Giant Magnetoresistance from an Electron Waveguide Effect in Cobalt-Copper Multilayers

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Calculations of the electrical conductivity and giant magnetoresistance of cobalt-copper multilayers show that these properties can be strongly affected by a waveguide effect. Majority electrons in cobalt have a lower Fermi momentum than in copper. This leads to total internal reflection of electrons whose momentum parallel to the interface exceeds a critical value. This waveguide effect will strongly influence the current distributions in the multilayer if the interfaces are sufficiently smooth, and it will contribute to the giant magnetoresistance if the scattering rates are significantly different in copper and cobalt. [S0031-9007(96)00092-0]

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Giant magnetoresistance (GMR) is a change in the electrical resistance of an inhomogeneous system that occurs when an applied magnetic field aligns the magnetic moments in different parts of a material. This phenomenon has aroused interest because it can be used to make magnetic field sensors and because it gives valuable insight into spin dependent transport. Since its discovery in 1988 [1,2], the source of the GMR effect has been the subject of much discussion. It is usually attributed to "spin dependent scattering," i.e., different scattering rates for majority and minority electrons. A detailed understanding of its origin, however, remains elusive.

In this Letter we show that majority electrons in cobalt-copper multilayers may undergo total internal reflection within the copper layers if the component of their Fermi momentum parallel to the layers exceeds the Fermi momentum of cobalt. These reflected or "channeled" electrons will therefore be confined to the copper layers, and, if the scattering rates are significantly lower in the copper than in the cobalt, they will give a large contribution to the majority current and a large contribution to the GMR. In order for this "waveguide" effect to occur, the interfaces must be smooth on an atomic scale.

Copper has eleven valence electrons per atom, 5.5 in each spin channel [3], while cobalt has nine valence electrons per atom, approximately 5.3 in the majority spin channel and approximately 3.7 in the minority channel. Figure 1 shows a cut through the majority spin Fermi surfaces of cobalt and copper. These are plots of the component of the wave vector perpendicular to the layers, $k_\perp$, as a function of the two dimensional wave vector in the plane of the layers, $\mathbf{k}_\parallel$. For the calculations illustrated by this plot, the layers are perpendicular to the (111) direction; and $k_\perp$ therefore describes propagation in the (111) direction. The particular cut shown is for $k_\parallel$ along

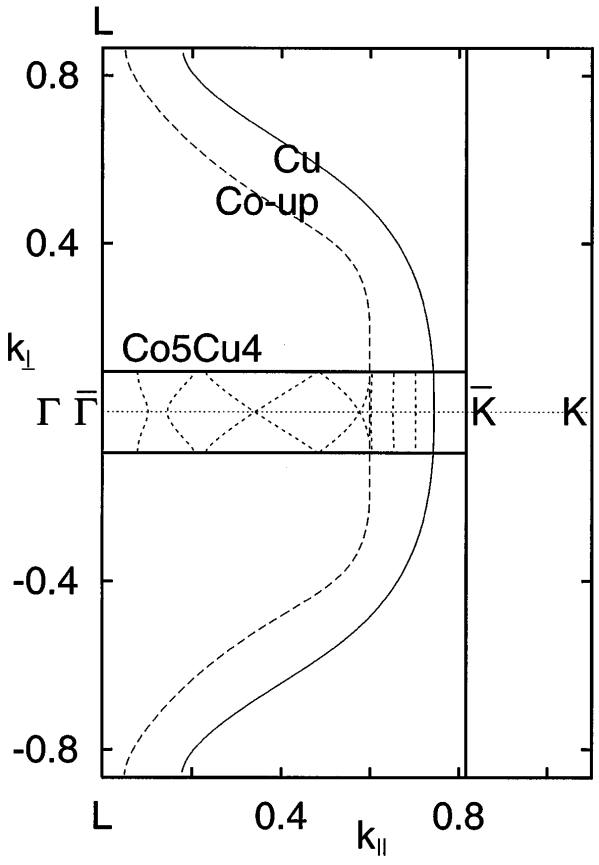

FIG. 1. Cuts through Fermi surfaces of bulk copper, majority bulk cobalt, and majority Fermi surface of a periodic Co_5Cu_4 (111) multilayer. The labels $\bar{\Gamma}$ and $\bar{K}$ refer to points at the center and corners, respectively, of the hexagonal two dimensional Brillouin zone. The points labeled Γ, L, and K refer to symmetry points in the three dimensional Brillouin zone. $k_\parallel$ and $k_\perp$ are expressed in units of $2\pi/a$, where a is the fcc lattice constant.

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the $\bar{\Gamma}$ to $\bar{K}$ direction in the hexagonal two dimensional Brillouin zone for fcc {111} layers. The feature we wish to emphasize is that regions of $\mathbf{k}_\parallel$ exist for which there are allowed values of $k_\perp$ for copper but no allowed values of $k_\perp$ for cobalt. Electrons in copper with these values of $\mathbf{k}_\parallel$ will be completely reflected by the copper-cobalt interface.

Figure 1 also shows the majority spin Fermi surface of a periodic multilayer consisting of alternating cobalt and copper layers. The layers consist of five atomic {111} planes of cobalt alternating with four atomic {111} planes of copper. The Fermi surface of the multilayer can be understood by imagining that the copper Fermi surface has been sliced into nine slices above and nine slices below the $k_\perp = 0$ plane, and the surface folded back in what is known as the "reduced zone scheme" construction. The actual Fermi surface of Co_5Cu_4 is then a distortion of this reduced zone Fermi surface of copper.

Note the two vertical "bands" in Fig. 1 which lie inside the copper Fermi surface but well outside the cobalt Fermi surface. These two bands correspond to regions of $\mathbf{k}_\parallel$ for which electrons can propagate in copper but not in cobalt. We shall show that they consist of electrons that are confined mainly within the copper layers. The fact that they have no dispersion in $k_\parallel$ means that they are localized in the direction perpendicular to the layers. These states can be thought of as two modes of an electron waveguide.

Interestingly, there is a region of small $k_\parallel$ near the "necks" in majority cobalt for which electrons can propagate in the cobalt but not in the copper. *These states contribute to channeling within the cobalt.* However, they have only a small effect on the total current.

We discovered these channeling modes as we were attempting to understand calculated results for the conductivity and giant magnetoresistance of cobalt-copper multilayers. We approached the problem of electron transport in systems which are inhomogeneous on a scale smaller than an electronic mean free path by calculating the nonlocal conductivity, $\sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}')$, which relates the current in direction μ at point $\mathbf{r}$ to the local applied field in direction ν at point $\mathbf{r}'$, $J_\mu(\mathbf{r}) = \sum_\nu \int d\mathbf{r}' \, \sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}') E_\nu(\mathbf{r}')$. In our calculations we made the approximation that the local applied field (which we define to be the change in the local field due to the externally applied electromotive force) is constant over an atomic cell. Then we defined $J_\mu(i)$ to be the average of the current in atomic cell i and $E_\nu(j)$ to be the local applied field at atom i. This allowed us to relate the current at site i in direction μ in an inhomogeneous system to the local applied field at site j in direction ν through the intersite conductivity $\sigma_{\mu\nu}(i, j)$; $J_\mu(i) = \sum_{\nu,j} \sigma_{\mu\nu}(i, j) E_\nu(j)$.

We calculated the intersite conductivity by evaluating the quantum mechanical linear response by means of the Kubo-Greenwood formula [4–7]. We wrote this formula in terms of the Green function $G(E, \mathbf{r}, \mathbf{r}')$ which we evaluated using multiple scattering theory. In particular, since we are primarily interested in layered systems, we have found it efficient to use the Layer-Korringa-Kohn-Rostoker technique [8] because it allows the efficient calculation of the Green function of a layered system. This technique is particularly effective for transport calculations because all calculations can be performed at a single energy.

In systems which consist of stacks of atomic planes which have a common underlying two-dimensional periodicity, it is convenient to calculate the nonlocal *layer* conductivity, $\sigma_{\mu\nu}(I, J)$, which is the current in direction μ in atomic plane I due to an applied electric field of unit magnitude in direction ν applied in atomic plane J [6]. $\sigma_{\mu\nu}(I, J)$ is given in terms of the nonlocal conductivity $\sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}')$ by integrating over the atomic cells in plane J and averaging over the atomic cells in plane I,

$$\sigma_{\mu\nu}(I, J) = N_I^{-1} \sum_{i \in I} \sum_{j \in J} \sigma_{\mu\nu}(i, j) \,. \tag{1}$$

Here N_I is the number of cells in plane I and the sums run over the cells in planes I and J, respectively.

We calculated the electronic structure and the nonlocal conductivity of periodic multilayers consisting of five {111} atomic planes of cobalt alternating with four (111) atomic planes of copper. This system is similar to one for which a very large GMR, $\Delta\rho/\rho > 0.35$, was observed [9] at room temperature. The stacking was assumed to be fcc for all of the layers. After the electronic structure was calculated self-consistently, the effective LDA potentials were shifted by an imaginary self-energy equal to $i\hbar/2\tau$ where τ is the electronic lifetime which was different in the copper and cobalt layers. This procedure is described in detail in Ref. [7]. The scattering rate for the copper layers was chosen to give the room temperature resistivity of typical sputtered copper films (2.8 $\mu\Omega$ cm) and the scattering rate for the cobalt layers was determined by the room temperature resistivity of typical cobalt films (14.8 $\mu\Omega$ cm) and by the assumption that the scattering rate in the minority channel was about 7 times higher than in the majority channel, a ratio equal to the ratio of the Fermi energy state densities in the two channels. Figures 2(a) and 2(b) show results of these calculations for the majority and minority channels, respectively, for the case in which all of the cobalt moments are aligned. Figure 2(c) shows the nonlocal conductivity for one of the channels for the case in which alternate layers of cobalt have their moments antialigned. Figure 2(d) shows the difference of the total nonlocal layer conductivity in both channels between the aligned and antialigned cases. The figures show $\sigma_{xx}(I, J)$ where x is a direction parallel to the {111} planes. The arrangement of the atomic planes as shown in the figures is $Cu_2|Co_5|Cu_4|Co_5|Cu_2$, periodically repeated. Thus atomic planes, I or J = 1, 2, 8–11, 17, and 18 are copper, while atomic planes 3–7 and 12–16 are cobalt.

The most striking feature of Fig. 2(a) is the large conductivity localized on the copper layers. The values of nonlocal conductivity $\sigma(I, J)$ when I and J are both in the same copper layer are larger than they would be in bulk copper. This surprising enhancement of the local conductivity in the copper is due to the electron channeling effect

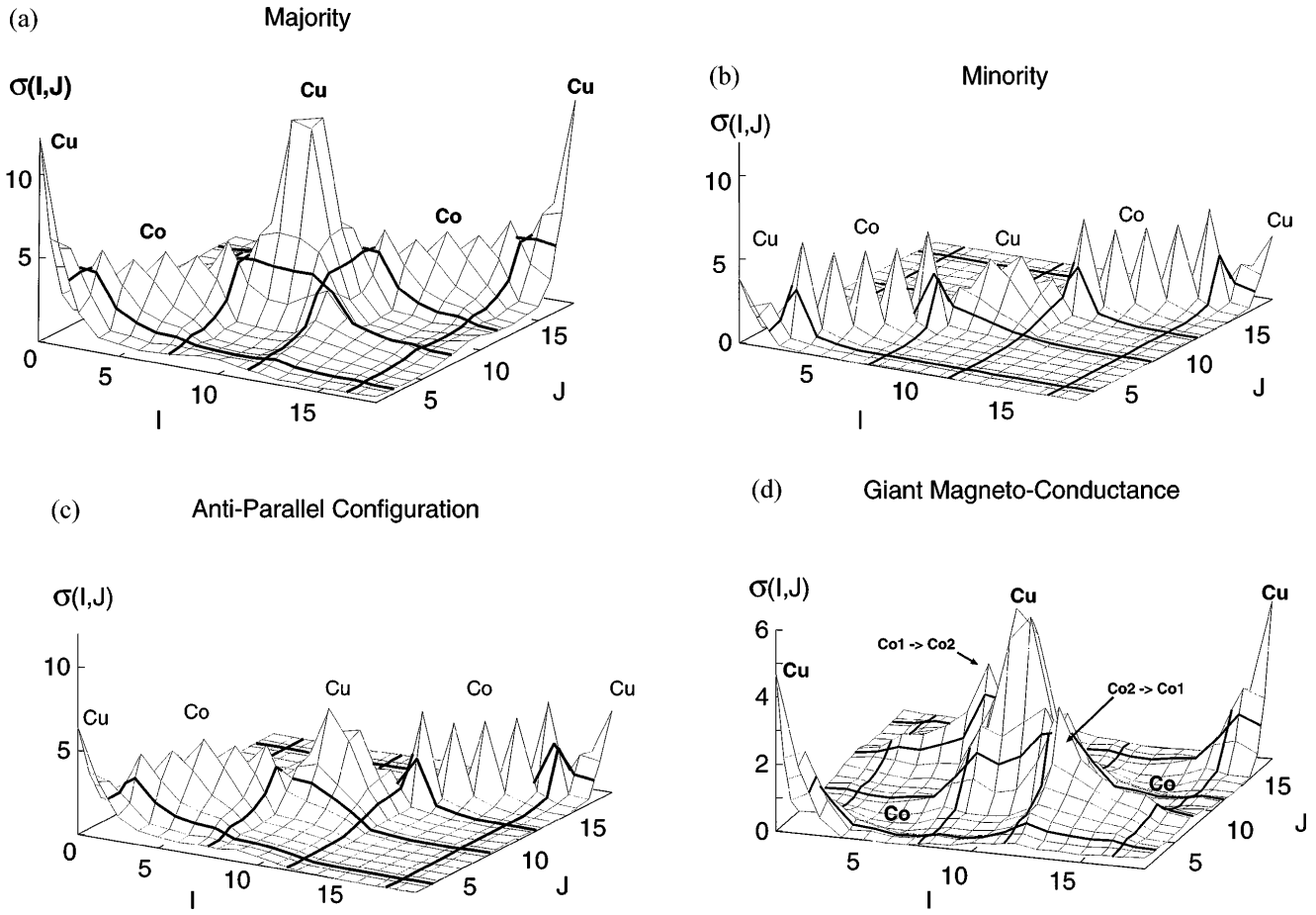

FIG. 2. Nonlocal layer dependent conductivities assuming different scattering rates for the cobalt and copper layers. (a) Majority spin conductivity for parallel alignment of cobalt moments, (b) minority spin conductivity for parallel alignment of cobalt moments, (c) conductivity for antiparallel alignment, and (d) giant magnetoconductance. Conductivity is in units of $10^{15}\ s^{-1} = 1113/\Omega\ cm$.

described above. Channeling effects also increase the conductivity of the antialigned moment configuration but not nearly so much as the majority aligned.

Figure 2(d) shows the contributions to the giant magnetoconductance, i.e., the difference between the conductivity of both channels for the moments aligned and the conductivity of both channels with the moments antialigned. In addition to the channeling effect which causes a large contribution to the GMR when I and J are both on the same copper layer there is an important contribution which arises from electrons which sense a field in one cobalt layer, propagate through the copper, and contribute to the current in a different cobalt layer. This effect causes the peak for $I = 12$ and $J = 7$ (or $I = 7$ and $J = 12$) and is more closely related to previous theories of GMR [10–12]. The GMR obtained by summing over the contributions shown in Fig. 2(d) is $\Delta\sigma/\sigma_{AP} = 0.34$. We also calculated the GMR for the case in which the scattering rates were the same in both spin channels in the cobalt with the common scattering rate chosen to give the observed resistivity of cobalt. The value of the GMR obtained for this case was 0.11, with a significant contribution coming from channeling. Note that channeling provides a mechanism for GMR distinct from "spin dependent scattering."

Figure 3 shows majority band contributions to the local conductivity $\sigma(I, I)$ for the interior atomic plane in the copper layer and the central atomic plane in the cobalt layer as a function of $\mathbf{k}_\parallel$ along the line from $\bar{\Gamma} \rightarrow \bar{K}$. One can see the large contribution to the conductivity in the copper plane coming from the two channeling peaks and the smaller conductivity in the cobalt plane coming from the cobalt channeling mode associated with the copper necks.

We also observed the electron channeling effect in cobalt-copper spin valves. We calculated the electronic structure and the nonlocal conductivity of a spin valve consisting of ten atomic {111} copper planes with ten {111} cobalt planes (with fcc stacking) on either side. We observed strong enhancement of the majority conductivity in the copper layers for parallel alignment when the scattering rate at the cobalt-copper interface was sufficiently low. For the same scattering rates assumed in the multilayer calculations displayed in Fig. 2, we observed a GMR, $\Delta\sigma/\sigma_{AP}$, of 0.26, with a major contribution coming from electron channeling. Five channeling modes were observed along the line $\bar{\Gamma} \rightarrow \bar{K}$ in the two dimensional Brillouin zone.

Our observation of electron channeling in calculations of the conductivity and giant magnetoresistance raises

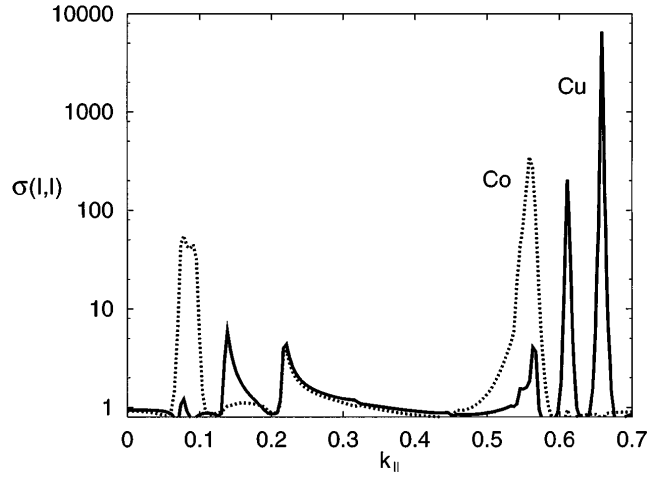

FIG. 3. Majority band contributions to the local layer dependent conductivity for points in the two dimensional zone along $\bar{\Gamma} \rightarrow \bar{K}$. The solid line is interior copper atomic plane, and the broken line is central cobalt plane. Units for $k_{\|}$ are au^{-1}.

the question of whether the interfaces were sufficiently smooth for this effect to have been important in experiments already performed and if not, whether the interfaces can be made smoother thereby producing larger values of GMR. In this regard we note that the calculated values of the GMR are in reasonable agreement with those observed experimentally in cobalt-copper multilayers. We do not mean to suggest that electron channeling is the only means to achieve GMR or even that it occurs in all systems. Our preliminary investigation of the Fermi surfaces of iron and chromium, for example, has not found an obvious channeling situation. The majority Fermi surface of permalloy should be very similar to that of cobalt so channeling would be expected to occur in the permalloy-copper system if the interfaces were structurally and magnetically perfect, which, unfortunately, we do not expect to be the case [13] unless, perhaps, they are coated with a thin layer of cobalt [14].

Our results are very different from the predictions of small or negative effects of electron channeling by Hood and Falicov [15] who treated the semiclassical free electron model and by Vedyayev *et al.* [16] who used the quantum free electron model. Levy [12] also concluded that potential steps such as might be used to model the copper cobalt interface in a free electron model should have only a small effect on the GMR. Our results differ from theirs at least in part because they employed the free electron model. This model *may* give a useful qualitative description of the majority electronic structure of copper cobalt, but it is not at all appropriate for minority cobalt. Channeling does not occur in copper for the minority channel of copper-cobalt {111} multilayers because there are no regions of $\mathbf{k}_{\|}$ for which there are copper states but no cobalt states.

It is important to distinguish the channeling or waveguide effect described here from the quantum well states that can lead to oscillatory interlayer magnetic coupling. These quantum well states occur in the *minority* channel for Co|Cu multilayers [17,18], whereas the channeling states occur in the *majority* channel. Furthermore, the quantum well states are associated with extremal vectors perpendicular to the layers and thus usually connect states which do not contribute to the conductivity parallel to the planes.

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