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Effect of interface randomness on electronic and magnetic structures of Fe/Cr multilayers

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Abstract. We have performed the realistic tight-binding band calculations for Fe/Cr/Fe sandwiches by taking into account the interface randomness within the coherent potential approximation. It is shown that the interface randomness yields significant modifications in electronic and magnetic structures near the interface. Magnitudes of local magnetic moments on Cr and Fe atoms near the interface become larger by increasing the degree of the interface randomness. We discuss the implications of our calculation for the magnetoresistance recently observed in Fe/Cr multilayers.

1. Introduction

Much attention has been paid to the magnetotransport property in multilayers in recent years. One of the current topics in this field is the giant magnetoresistance (GMR) observed in Fe/Cr multilayers (Baibich *et al* 1988, Binasch *et al* 1989). Various experiments such as light scattering (Grünberg *et al* 1986, Saurenbach *et al* 1988), spin-polarized low energy diffraction (Carbone and Alvarado 1987) and neutron diffraction (Hosoito *et al* 1990) show that magnetic moments on successive Fe layers couple antiferromagnetically across intervening Cr layers when the Cr layer thickness is less than about 20 Å (Nguyen *et al* 1988, Krebs *et al* 1989). Recently Parkin *et al* (1990) observed the Rudenman–Kittel–Kasuya–Yosida (RKKY)-type oscillation in the Fe–Fe couplings with a period of 18–29 Å out to a Cr thickness of about 50 Å. This antiferromagnetic coupling between successive Fe layers is expected to play an essential role in the observed GMR. When an external field is absent, the coupling between successive Fe layers is antiferromagnetic and the spin-dependent scattering at interfaces leads to a large resistivity. When a strong field is applied, on the other hand, Fe moments order ferromagnetically and the resistivity is reduced on account of the disappearance of the spin-dependent scattering. Since the discovery of GMR in Fe/Cr multilayers, a similar phenomenon has been found in many multilayers such as Co/Cr, Co/Ru (Parkin *et al* 1990) and Co/Cu/NiFe/Cu (Shinjo and Yamamoto 1990). Extensive experimental studies are now in progress to discover systems with more significant GMRs.

On the theoretical side, the mechanism of spin-dependent scattering has been proposed by several authors (Camley and Barnas 1989, Barnas *et al* 1990, Levy *et al* 1990). The origin of the antiferromagnetic coupling has been discussed based on detailed band calculations using the local spin density functional method (Levy *et al* 1990a) or the realistic tight-binding model (Hasegawa 1990b, 1991, Stoeffler and Gautier 1990).

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The exchange interaction, J, between Fe moments across m-layer Cr, calculated by Hasegawa (1990b), is shown to be positive (ferromagnetic) for $0 \leq m < 1$ while J becomes negative (antiferromagnetic) for $1 \leq m < 6$. This is consistent with the antiferromagnetic couplings observed in Fe/Cr/Fe multilayers with a Cr thickness less than about 20 Å (Nguyen *et al* 1988, Krebs *et al* 1989). Owing to a limit in computer capability, this type of band calculation is restricted to the systems with small $m(\leq 6)$, and cannot explain the RKKY-type long range oscillation observed in thicker Cr layers (Parkin *et al* 1990). This RKKY-type oscillation is reproduced in the other type of calculations based on the simplified model taking into account s electrons and s–d hybridization (Wang *et al* 1990, Edwards and Mathon 1991). They cannot, however, adequately account for the short range behaviour in the observed Fe–Fe couplings. Thus the two approaches are complementary.

In these band calculations (Levy *et al* 1990a, Hasegawa 1990b, 1991, Stoeffler and Gautier 1990), interfaces in Fe/Cr multilayers are assumed to be ideal; Fe and Cr interfaces are taken to be completely separated. This is, however, not the case in real systems where some Cr atoms exist in Fe interface layers and vice versa. Quite recently Petroff *et al* (1991) reported that when the interface randomness is increased in Fe/Cr/Fe multilayers, their GMR becomes more significant. This suggests that the interface randomness would play an important role in the GMR of Fe/Cr/Fe multilayers.

It is the purpose of the present paper to investigate theoretically the effect of the interface randomness on electronic and magnetic structures in Fe/Cr/Fe multilayers. We introduce the randomness into the Fe and Cr interfaces of Fe/Cr/Fe sandwiches described by the realistic tight-binding model. The interface randomness introduced is treated within the coherent potential approximation. The distribution of local magnetic moments on Fe and Cr layers is calculated by changing the degree of the interface randomness.

The outline of this paper is as follows: in section 2 we describe the model and computation method adopted in the present study. In section 3, the calculated results are reported. The final section (section 4) is devoted to supplementary discussions.

2. Model and computational method

We assume a sandwich in which both Fe and Cr atoms lie on a common BCC lattice with (001) interface (Hasegawa 1990a). The layer parallel to the interface (001) is identified by the index, n, which is 1 for the top layer. The crystalline anisotropy is neglected for simplicity in the calculation. For a given multilayer we employed the model Hamiltonian:

$$H = H_0 + H_I \tag{1}$$

where H_0 and H_I denote the one-electron and interaction terms, respectively. The one-electron part is expressed by the tight-binding d-band Hamiltonian given by

$$H_0 = \sum_{\sigma} \sum_{j} \sum_{m} E_j a^{\dagger}_{jm\sigma} a_{jm\sigma} + \sum_{\sigma} \sum_{j,j'} \sum_{m,m'} t^{mm'}_{jj'} a^{\dagger}_{jm\sigma} a_{j'm'\sigma} \tag{2}$$

where $a^{\dagger}_{jm\sigma}$ ($a_{jm\sigma}$) is a creation (annihilation) operator of a σ-spin electron of the orbital m on the lattice site j, E_j is the core potential and $t^{mm'}_{jj'}$ stands for the two-centre transfer integrals which are given after the canonical band theory (Pettifor 1977) as

$$dd(\sigma, \pi, \delta) = (-6, 4, -1)(W_d/2.5)(S/R)^5. \tag{3}$$

Here R is the interatomic distance, S the Wigner–Seitz radius and W_d is the d-bandwidth

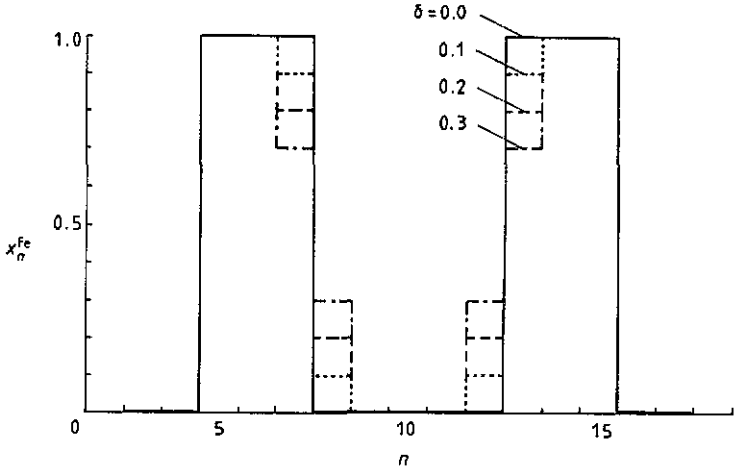

Figure 1. Concentration distribution for Fe, x_n^{Fe}, against the layer index n in Fe/Cr/Fe layers; the randomness characterized by a parameter δ is introduced in the interfaces (see text).

parameter. Transfer integrals are included up to the second-nearest-neighbour sites and those between different kinds of atoms are assumed to be given by their geometrical averages (Pettifor 1977).

The interaction term in equation (1) is given by

$$H_I = (1/4) \sum_j (U_j N_j^2 - J_j M_j^2) \tag{4}$$

where N_j (M_j) denotes the charge (magnetic moment) operator on the site j, and U_j and J_j are Coulomb and exchange interactions, respectively.

We adopted the multilayer whose configuration is given by (Hasegawa 1990a, b) $(Cu)_2/(Cr)_2/(Fe)_3/(Cr)_5/(Fe)_3/(Cr)_2/(Cu)_2/Cu(001)$. Semi-infinite Cu(001) simulates the non-magnetic substrate employed in the experiments and the outer Cr layers are added as buffers. We introduced the randomness into the interface layers at $n = 7, 8, 12$ and 13 of the inner $(Fe)_3/(Cr)_5/(Fe)_3$ layers as follows (see figure 1). It is assumed that Cr atoms may exist on the interface Fe layer with a fractional δ, and vice versa. Then the concentration of Fe (Cr) atoms on layer n, $x_n^{Fe}(x_n^{Cr})$, is given by

$$x_n^{Fe} = 1 - x_n^{Cr} = 1 - \delta \qquad \text{for } n = 7 \text{ and } 13$$

$$x_n^{Fe} = 1 - x_n^{Cr} = \delta \qquad \text{for } n = 8 \text{ and } 12.$$

The degree of the interface randomness is expressed by a parameter δ, which is zero for ideal, perfect interfaces. The effect of the interface randomness introduced is taken into account by employing the extended coherent potential approximation (Shiba 1971). After some manipulations, we obtain the self-consistent equations determining the number of electrons and local magnetic moments of atom α (=Fe and Cr) on layer n as follows:

$$N_n^\alpha = N_{n\uparrow}^\alpha + N_{n\downarrow}^\alpha, \; M_n^\alpha = N_{n\uparrow}^\alpha - N_{n\downarrow}^\alpha \tag{5}$$

Table 1. Parameters (in units of eV) used in the calculation.

Atom	E_n	W_d	U_n
Cr	5.80	8.00	0.67
Fe	3.80	6.12	0.80
Cu	0.00	4.08	0.80

with

$$N_{n\sigma}^{\alpha} = \int^{\varepsilon_F} d\varepsilon\, \rho_{n\sigma}^{\alpha}(\varepsilon) \tag{6}$$

$$\rho_{n\sigma}^{\alpha}(\varepsilon) = (-1/\pi)\,\mathrm{Im}[K_{n\sigma}(z)/[1 - ((\Xi_{n\sigma}(z) - L_{n\sigma}^{\alpha}(z))K_{n\sigma}(z)]/r^{\alpha}] \qquad z = \varepsilon + \mathrm{i}0. \tag{7}$$

In equations (5) to (7), $r^{\alpha} = W_d^{\alpha}/W_d^{\mathrm{Cr}}$ (α = Fe and Cr), and $K_{n\sigma}(z)$ is the local coherent Green function of σ-spin electrons on layer n of the alloy, which is evaluated by the transfer matrix method for a given set of the coherent locators, $\Xi_{n\sigma}(z)$ (Falicov and Yudurain 1975, Hasegawa 1986). They are given as the solution of the CPA equation:

$$K_{n\sigma}(z) = \langle K_{n\sigma}(z)/[1 - (\Xi_{n\sigma}(z) - L_{n\sigma}^{\alpha}(z))K_{n\sigma}(z)]\rangle^{\alpha} \tag{8}$$

with

$$L_{n\sigma}^{\alpha}(z) = (z - E_{n\sigma}^{\alpha})/r^{\alpha} \tag{9}$$

$$E_{n\sigma}^{\alpha} = E_{\alpha} + \tfrac{1}{2}(U_{\alpha}N_n^{\alpha} - \sigma J_{\alpha}M_n^{\alpha}) \tag{10}$$

where the bracket $\langle\ \rangle^{\alpha}$ stands for the configuration average over α. It is easy to see that the coherent locator on interface layers with no randomness ($\delta = 0$) is simply given by

$$\Xi_{n\sigma}(z) = L_{n\sigma}^{\alpha}(z). \tag{11}$$

The average magnetic moment on layer n, M_n, is given by

$$M_n = \langle M_n^{\alpha}\rangle^{\alpha}. \tag{12}$$

We assumed $U_j = J_j$ to reduce the number of parameters and treated them within the Hartree–Fock approximation. The U value for Fe was chosen such that we obtain the ferromagnetic ground state with magnetic moments of 2.2 μ_B. We chose U for Cr so as to obtain the commensurate antiferromagnetic states with the sublattice moment of 0.6 μ_B. These are consistent with the local spin density functional calculations for BCC Fe (Moruzzi *et al* 1978) and Cr (Kübler 1980, Kulikov *et al* 1981). The U value for Cu was assumed to be the same as that of Fe. The number of d-electrons for Cr, Fe and Cu were taken as 5.0, 7.4 and 10.0 per atom, respectively. The core potentials, E_j, were chosen to preserve the local charge neutrality, neglecting slight deviations near the interfaces (Hasegawa 1990b). The band parameters, W_d, U_n and E_n, employed in our calculations are summarized in table 1.

The averages of local magnetic moments and number of electrons, M_n^{α} and N_n^{α}, were calculated self-consistently by an iterative method (Hasegawa 1986). The iteration was continued until initial and resultant M_n^{α} and N_n^{α} agreed within an assumed accuracy of 0.025 μ_B/atom and electrons/atom. By adopting a variety of initial trial solutions, we repeated our calculations looking for solutions which are locally stable in the configuration space.

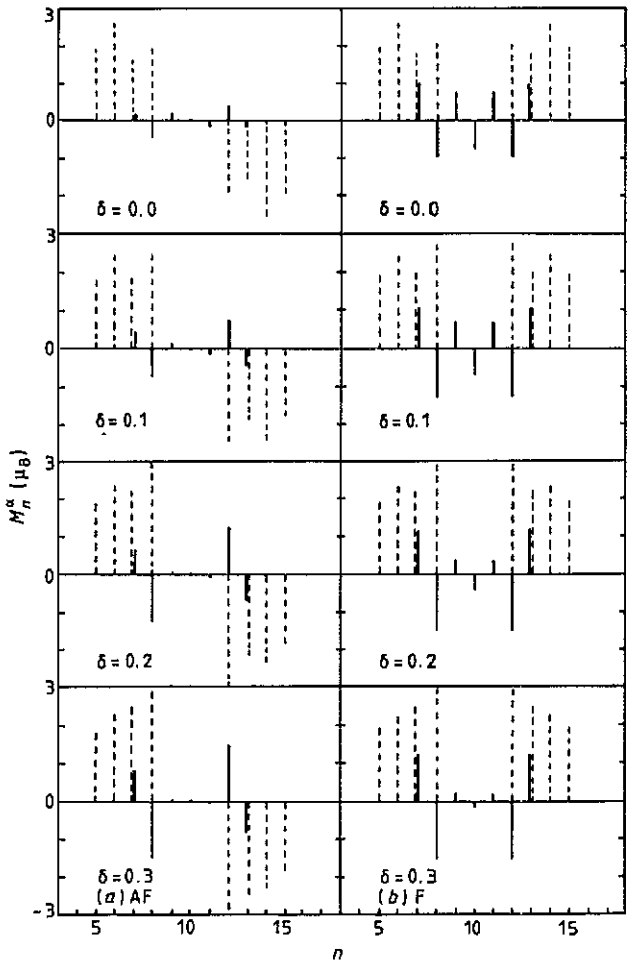

Figure 2. Local moment distribution of (*a*) AF and (*b*) F solutions in the inner Fe/Cr/Fe layers by changing the degree of interface randomness, δ, local moments on Cr and Fe layers being shown by full and dashed curves, respectively.

3. Calculated results

In the previous calculation for Fe/Cr/Fe sandwiches with ideal interfaces (Hasegawa 1990b, 1991), we obtained the stable F and AF solutions; in the former (latter) solution, magnetic moments on successive Fe layers are parallel (antiparallel). This is also realized again in the present calculation including the interface randomness.

Figures 2(*a*) and (*b*) show the calculated moment distributions of the AF and F solutions in the inner Fe/Cr/Fe layers, respectively; local moments on the outer, buffer Cr layers in this calculation are almost the same as in the previous calculation (Hasegawa 1990b, 1991). Results for the perfect interface, $\delta = 0$, are shown in the top figures, where Cr moments on $n = 7$ and 13 (Fe moments on $n = 8$ and 12) are plotted as local moments in the single-impurity limit ($\delta \rightarrow 0$). A local moment of *impurity* Cr is antiparallel to that of *host* Fe (Friedel 1958). Conversely, an *impurity* Fe moment is parallel to that of a *host* Cr moment.

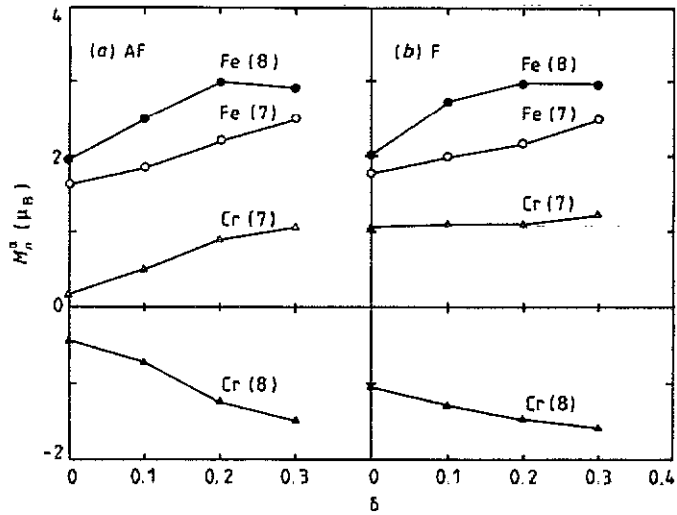

Figure 3. Local moments on interface Fe and Cr layers in (*a*) AF and (*b*) F solutions against δ, numbers in the brackets denoting the layer index n.

When the interface randomness, δ, is introduced, local moments near the interfaces are modified. Figures 3(*a*) and (*b*) show Cr and Fe moments at interfaces in the AF and F solutions, respectively, as a function of δ. We note that as δ is increased, the magnitudes of Fe and Cr moments at the interfaces are much increased.

4. Discussion

Our calculation has shown that the effect of interface randomness on the electronic and magnetic structures is significant in Fe/Cr/Fe multilayers, which is expected to modify their magnetotransport property. In order to understand the observed randomness dependence of the GMR in Fe/Cr/Fe multilayers (Petroff *et al* 1991), we consider the spin-dependent scattering at interfaces (Camley and Barnas 1989, Barnas *et al* 1990, Levy *et al* 1990b). Here we assume that the spin-dependent scattering potentials, V_n^{ex}, at Fe/Cr interfaces given by

$$V_n^{ex} = \tfrac{1}{2}U_{Cr}M_n^{Cr} - \tfrac{1}{2}U_{Fe}M_n^{Fe} \tag{13}$$

are important. Their square averages become

$$\langle (V_n^{ex})^2 \rangle = \delta(1-\delta)(U/2)^2(M_n^{Cr} - M_n^{Fe})^2 \tag{14}$$

where $U = U_n^{Cr} \sim U_n^{Fe}$. Equation (14) suggests that, as the interface randomness, δ, is increased, the GMR is increased because $\langle (V_n^{ex})^2 \rangle$ is increased not only by an increase in the factor $\delta(1-\delta)$ but also by an increase in the term $(M_n^{Cr} - M_n^{Fe})^2$ arising from an enhanced magnitude of local moments (figure 3). This is *qualitatively* consistent with the experiment by Petroff *et al* (1991) showing that the GMR becomes more significant with increased interface randomness in Fe/Cr multilayers. For a *quantitative* discussion, it would be necessary to include the contribution from the interface scatterings caused by bulk scattering asymmetry (Fert and Campbell 1976) and, more basically, to develop

an advanced theory for the GMR explicitly including the interface randomness. It would also be necessary to make similar studies on other systems besides Fe/Cr/Fe multilayers both by experimental and theoretical methods.

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