Journal of Magnetism and Magnetic Materials 140–144 (1995) 503–504

ELSEVIER

journal of magnetism and magnetic materials

Giant magnetoresistance from first principles

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Abstract

The transport properties of Co/Cu multilayers are calculated from first principles in the ballistic regime. Magnetoresistances as large as 120% are obtained in the geometry with the current perpendicular to the interface plane. The s–d hybridization is found to play an essential role in giving rise to this giant magnetoresistance effect.

We present a theoretical study of the giant magnetoresistance (MR) in antiferromagnetically coupled magnetic multilayers which emphasizes the importance of band structure effects. Giant MR arises when the anti-parallel magnetizations of adjacent magnetic layers are forced to become parallel by an external magnetic field [1]. Electrical transport experiments are carried out in the Current-Perpendicular-to-the-interface-Plane (CPP) geometry [2–5] as well as in the more conventional Current-In-Plane (CIP) geometry.

Our aim is to examine the effect of realistic band structures on the transport properties of transition metal multilayers. The Landauer–Büttiker formalism that has been used previously to study transport in a semiclassical effective mass approximation [6,7] can be readily extended to include band structure effects. The Landauer conductance formula [8] is then rewritten by labeling the ingoing and outgoing states at the Fermi energy by the component $q_{\perp\hat{n}}$ of the crystal momentum inside the first Brillouin zone perpendicular to the transport direction $\hat{n}$, the band index ν and the spin index σ:

$$G = \frac{e^2}{h} \sum_{q_{\perp\hat{n}}\nu\sigma, q'_{\perp\hat{n}}\nu'\sigma'} |t_{q_{\perp\hat{n}}\nu\sigma;q'_{\perp\hat{n}}\nu'\sigma'}|^2. \qquad (1)$$

The calculation of the transmission probabilities $|t_{q_{\perp\hat{n}}\nu\sigma;q'_{\perp\hat{n}}\nu'\sigma'}|^2$ from incident mode $q_{\perp\hat{n}}\nu\sigma$ to transmitted mode $q'_{\perp\hat{n}}\nu'\sigma'$ is in general difficult. We therefore begin by considering the perfectly ballistic regime of a point contact [9], where we only have to count the number of transverse modes N_σ. This regime should be experimentally accessible. Furthermore, Asano et al. [10] have pointed out that whereas the existence of CIP-MR depends critically on interface impurity scattering, this is not true of CPP-MR. The ballistic (Sharvin) conductance is proportional to the sample cross section A and the projections $S_{\nu\sigma}$ of the Fermi surfaces for the different bands on the plane normal to $\hat{n}$ [11,12]:

$$G_{\hat{n}} = \frac{e^2}{h}\sum_\sigma N_\sigma = \frac{e^2}{h}\frac{A}{4\pi^2}\frac{1}{2}\sum_{\nu\sigma} S_{\nu\sigma}(\hat{n})$$

$$= \frac{e^2}{h}\frac{A}{4\pi^2}\frac{1}{2}\sum_{\nu\sigma}\int \mathrm{d}q\,|\hat{n}\cdot\nabla_q \epsilon_{\nu\sigma}(q)| \times \delta(\epsilon_{\nu\sigma}(q) - E_F). \qquad (2)$$

To evaluate Eq. (2) we calculated the bandstructures $\epsilon_{\nu\sigma}(q)$ from first principles in the local-spin-density approximation using the linear muffin-tin orbital method in the atomic spheres approximation [13] for a series of (100) oriented Co_n/Cu_n multilayers. The unit cell contains n atomic layers of Co followed by n atomic layers of Cu. The charge and spin densities in the parallel configurations were calculated self-consistently and the corresponding band structures determined. For $n \geq 3$ the bandstructures in the anti-parallel configuration were calculated from a potential obtained by interchanging the spin densities from the parallel configuration on alternating Co_n/Cu_n cells. The influence of calculating the spin-densities self-consistently was studied for $n = 1$, 2 and found to be unimportant. We adapted the linear analytic tetrahedron method [14] to obtain the number of channels from the band structure and a large number of k-points was used to obtain well converged results. For example, the band structure was calculated at as many as 55 000 points in the full Brillouin zone for the Co_4/Cu_4 results discussed below.

Fig. 1 shows the projections of the Fermi surfaces in the CPP direction for the two spins of a (100) oriented Co_4/Cu_4 multilayer in the parallel configuration. The

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SSDI 0304-8853(94)00575-3

total black area is only a rough measure of the conductance because some sheets of Fermi surface might be projected on top of one another. Although not visible in the figure, this effect is taken into account correctly in the numerical results. The fourfold symmetry reflects the symmetry of the underlying lattice. The 'white rings' are gaps due to the periodic potential of the multilayer. The Fermi surface of the multilayer minority spin is complicated because of the d-bands in cobalt. Localized quantum well states are observed for the minority spin (thin lines). The projection (for either of the two degenerate spins) in the anti-parallel configuration (not shown) resembles the projection for the minority spin but the number of gaps is twice as large because the size of the unit cell is doubled.

Fig. 2 summarizes our results for a series of (100) oriented Co_n/Cu_n multilayers in the CPP geometry. The calculated CPP-MR for large layer thicknesses is comparable to experimental values ($\sim 90\%$ for (1.2 nm Co + 1.1 nm Cu) (100) oriented multilayers [5]), even though impurity scattering has been completely neglected. We emphasize that *no* empirical parameters or other phenomenological input have been used. Neglecting the sp–d hybridization in the calculation reduces the CPP-MR to almost zero from which we conclude that this hybridization is of crucial importance to describe the giant MR effect. For the CIP, on the other hand, the calculated MR is much smaller and impurity scattering appears to be much more important.

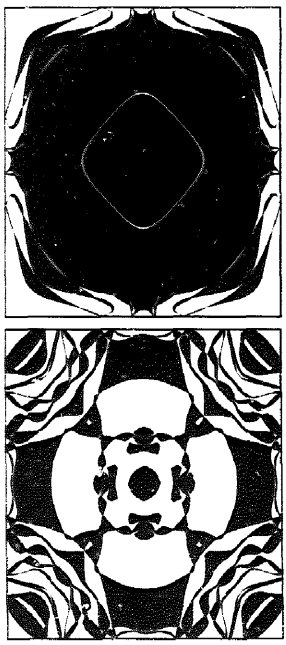

Fig. 1. The projections of the Fermi surfaces on a plane parallel to the interfaces for the majority (top) and the minority spin (bottom) of a (100) oriented Co_4Cu_4 multilayer in the parallel configuration. The black parts represent the projected Fermi surfaces inside the first Brillouin zone. The Γ-point is in the middle of the figures.

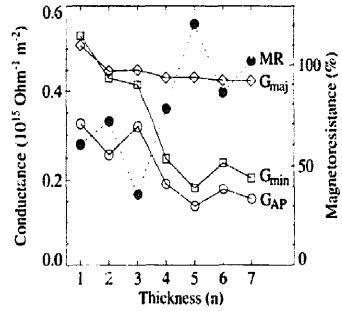

Fig. 2. The thickness dependence of the MR (●) and of the conductances G for the majority (◇) and the minority (□) spin in the parallel configuration and for both spins in the anti-parallel configuration (○). The MR is defined as $(G_{maj} + G_{min} - 2G_{AP})/2G_{AP}$.

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