroused by the Gd doping. Figure 2 shows the exchange coupling constant (J) between Gd and Fe atoms as a function of the Gd–Fe distance. Here, $J = E_{\rm AFM}–E_{\rm FM}$, where $E_{\rm AFM}$ and $E_{\rm FM}$ are the total energies of the AFM and the FM states, respectively. A positive J means ferromagnetic coupling, while a negative J indicates antiferromagnetic coupling. From the figure, it is observed that the magnetic coupling between Fe and Gd atoms is sensitive to the inter-atomic distance. Especially, when $d < 3.80$ Å, J is positive; when $d > 3.80$ Å, it becomes negative. Therefore, there exists a critical Gd–Fe distance for the transition from ferromagnetic coupling to antiferromagnetic coupling. As seen in Fig. 1, the distances of the nearest neighbor Gd and Fe atoms for $x \leq 0.75$ are all less than 3.80 Å. Thus, the magnetic coupling between Gd and Fe atoms is FM with $x \leq 0.75$. However, for $x = 1.0$, there exist two high-position Gd atoms (spin down) and two low-position Gd atoms (spin up). For the high-position Gd atoms, the distance (4.587 Å) between Gd and Fe atoms is larger than 3.80 Å, which responds to the antiferromagnetic coupling. For the low-position Gd atoms, the distance (2.749 Å) between Gd and Fe atoms is less than 3.80 Å, which responds to the ferromagnetic coupling.

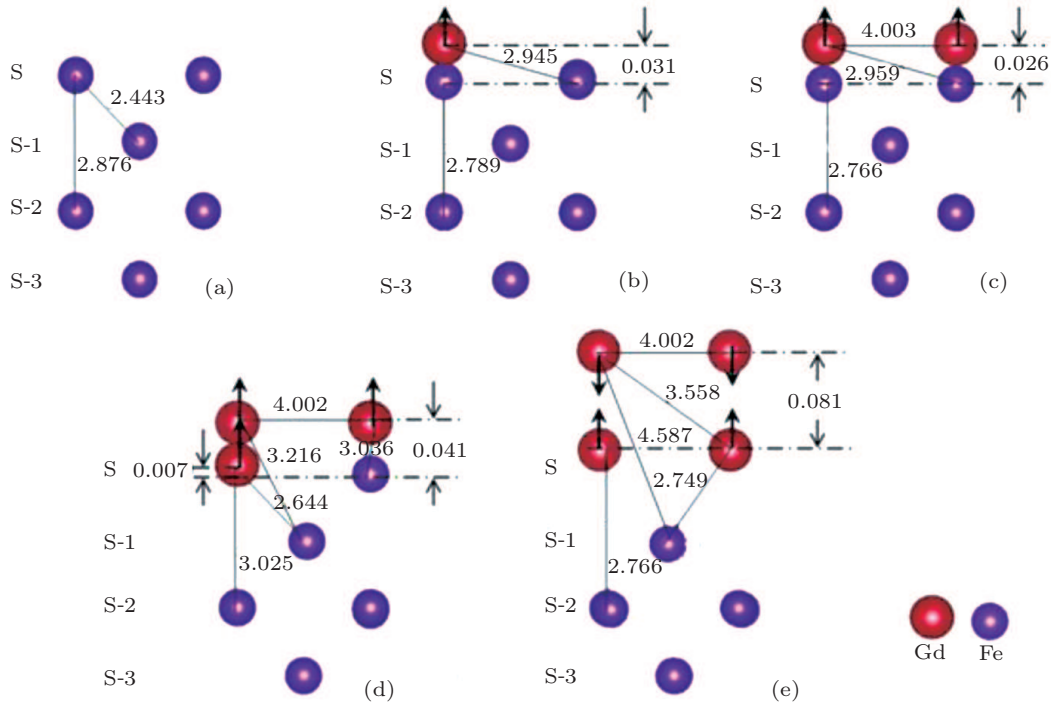


Fig. 1. (color online) Side views of the atom arrangements for the top four layers of $Fe_{1-x}Gd_x$/Fe (001): (a) $x = 0.0$, (b) $x = 0.25$, (c) $x = 0.5$, (d) $x = 0.75$, (e) $x = 1.0$.

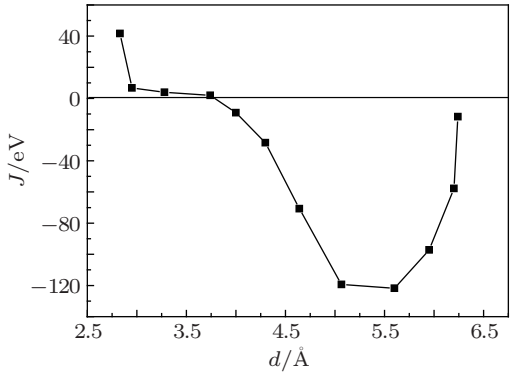


Fig. 2. Exchange coupling constant J between Gd and Fe atoms as a function of the Gd–Fe distance.

Figure 3 shows the Fermi energy and the work function as a function of Gd doping content x on the surface layer for Fe(001). From the figure, it can be found that for $x \leq 0.5$, with increasing x, the Fermi energy is increased and the work function is decreased except for $x = 0.5$. Table 2 lists the calculated

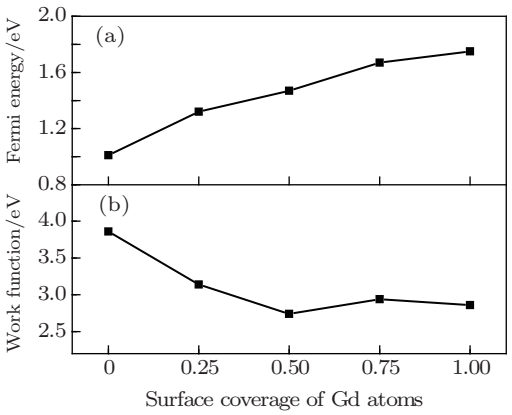


Fig. 3. (a) Fermi energy $E_{\rm F}$ and (b) work function Φ as a function of Gd doping content x on the surface layer for Fe (001).

Fermi energies E_F, work functions Φ, and magnetic moments M of the topmost three layer atoms for Gd_xFe_{1-x}/Fe(001) surfaces. As shown in Table 2, the work functions of Fe (001) can be reduced by Gd doping, which is consistent with the experimental results in Ref. [6]. It is believed that the effect of a layer of adsorbate on the work function of a surface is governed by the electronegativity of the adsorbate.[40–43] The electronegativity of Gd (1.21) is less than that of Fe (1.83), which results in an excess of positive charge on the surface layer and negative charge below the surface layer. This leads to a positive dipole, which gives rise to the reduction of the work function. Moreover, with the increase of the Gd doping content, the Fermi energy E_F is elevated due to the electron transfer from Gd to Fe. At the same time, the change of the Fermi energy E_F will also give rise to one of the magnetic moments of Gd and Fe atoms.

Table 2. The calculated Fermi energies E_F, work functions Φ, and magnetic moments M of the topmost three layer atoms for each Gd_xFe_{1-x}/Fe(001) film.

x		0.0	0.25	0.5	0.75	1.0
S	M(Gd)/μ_B		5.015	6.74, 6.17 ($\bar{M}=6.46$)	2.31, 7.31, 7.31 ($\bar{M}=5.64$)	–7.65, –7.65, 6.96, 6.96 ($\bar{M}=7.30$)
	M(Fe)/μ_B	2.98	2.56, 2.56, 2.97 ($\bar{M}=2.70$)	2.10, 2.10	1.90	
S-1	M(Fe)/μ_B	2.27	2.24	2.21	2.22	2.38
S-2	M(Fe)/μ_B	2.37	2.36	2.27	2.30	2.35
	E_F/eV	1.01	1.32	1.47	1.67	1.75
	Φ/eV	3.86	3.14	2.74	2.94	2.86

Figure 4 shows the schematic density of states $N(E)$ of ferromagnetic Fe–Gd metal alloy occurring in the presence of an effective magnetic field $H_{\rm eff}$ ($H_{\rm eff}=H+H_W$), where H is the external magnetic field, and H_W is the Weiss molecular field that is proportional to the exchange coupling constants. There is an energy shift of $-\mu_B H_{\rm eff}$ ($+\mu_B H_{\rm eff}$) for electrons with magnetic moments parallel (antiparallel) to the applied magnetic field. The electrons which flip their magnetic moments from $+\mu_B$ to $-\mu_B$ are those contained in the energy interval around the Fermi level, their number is donated by ΔN. Then, we have[22]

$$\Delta N = [N_\downarrow(E_F)+N_\uparrow(E_F)]\mu_B H_{\rm eff} \times\{1-[N_\downarrow(E_F)-N_\uparrow(E_F)]/[N_\downarrow(E_F)+N_\uparrow(E_F)]\}, \quad (1)$$

and the change of the Fermi level is given by

$$\Delta E_F = [N_\downarrow(E_F)-N_\uparrow(E_F)]\mu_B H_{\rm eff}/[N_\downarrow(E_F)+N_\uparrow(E_F)], \quad (2)$$

where $N_\downarrow(E_F)$ and $N_\uparrow(E_F)$ are the density-of-states at the Fermi level for down and up spins, respectively. Moreover, when the electrons transfer from the surface magnetic atoms to the substrate atoms, the numbers of electrons with up and down spins filling in near the Fermi level are different. It is found that the added electrons in Fig. 4 with up spins are more than those with down spins. Therefore, with increasing the number of the transfer electrons, the net magnetic moment should be increased and the Fermi level should be ascended. As Fe is replaced by Gd, the electrons of Gd will transfer into the Fermi surface of Fe. As a result, the doping of Gd will give rise to the lifting of the Fermi energy level, the decrease of the magnetic moment of Gd, and the increase of the Fe moment. However, compared to the results in Table 2, the Fe moments are instead reduced by the Gd doping, which means that there exist other factors influencing the Fe magnetic moment except for the electron transfer. The complex influence roles on the magnetic moment will be discussed in the following text.

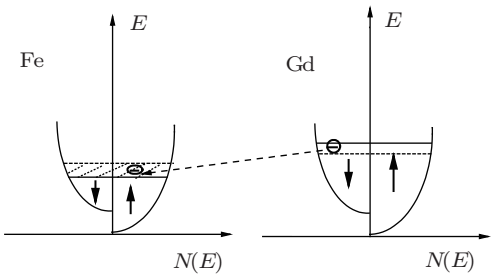


Fig. 4. Schematic density of states N(E) of ferromagnetic Gd and Fe metals.

The electron transfer is an important factor affecting the work function. Figure 5 shows the contour plot of the difference of the electron density for $Fe_{1-x}Gd_x$/Fe (001) with $x=0.25$, 0.5, 0.75. From the figure, it can be clearly seen that there exist strong Gd–Fe and Gd–Gd interactions for each $Fe_{1-x}Gd_x$/Fe (001) film. At the same time, for $Fe_{1-x}Gd_x$/Fe (001) ($x=0.25$, 0.50, 0.75, 1.00), the charge transfer from Gd to Fe leads to a positive dipole formed on the surface, which is responsible for the decrease of the work function. The change of the work function is mainly determined by the change of the Fermi level. However, the change of the surface structure can also influence the change of the work function. As shown in Fig. 1, the distance $d_{\rm Fe-Gd}$ between the Fe layer and the Gd layer increases from 0.031 Å to 0.081 Å with the increase of

Gd doping content x, except for $x = 0.5$ with 0.026 Å. The Gd–Fe interactions for $x = 0.5$ with least $d_{\mathrm{Fe-Gd}}$ (0.026 Å) are stronger than those for $x = 0.25$ and 0.75, which leads to the highest surface positive dipole. It was reported that the change of work function $\Delta\Phi$ is proportional to the surface dipole.[37] Therefore, the unusual reduction of the work function of $Fe_{0.5}Gd_{0.5}$/Fe (001) should be attributed to less $d_{\mathrm{Fe-Gd}}$.

From Table 2, it is found that the magnetic moments of Fe and Gd on the surface layer can be strongly influenced by Gd doping. As seen in Table 1, for pure Fe and Gd atoms, their surface magnetic moments are $2.98\mu_{\mathrm{B}}$ and $7.73\mu_{\mathrm{B}}$, respectively. On the Fe(001) surface, as one Fe atom is replaced by one Gd atom, on the one hand, the electrons of the Gd atom will be transfered into the Fermi surface of Fe, which will give rise to the decrease of the Gd magnetic moment and the increase of the Fe moment; on the other hand, the coupling interaction between Gd and Fe atoms has the Weiss molecular field H_{W} acting on the Fe atom reduced, which leads to the decrease of the Fe magnetic moment. Therefore, the combined actions of both factors above make the Gd and Fe magnetic moments decrease. Moreover, with increasing the Gd doping content, the average moment of the Fe atom on the surface layer is further reduced. For a low Gd doping content ($x \leq 0.25$), the moment of Fe on the surface layer is higher than that for bulk Fe, which is attributed to the surface effect.[43–46] While for $x > 0.25$, the strong Gd–Fe interaction leads to the decrease of the moment of Fe, which is consistent with the results in Ref. [47]. However, the changes of Gd magnetic moments are more complex. For all Gd_xFe_{1-x}/Fe (001) films, the average moments of Gd are lower than its surface magnetic moments ($7.73\mu_{\mathrm{B}}$), which is due to the coupling interaction between Gd and Fe. When $x \geq 0.5$, there exist the pairing Gd atoms moving outward away from the surface, as seen in Fig. 1. The magnetic moments of the pairing Gd atoms above are near the surface magnetic moments of Gd, which is attributed to a strong Gd–Gd interaction and a weak Gd–Fe interaction. For $x = 0.75$, there are two pairing Gd atoms at higher levels and one Gd atom at lower levels. Moreover, the Gd atom at lower levels has a small magnetic moment with $M = 2.31\mu_{\mathrm{B}}$ due to the strong Gd–Fe coupling.

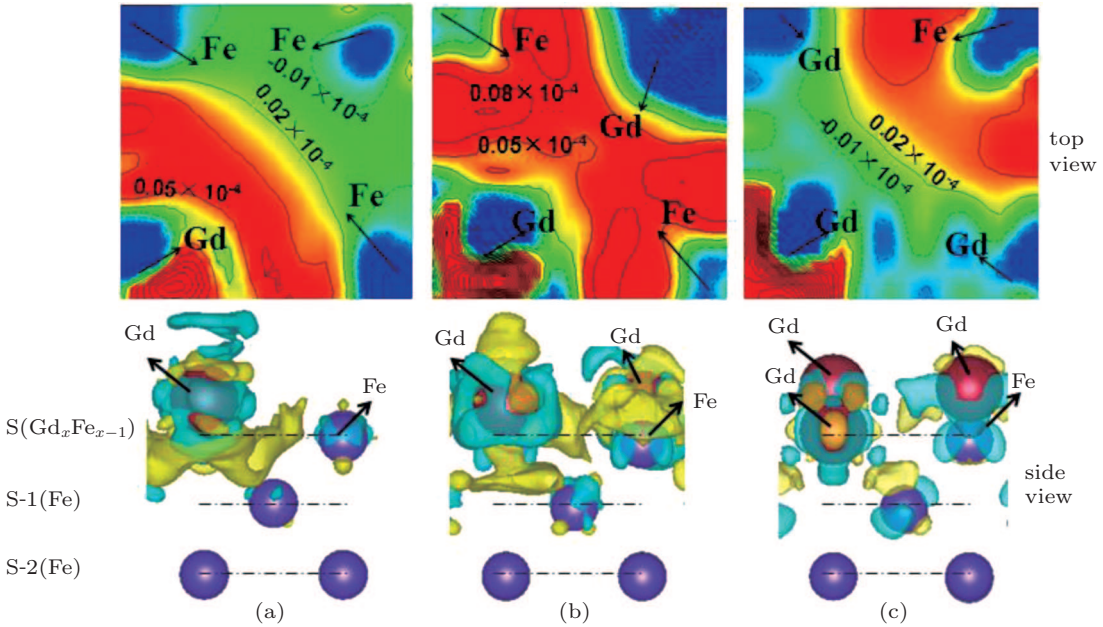


Fig. 5. (color online) Contour plot of the difference of the electron density (in e/Å ^{3}) for (a) $x = 0.25$, (b) $x = 0.5$, and (c) $x = 0.75$. Solid and dashed lines are used to label contours whose values are larger and less than zero for the 2D maps of the top view, while in 3D maps of the side view for the top three layers, positive and negative values are shown by yellow and blue, respectively.

4. Conclusion

In conclusion, we have investigated the effects of the Gd doping on the magnetism and work function of $Fe_{1-x}Gd_x$/Fe (001). It is found that the Gd doping gives rise to the restructure of the surface atoms of $Fe_{1-x}Gd_x$/Fe (001), which leads to the transition of magnetic coupling between Gd and Fe atoms from FM with $x \leq 0.75$ to mixed AFM and FM with $x = 1.00$. As the Fe atoms are replaced by the Gd atoms, the charge transfer from Gd to Fe appears. The electronegativity of Gd is less than that of Fe, which leads to a positive dipole. This is responsible for the decrease of the work function with increasing Gd doping content. Moreover, it is found that the electron transfer, Gd–Gd and Gd–Fe couplings do jointly determine the changes of the magnetic moments of Fe and Gd on the surface layer. Of course, after Gd doping, the complex surface restructure should be one of the main origins of the various changes of Gd and Fe magnetic moments.

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