Thickness-Dependent Interface Magnetism of Fe/Cr/Fe Trilayers

S. V. MAN'KOVSKY,[1] D. BALDOMIR,[2] M. PEREIRO[2]

[1]*G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, 36 Academician Vernadsky Blvd., UA-03680 Kiev-142, Ukraine*

[2]*Facultade de Fisica, Universidad Santiago de Compostela, 15706 Santiago de Compostela, Spain*

Received 10 September 2001; accepted 6 February 2002

DOI 10.1002/qua.10398

ABSTRACT: Electronic structure and magnetic properties of $Fe_N/Cr_3/Fe_N$ bcc(100) trilayers (N is the number of atomic layers) are studied on the basis of ab initio calculations performed within the framework of the density functional theory in the local spin density approximation, using the full-potential LAPW method in slab geometry. According to our calculations, the magnetic moment of a surface Fe layer increases monotonically from 2.45 μ_B for $N = 1$ to 2.92 μ_B for $N = 3$ and practically does not change at further increase of the Fe film thickness. However, the magnetic moment in the interface Fe layer changes nonmonotonically with the Fe film thickness increase and is close to the surface value at $N = 5$ and 7.
Int J Quantum Chem 91: 234–238, 2003

Key words: density-functional calculations; magnetic films; interface states; chromium; iron

Introduction

Fe/Cr multilayers and Fe/Cr/Fe (Cr/Fe/Cr) sandwich systems attract the attention because of their interesting features related to the oscillatory interlayer coupling and GMR effect. Magnetic properties of these systems were intensively studied depending on the thickness of Cr spacer and Fe film [1–8], although the influence of Fe film thickness was not taken extensively in consideration. They are related to the formation in such layered systems of 2-D quantum wells with confined electronic states, called the quantum well (QW) states [9–13], namely, the QW states are supposed to be responsible for the oscillatory interlayer coupling in layered systems and this was discussed, for example, in Refs. [14, 15]. The confinement of electronic states results also in the formation of thickness-dependent magnetic moment in Pd film on Ag substrate (at low coverage), as was found by Mirbt et al. [13] in ab initio calculations, which is conditioned by the appearance of QW states in these systems and by the thickness dependence of the energy of these states.

Correspondence to: S. V. Man'kovsky; e-mail: mankov@imp.kiev.ua.

TABLE I
Layer projected magnetic moments (in μ_B) for $Fe_N/Cr_3(100)/Fe_N$ systems.

n	Cr	Cr	Fe	Fe	Fe	Fe	Fe	Fe	Fe
1	0.62	−0.62	2.45						
2	0.35	−0.48	1.94	2.86					
3	0.71	−0.75	2.00	2.43	2.92				
4	0.49	−0.51	2.16	2.49	2.27	2.97			
5	0.64	−0.93	3.12	1.79	2.41	2.35	2.97		
6	0.58	−0.65	2.20	2.34	2.24	2.41	2.25	2.96	
7	0.50	−0.71	2.86	1.78	2.25	2.20	2.27	2.24	2.94

Computational Details

In the present work, we studied the electronic structure and magnetic properties of $Fe_N/Cr_3/Fe_N$ bcc(100) trilayers. Calculations were performed taking into account the same lattice constant value for Fe and Cr, i.e., $a_0 = 5.44$ a.u., which is the bulk bcc Cr lattice constant. The reason for making such a choice was that we have seen small differences of the results when these constants were taken differently. Ab initio electronic structure calculations were performed on the basis of a density-functional theory in the local spin density approximation. The exchange correlation potential was used in the form of Vosko et al. [16]. Kohn–Sham equations were solved using the full-potential LAPW method in slab geometry [17, 18]. The valence states were calculated in a scalar-relativistic approximation. A grid of 15 $\vec{k}$ points in an irreducible wedge of the 2-D BZ was used in the iterations and of 45 $\vec{k}$ points in the final iteration. Inside the muffin-tin spheres, basis functions with angular momentum components up to $l = 8$ were included. More than 60 augmented plane waves per atom was used for a variational basis set.

Results and Discussion

The layer-by-layer magnetic moment distributions in a unit cell for $Fe_N/Cr_3/Fe_N$ trilayers with different N values are presented in Table I. We found in our calculations that the magnetic moment of a surface Fe layer increases monotonically from 2.45 μ_B for $N = 1$ to about 2.97 μ_B for $N \geq 3$ (Fig. 1, squares). At the same time, the behavior of the magnetic moment in the interface Fe layer, according to our calculations, is nonmonotonic (Fig. 1, circles). Magnetic properties of the Fe/Cr/Fe system at small N ($N = 1, 2, 3$) were discussed in Ref. [19]. When $N > 3$, significant changes in the charge distribution near the interface Fe layer appear when the Fe film thickness is increased. Figure 2 shows that these changes are conditioned by variations of the density of minority-spin electrons, while the majority-spin density does not change significantly. Thus, the decrease of the density of minority-spin electrons in the Fe interface layer in the cases of $N = 5$ and 7 (see Figs. 1 and 2) results in a large magnetic moment in this layer that implies modification of the magnetic moment in the neighboring layers. The density of states (DOS) pictures (Fig. 3) shows that the exchange splitting of the majority- and minority-spin states is greater in the case of $N = 5$ (as well as at $N = 7$) and DOS of the occupied minority-spin states in this case is essentially smaller than at $N = 6$. Taking into account these properties, let us discuss below the following problems.

The first is to know the reason for the appearance of a large magnetic moment, m_{if}, in the interface Fe

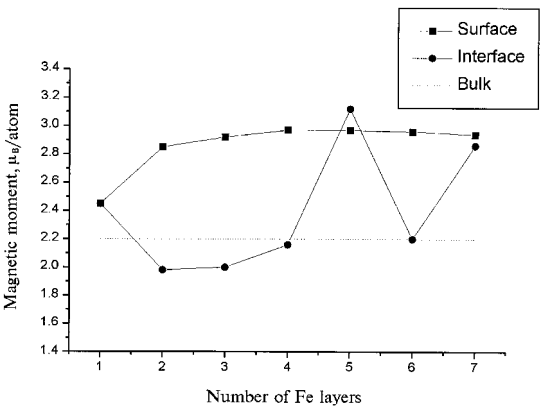

FIGURE 1. Behavior of the surface (squares) and interface (circles) Fe magnetic moments vs. the Fe film thickness.

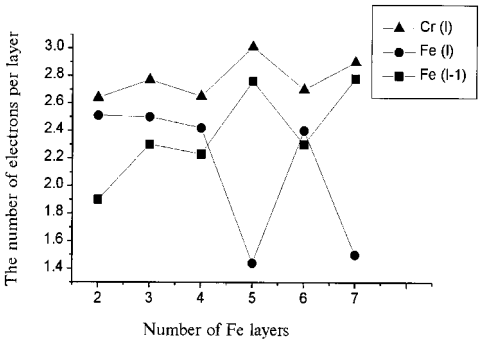

FIGURE 2. Minority-spin charge near the Fe/Cr interface vs. the number of Fe layers in an $Fe_N/Cr_3/Fe_N$ sandwich.

layer (when $N = 5$ and $N = 7$). The second is to find the explanation for the magnetic moment, m_{if}, changes in the interface Fe layer associated with the change of the Fe film thickness (note that we did not discuss here any oscillatory behaviour of m_{if} because the calculations were performed only for several values of N).

For this purpose, we studied an ideal nonmagnetic state of the system. The electronic structure calculations performed have shown that the densities of states in the interface Fe layer are close to

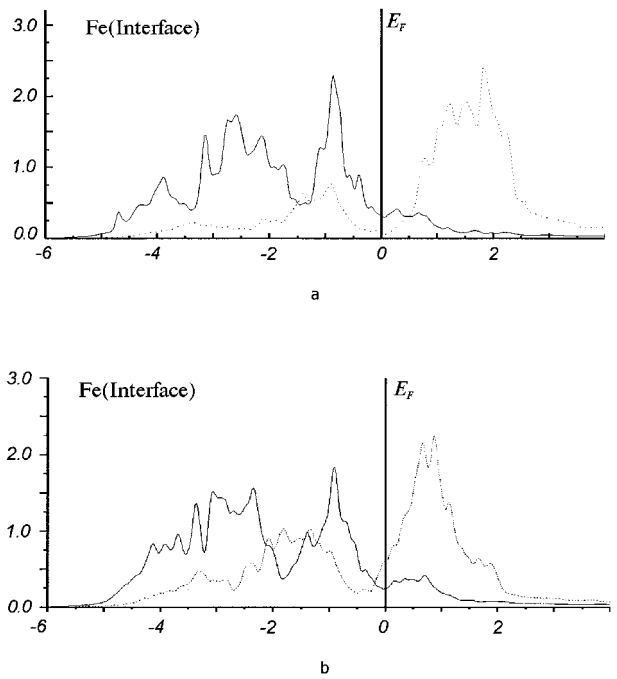

FIGURE 3. DOS for the interface Fe *d*-states in $Fe_N/Cr_3/Fe_N$ sandwiches with $N = 5$ (a) and $N = 6$ (b). Solid lines correspond to majority-spin states and dotted lines to minority-spin states.

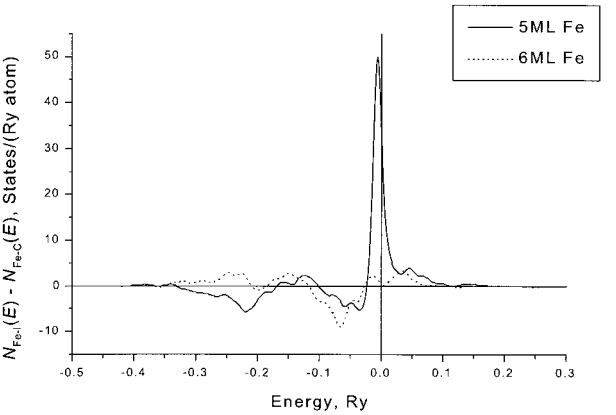

FIGURE 4. Difference between the DOS in the interface and third Fe layers for $Fe_N/Cr_3/Fe_N$ sandwiches when $N = 5$ (solid line) and $N = 6$ (dotted line).

DOS in bulk Fe (both at $N = 5, 7$ and at $N = 4, 6$) and differ from the surface DOS conditioned by the restricted number of nearest neighbors for the surface atoms. Therefore, the large magnetic moment in an interface Fe layer cannot be explained in a similar form as it happens for the increasing of the surface magnetic moment. However, considering the difference between DOS corresponding to the interface and bulk Fe layers (Fig. 4), we can see the pronounced peak below the Fermi level, when $N = 5$ and 7, whereas in the other cases ($N = 2, 4, 6$) it is not observed. This testifies to the existence of the electronic states near the Fermi level, which are distinctly localized in the interface Fe layer. Apparently, it cannot be expected that these states will influence significantly the value of the exchange splitting of electronic states (similarly to that observed in a surface layer) by the reasons mentioned above. Nevertheless, the exchange splitting results in a shift up (in the energy scale) of the states of minority-spin electrons, largely localized in the interface Fe layer, and they become unoccupied above the Fermi level. At the same time, the states of majority-spin electrons shift down in the energy scale. The unoccupied states of majority-spin electrons are not the interface resonances and therefore they are not localized significantly in any layer. Moreover, these states become almost fully occupied in the magnetic state. For these reasons, the quantity of electrons in the interface layer becomes smaller, and this occurs at the cost of minority-spin electrons. Therefore, the magnetic moment increases in the interface Fe layer and this increase is accompanied by the charge distributions mentioned above.

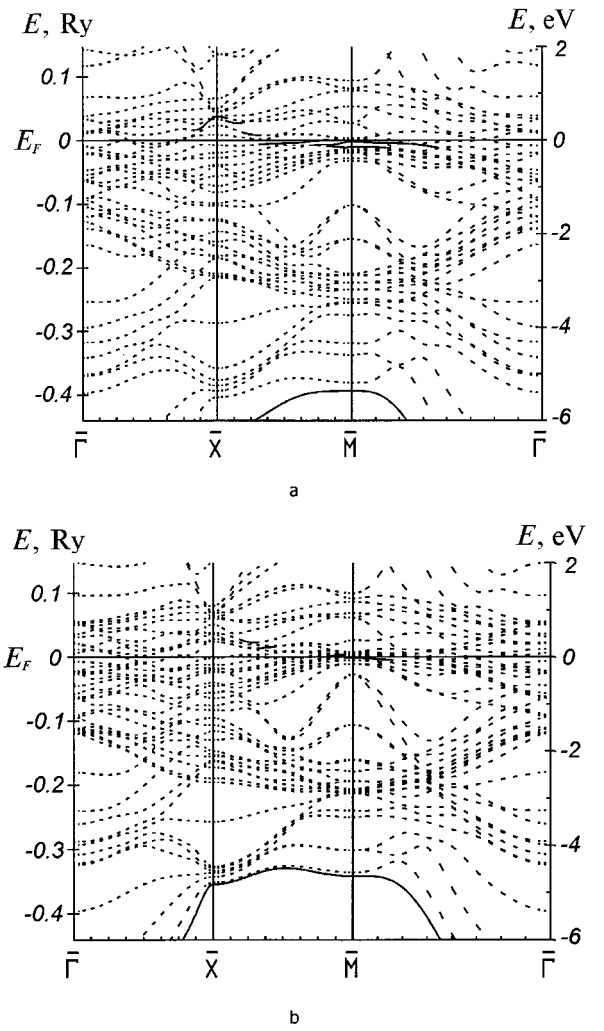

FIGURE 5. Energy bands of the even states of paramagnetic $Fe_N/Cr_3/Fe_N$ sandwiches when $N = 5$ (a) and $N = 6$ (b). Solid lines represent the states with more than 50% localization in the interface Fe layer.

The availability of the electronic states near the Fermi level, which are distinctly localized in the interface Fe layer, depends, as mentioned above, on the thickness of Fe film. Note that the interface states, as well as the surface states, should not depend on the thickness of a film because they decay fast into the film. Another pattern takes place in the case of interface (surface) resonant states. They are not localized in the restricted number of layers and, therefore, they can form the QW states when the system becomes confined (as takes place in multilayers and sandwiches). The energy position of QW states changes with the variation of the film thickness [11–13], while the resonance states arise at well-defined energy values, which depend mainly on the behavior of the potential near the interface. When the energy difference between them increases, the resonance states become more apparent in the electron energy spectrum. Just such a situation takes place in the case discussed above. Figure 5 shows the energy bands of the even states for paramagnetic $Fe_NCr_3Fe_N$ systems with $N = 5$ (a) and $N = 6$ (b). In the case of $N = 5$, we can clearly see near the $\bar{M}$ and $\bar{X}$ points and in $\bar{X}$–$\bar{M}$ direction the states significantly localized in the interface Fe layer (more than 50%). These states are responsible for the peak in the DOS differences presented in Figure 4. When $N = 6$ [Fig. 5(b)], such interface resonances practically are absent.

Conclusions

In summary, we performed ab initio calculations of the electronic structure of $Fe_NCr_3Fe_N$ sandwiches in magnetic and nonmagnetic states. We found the nonmonotonic behavior of the magnetic moment in the interface Fe layer, which is conditioned by formation in system considered of the quantum well states. Under certain conditions, these states can introduce resonances with a high degree of localization in the interface layer, which are responsible for the appearance of a large magnetic moment in this layer.

References

1. Walker, T. G.; Pang, A. W.; Hopster, H.; Alvarado, S. F. Phys Rev Lett 1992, 69, 1121.
2. Schmitte, T.; Schteyer, A.; Leiner, V.; Siebrecht, R.; Theis-Bröhl, K.; Zabel, H. Europhys Lett 1999, 48, 692.
3. Schmidt, C. M.; Bürgler, D. E.; Schaller, D. M.; Meisinger, F.; Güntherodt, H.-J. Phys Rev B 1999, 60, 4158.
4. Perkin, S. S. P.; More, N.; Roche, K. P. Phys Rev Lett 1990, 64, 2304.
5. Heinrich, B.; Cochran, J. F.; Monchesky, T.; Urban, R. Phys Rev B 1999, 59, 14520.
6. Bruno, P. Europhys Lett 1993, 23, 615.
7. Barnas, J. J Magnetism and Magnetic Materials 1992, 111, L215.
8. Vedyayev, A.; Cowache, C.; Ryzhanova, N.; Dieny, B. J Phys Condens Matter 1993, 5, 8289.
9. Ortega, J. E.; Himpsel, F. J.; Mankey, G. J.; Willis, R. F. Phys Rev B 1993, 47, 1540.
10. Pérez-Díaz, J. L.; Muñoz, M. C. Phys Rev B 1996, 53, 13583.
11. Niklasson, A. M. N.; Nordström, L.; Mirbt, S.; Johansson, B.; Skriver, H. L. J Phys Condens Matter 1999, 11, 975.

12. Klasges, R.; Schmitz, D.; Carbone, C.; Eberhardt, W.; Lang, P.; Zeller, R.; Dederichs, P. H. Phys Rev B 1998, 57, 696.
13. Mirbt, S.; Johansson, B.; Skriver, H. L. Phys Rev B 1996, 53, R13310.
14. Ortega, J. E.; Himpsel, F. J. Phys Rev Lett 1992, 69, 844.
15. Edwards, D. M.; Mathon, J.; Muniz, R. B.; Phan, M. S. Phys Rev Lett 1991, 67, 493.
16. Vosko, S. W.; Wilk, L.; Nusair, M. Can J Phys 1980, 58, 1200.
17. Cherepin, V. T.; Ostroukhov, A. A.; Tomilenko, V. N. Poverkhnost Surface 1986, 6, 43 (in Russian).
18. Weinert, M. J Math Phys 1981, 22, 2433.
19. Man'kovsky, S. V.; Cherepin, V. T. Czech J Phys 1999, 49, 1597.