Quantum calculation of giant magnetoresistance in layered magnetic films

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We compute the magnetoresistance of a step-potential model of an FeCr multilayer. We use a Boltzmann-equation method incorporating exact quantum-mechanical wave functions obtained by a transfer-matrix method. The only parameters required are the (spin-dependent) potentials and effective masses of the bulk materials, and the bulk and surface densities of point scatterers. Oscillatory magnetoresistances of the order of several percent are obtained *without* spin-dependent scattering, due to Fermi-surface necking effects.

In this Brief Report we give results for the magnetoresistance (MR) in a simple model of an FeCr multilayer, which has been found experimentally[1] to exhibit a large ("giant") MR. This effect has been observed in many different systems,[2] which suggests that it is not sensitive to details of the band structure of specific materials, so that a simple model based on free-electron-like band structures might be adequate to explain the data semiquantitatively.

We model the multilayer by a potential function which is constant within each layer, but which may depend on spin. The system has Fe magnetic layers alternating with Cr spacer layers, so if the Fe layers are aligned ferromagnetically, the overall periodic unit consists of two layers. This is the well-known Kronig-Penney model, for which the wave functions can be calculated analytically. We have developed a transfer-matrix scheme[3] that gives the exact result for an arbitrary number of layers, so we can handle the antiferromagnetic case (a four-layer period), as well as nonperiodic multilayers of arbitrary thickness. We calculate the wave functions at a sample of several hundred points on the Fermi surface for each spin, and solve the Boltzmann equation[3] to obtain the conductivity parallel to the layer planes. The result depends on the relative alignment of the magnetic layers, which is antiferromagnetic (AF) at zero magnetic field (for suitable choices[4] of Cr layer thickness d_{Cr}) and switches to ferromagnetic (F) at high field. The difference between the F and AF conductivity results determines the MR.

The scattering kernel used in the Boltzmann equation depends on the scattering mechanism assumed. We assume a distribution of delta function scattering potentials $V_0\ \delta(\mathbf{r}-\mathbf{r}_{\mathrm{SC}})$ located at points $\mathbf{r}_{\mathrm{SC}}$, both in the bulk (where their density in layer L is ρ_L^b) and at the interfaces (where their areal density at interface I is ρ_I^i). The scattering probability from state $\mathbf{k}$ to a volume element $d\mathbf{k}'$ is[3]

$$Q(\mathbf{k},\mathbf{k}')d^3k' = \hbar^{-1}V_0^2 D^{-1}(2\pi)^{-2}(d^2k'_{\mathrm{FS}}/\hbar v) \times \Big[\sum_I \rho_I^i |\psi_{\mathbf{k}}^*(z_I)\psi_{\mathbf{k}'}(z_I)|^2 + \sum_L \rho_L^b \int_0^D |\psi_{\mathbf{k}}^*(z)\psi_{\mathbf{k}'}(z)|^2 dz\Big] \quad (1)$$

where z_I is the position of the Ith interface, D is the total periodicity distance (the sum of 2 or 4 layer thicknesses in the F and AF case, respectively), v is the velocity, and $d^2\mathbf{k}'_{\mathrm{FS}}$ is the area of Fermi surface contained in $d^3\mathbf{k}'$. We have used the exact values of $\psi_k(z_I)$ at the interfaces in Eq. (1); interference effects can cause it to vary considerably. The bulk term in Eq. (1) is an average over z and varies much less; we have used $\psi=1$ for simplicity. The relaxation rate $\tau_{\mathbf{k}}^{-1}$ for state $\mathbf{k}$ is obtained by integrating Eq. (1) over the Fermi surface. The in-plane conductivity is an integral of the relaxation time over the Fermi surface;[3] if we denote the effective mass by m^* and assume it is the same for all layers,

$$\sigma=\sigma_{xx}=(2\pi)^{-3}e^2 m^{*-1}\int (v_x k_x \tau_{\mathbf{k}}/v)d^2k_{\mathrm{FS}} . \quad (2)$$

The scattering probability due to interface I in Eq. (1) is proportional to $V_0^2\rho_I^i$. In choosing a model for this quantity, we note that interfacial roughness is found experimentally[5] to enhance the giant magnetoresistance. The scattering centers in this case are atoms situated on the wrong side of the interface; the perturbation to the potential at such an impurity site is the difference between the atomic potentials of the two materials. Within our step-potential model, this is just the potential jump ΔV_I at a step I. Allowing also for interface scattering due to impurities or lattice defects, which does not depend on the potential difference, we thus parametrize the interface scattering by

$$V_0^2\rho_I^i = S_{\mathrm{si}} + S_{\mathrm{sd}}(\Delta V_I)^2 . \quad (3)$$

For notational consistency, we parametrize the bulk scattering by

$$V_0^2\rho_L^b = S_{\mathrm{bulk}} \quad (4)$$

so that the free parameters S_{si}, S_{sd}, and S_{bulk} control the spin-independent, spin-dependent, and bulk scattering respectively.

Most previous giant MR calculations have been based on the semiclassical Boltzmann-equation approach of Sondheimer and Fuchs,[6,7] in which reflection or refraction of electrons at interfaces is taken into account through reflection and transmission coefficients (usually free parameters, although they have also been calculated from quantum scattering theory[8]). Our fully quantum-

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mechanical approach goes beyond this in that it accounts for interference between waves reflected at different interfaces. Interference effects are probably negligible for large layer spacing d, but may be important for the thinner (10–20 Å) layers that have now been investigated experimentally.[4] Quantum-mechanical calculations have also been carried out by a tight-binding method for clusters[9] and sandwich structures,[10] and by a more abstract approach based on a Kubo formalism[11] and leading to a local or nonlocal[12] conductivity from which the overall conductivity of the layered structure is obtained by integration.

In the free-electron model, the electron density is related to the Fermi energy E_F, Fermi wave vector k_F and potential V by

$$N=(2\pi)^{-3}(4\pi/3)k_F^3 , \quad E_F-V=(\hbar^2/2m^*)k_F^2 . \quad (5)$$

In a free-electron model of a real material, N represents the density of itinerant electrons, moving in a weak pseudopotential determined by the core potentials and the electrons bound in the cores. Thus the number of itinerant electrons per atom need not be an integer—these are plane wave states, which may include admixtures of both s- and d-like orbitals. In the present calculation we need to choose three potentials $V_{\mathrm{Fe}+}$, $V_{\mathrm{Fe}-}$, and V_{CR}, where + and − refer to the spin directions. We have taken the relative values of these V's from the work of Inoue *et al.*[13] Relative to the mean Fe potential, these are $V_{\mathrm{Fe}\pm}=\pm 0.81$ eV, $V_{\mathrm{Cr}}=0.56$ eV. To set the absolute levels (i.e., the Fermi energy), we have chosen N_{FE^+} to be 2 electrons/atom = 30 Å^{-3}. Setting the energy origin at E_F, this gives $k_F=1.93$ Å^{-1} and $V_{\mathrm{Fe}^+}=-3.52$ eV. The resulting values of all the potentials are given in Table I.

We have assumed the Fe and Cr layers are of equal thickness d, and used values of d from 1.0 to 12.0 Å. The lower values are experimentally unrealizable, but note that d can be scaled up or down by changing the assumed itinerant-electron density. We show some sample Fermi surfaces in Fig. 1; note that the left-hand (inner) sheets are quite free-electron-like (a circle sliced by horizontal planes).

We use the conservative (intrinsically <1) definition

$$\mathrm{MR}\equiv\frac{1/\sigma(\mathrm{F})-1/\sigma(\mathrm{AF})}{1/\sigma(\mathrm{AF})} \quad (6)$$

for the magnetoresistance. (Note that we use the traditional sign here: MR > 0 if the resistance increases with field.) The magnetoresistance result with only bulk scattering and no interface scattering (Fig. 2) is easiest to understand. The conductivities of + and − spins in the F case, and the spin-independent conductivity in the *AF* case, are only weakly dependent on layer thickness d. The relaxation rate τ^{-1} is just proportional to $N(E)S_{\mathrm{bulk}}$, where $N(E)$ is the density of (final) states at the Fermi level. The conductivity σ is proportional to $n\tau$, where n is the electron density, so

$$\sigma \propto n/N(E)S_{\mathrm{bulk}} . \quad (7)$$

Both n and $N(E)$ are larger for the majority spin than the minority, but n differs more [in a free electron model, $N(E)\propto k_F$ but $n\propto k_F^3$] so $\sigma_{\mathrm{F}^+}>\sigma_{\mathrm{F}^-}$. If σ_{AF} (per spin) were exactly midway between these two, the MR would exactly vanish; it can be seen from Fig. 1 that it is slightly positive. This cannot be understood from a purely free electron model, which predicts it to be negative. With a perturbing potential, however, the circular Fermi surface is distorted near the Brillouin zone boundaries (the horizontal line $k_z=\pi/D$ in Fig. 1) in such a way as to decrease its area and the density of states. Because the periodicity D is larger ($4d$) in the AF case than in the F case ($2d$), the Brillouin zone is smaller, so the Fermi circle in Fig. 1(c) is chopped into more slices. This reduces the density of states more in the AF case, so its conduc-

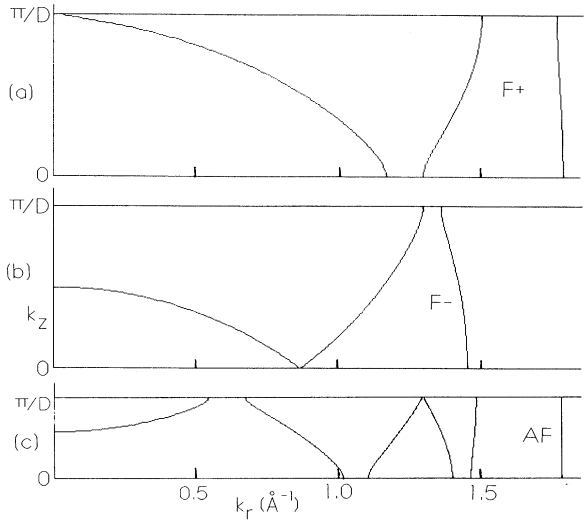

FIG. 1. Cross sections of the Fermi surface for the (a) majority spin, (b) minority spin in the ferromagnetic configuration, and (c) the antiferromagnetic configuration of FeCr, using $d=2.685$ Å (the point marked "1a" in Fig. 2). The vertical axis (k_z) is the component perpendicular to the layer planes, and k_r is parallel to them. The FS is a solid of revolution about the vertical axis. In the repeated zone scheme, the leftmost piece is a "lens" and the other pieces are undulating cylinders. The FS is a screen dump from an IBM-PC program that calculates the MR; anyone interested in a copy should contact the authors.

TABLE I. The parameters used in the calculations. Only one of S_{si} and S_{sd} is nonzero in each calculation. The overall scale of the scattering strengths S is irrelevant; only the relative values affect the MR. S_{si} was chosen so $S_{\mathrm{si}}/S_{\mathrm{sd}}=(\hbar^2/2m^*)^2$.

m^*	$4m_e$
V_{Fe^+}	−3.515 eV
V_{Fe^-}	−1.896 eV
V_{Cr}	−2.148 eV
S_{bulk}	0.358 (eV)^2 Å^{-3}
S_{si}	0.946 (eV)^2 Å^{-2}
S_{sd}	1.0 Å^{-2}

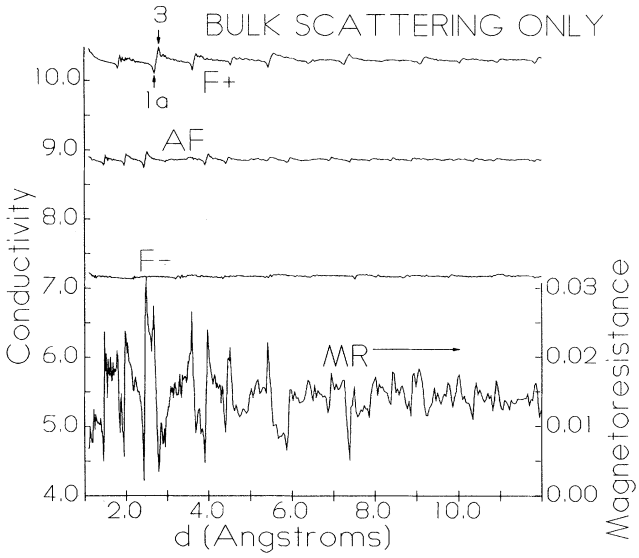

FIG. 2. Conductivities (scale at left, arbitrary units) and magnetoresistance (scale at right) for the case of bulk scattering ($S_{\text{bulk}}=0.358$ eV^2 Å^{-3}, $S_{\text{si}}=S_{\text{sd}}=0$), as a function of layer thickness d, assumed the same for all layers. The conductivities for $\pm$ spins in the ferromagnetic state are labeled $F\pm$, while the AF σ is spin independent. Fermi surfaces at points labeled "1a" and "3" are shown in Figs. 1(a) and 3.

tivity is larger, giving a positive MR as seen in Fig. 2.

Another notable feature of Fig. 2 is the strong oscillation of the MR, especially for small d. Its origin can be seen in the conductivity curves, which have regularly spaced anomalies consisting of a minimum, a rapid rise, and a maximum. The Fermi surface at the minimum labeled "1a" in Fig. 2 was shown in Fig. 1(a). It can be seen that the Fermi surface (which moves outward relative to the Brillouin zone as d increases) has just hit the zone boundary $k_z=\pi/2d$. The conductivity is a minimum because the FS area is a maximum at this value of d, as it is about to shrink to the undulating cylinder in Fig. 3, corresponding to the point labeled "3" in Fig. 2. The area has a minimum and begins to increase again when a new lens pops into existence at $k_r=0$ (Fig. 3), leading to the conductivity maximum ("3") in Fig. 2. The other anomalies in Fig. 2 have similar origins, except that every second new lens forms at $k_z=0$ instead of $k_z=\pi/D$. The period (about $\Delta d=0.95$ Å^{-3}) is close to the free-electron prediction $\pi/2k_F$. Variations with this periodicity Δd would of course not be directly observable, although Δd can be made larger by assuming a smaller

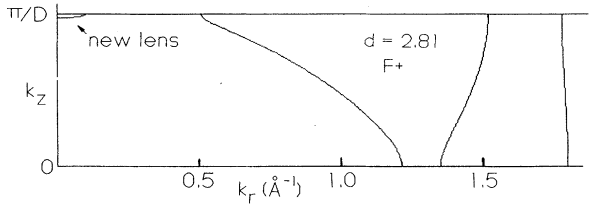

FIG. 3. Fermi surface, as in Fig. 1(a) but for $d=2.81$ Å.

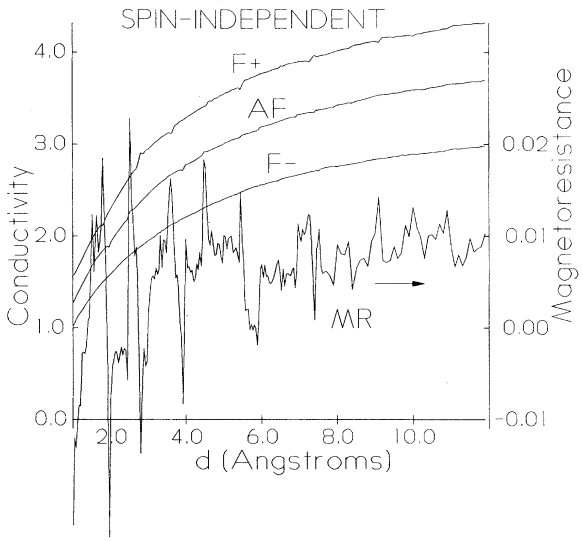

FIG. 4. Conductivities and magnetoresistance for the case of spin-independent interface scattering ($S_{\text{bulk}}=0.358$ eV^2 Å^{-3}, $S_{\text{si}}=0.358$ eV^2 Å^{-2}, $S_{\text{sd}}=0$). Notation is as in Fig. 2.

effective itinerant-electron density. These oscillations should not be confused with the oscillations in magnetic coupling[4] that lead to antiferromagnetic coupling in the first place; we have assumed antiferromagnetic coupling at all values of d. Most explanations of the periodicity Δd of the coupling oscillations involve features on the scale of $2\pi/\Delta d$ in the bulk FS,[14] whereas in the present context the FS itself depends on d.

We show in Fig. 4 the conductivities and MR when there is spin-independent interface, as well as bulk,[15] scattering. For large d, the interfaces become irrelevant and the conductivities approach those in Fig. 2 (bulk scattering only). For smaller d, all conductivities de-

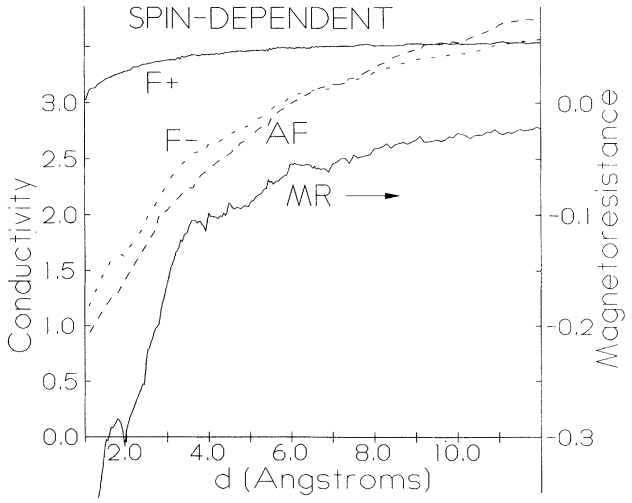

FIG. 5. Conductivities and magnetoresistance for the case of spin-dependent interface scattering ($S_{\text{bulk}}=0.358$ eV^2 Å^{-3}, $S_{\text{sd}}=0.358$ Å^{-2}, $S_{\text{si}}=0$). Notation is as in Fig. 2.

crease due to interface scattering. There are still substantial (several percent) oscillations in the MR, but it is still positive.

We obtain the negative MR that is found experimentally in giant-MR systems only by including spin-dependent scattering; these results are shown in Fig. 5. Now the minority spin conductivity (labeled $F-$) is much larger than the majority one, because the potential jump at the Fe-Cr interface is much smaller (Table I) giving weaker impurity scattering [Eq. (3)]. Quantitative comparison is not possible because we have chosen the surface density of scatterers arbitrarily, but it is clearly possible to get negative magnetoresistances of the order of those found experimentally, with reasonable scatterer densities.

Recent results for granular films[16] suggest that the giant MR effect does not even depend critically on the existence of ordered layers, but only on the juxtaposition of domains of different magnetization. However, it is not yet possible to handle the effects of disorder theoretically in a credible way, so a layered model is probably the best one to study at present. In fact, a reasonable model for the behavior of a granular film might be obtained by averaging the results for layered systems over the angle between the field and the layers, thus including the CPP (current parallel to planes) and CIP (current in plane) geometries as limiting cases. Although we have given results here only for the CIP case, our method[3] is generalizable to CPP as well.

The transfer matrix method makes it possible to calculate the electron wave functions in a model magnetic multilayer efficiently and rapidly enough that one can average over the Fermi surface and evaluate the giant magnetoresistance. We have done so using spin-dependent delta function scatterers situated at layer interfaces (a surface roughness model) and found that this yields experimentally reasonable magnetoresistances.

[1]M. N. Baibich, J. M. Broto, A. Fert, F. Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. **61**, 2472 (1988).

[2]B. Dieny, V. S. Speriosu, S. Menin, S. S. P. Parkin, B. A. Gurney, P. Baumgart, and D. R. Wilhoit, J. Appl. Phys. **69**, 4774 (1991).

[3]P. B. Visscher (unpublished).

[4]S. S. P. Parkin, N. More, and K. P. Roche, Phys. Rev. Lett. **64**, 2304 (1990).

[5]D. Stoeffler and F. Gautier, Phys. Rev. B **44**, 10 389 (1991).

[6]K. Fuchs, Proc. Cambridge Philos. Soc. **34**, 100 (1938); H. Sondheimer, Adv. Phys. **1**, 1 (1952).

[7]R. E. Camley and J. Barnaś, Phys. Rev. Lett. **63**, 664 (1989); J. Barnaś, A. Fuss, R. E. Camley, P. Grünberg, and W. Zinn, Phys. Rev. B **42**, 8110 (1990).

[8]R. Q. Hood and L. M. Falicov, Phys. Rev. B **44**, 9989 (1991).

[9]H. Itoh, J. Inoue, and S. Maekawa, Phys. Rev. B **47**, 5809 (1993).

[10]A. Oguri, Y. Asano, and S. Maekawa, J. Phys. Soc. Jpn. **61**, 2652 (1992).

[11]P. M. Levy and S. Zhang, Phys. Rev. Lett. **65**, 1643 (1990).

[12]P. M. Levy, Bull. Am. Phys. Soc. **37**, 683 (1992).

[13]J. Inoue, A. Oguri, and S. Maekawa, J. Phys. Soc. Jpn. **60**, 376 (1991).

[14]P. Bruno and C. Chappert, Phys. Rev. Lett. **67**, 1602 (1991); D. M. Edwards, J. Mathon, R. B. Muniz, and M. S. Phan, Phys. Rev. Lett. **67**, 1476 (1991); R. Coehoorn, Phys. Rev. B **44**, 9331 (1991).

[15]Without bulk scattering, if the wave function happens to vanish at all interfaces, the relaxation time is infinite, leading to computational difficulties.

[16]A. E. Berkowitz, J. R. Mitchell, M. J. Carey, A. P. Young, S. Zhang, F. E. Spada, F. T. Parker, A. Hutten, and G. Thomas, Phys. Rev. Lett. **65**, 3745 (1992).