Electrical Conductivity of Magnetic Multilayered Structures

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The electrical transport properties of magnetic multilayered structures are dominated by three ingredients: (1) the scattering within layers that changes from one layer to another, (2) the *additional* scattering resistivity due to the roughness of the interfaces between layers, and (3) the resistivity that depends on the orientation of the magnetization of the magnetic layers. In the quasiclassical approach the boundary scattering is treated *differently* from other sources. Here we present a *unified* treatment of all sources of resistivity, and determine the origin of the giant magnetoresistance observed in Fe/Cr superlattices.

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Recent studies of the transport properties of iron-chromium superlattices found an extraordinary reduction of resistivity, by as much as a factor of 2, in magnetic fields of 2 T.[1-4] Extant analyses of transport phenomena in layered structures are based on the pioneering work of Fuchs[5] and Sondheimer;[5] this was initially applied to the resistivity of thin films due to surface roughness, and extended to multilayers by Carcia and Suna.[6] Recently, the giant magnetoresistance of iron-chromium multilayered structures was analyzed by using this quasiclassical approach by including the spin-dependent interface scattering as well as a spin-dependent bulk scattering.[7] This approach does not treat the interface roughness scattering on an equal footing with that coming from the bulk.

What is needed is a *unified* treatment of the scattering from the interfaces and bulk. We have derived the conductivity and magnetoresistance of magnetic superlattices by using the quantum approach first used by Těsanović, Jarić, and Maekawa to discuss the resistivity of *thin* films coming from the roughness of their surface.[8] To determine the electrical transport properties of these multilayered structures we have extended their approach by considering the surface-roughness scattering from an array of interfaces, not just one, and by making the scattering dependent on spin. While our primary intention is to apply our result to periodic superlattices, our formalism is *equally* applicable to cases where there is no periodicity and to sandwich structures of finite thickness, e.g., Fe/Cr/Fe.[2,3,7] We find, *inter alia*, that while the translationally invariant homogeneous transport properties of these inhomogeneous structures are characterized by a mean free path which is related to the *diagonal* part of the conduction-electron Green's function, their position dependence comes from the *off-diagonal* parts of the Green's function. Here we present our derivation of the position-dependent conductivity of magnetic superlattices, and we apply our result to analyze the giant magnetoresistance of iron-chromium superlattices in terms of the spin-dependent bulk and interface scattering.

We model the transport properties of Fe/Cr magnetic superlattices by considering conduction electrons subject to *bulk* scattering which occurs within the layers, and *interfacial roughness* scattering which occurs at the interfaces between the iron and chromium layers. We confine ourselves to low temperatures and neglect phonon and magnon scattering; the latter should determine the temperature dependence of the magnetoresistance. The scattering at the interfaces comes from their roughness; iron atoms find themselves in the chromium layer and vice versa. As the iron layers are magnetized this produces *spin-dependent interfacial roughness* scattering.[1] The bulk scattering comes from imperfections and impurities in the iron and chromium layers. By following Těsanović, Jarić, and Maekawa[8] we represent the surface-roughness scattering by a potential that is random in the plane of the interface and a δ function in the third dimension. We consider the iron and chromium layers to be parallel to the x-y plane and to be stacked along the z direction. We denote the thickness of the iron and chromium layers as a and b, and in order to consider antiferromagnetic ordering we take the period of the superlattice (along z) to be $T \equiv 2(a+b)$. The scattering potential giving rise to resistivity is

$$V(\mathbf{r},\hat{\sigma}) = \sum_i V_i^b(\hat{\sigma})\delta(\mathbf{r}-\mathbf{R}_i) + \sum_l V_l^s(\hat{\sigma}) f_l(\boldsymbol{\rho})\delta(z-z_l)\,, \quad (1)$$

where $\mathbf{r} \equiv (\boldsymbol{\rho}, z)$ (z is normal to the layers), $\mathbf{R}_i$ is the position of an impurity or defect, z_l is the position of the lth Fe/Cr interface, $f(\boldsymbol{\rho}=(x,y))$ represents interface roughness, the sum over i is per unit volume, and the sum over l is per unit length. The spin-dependent poten-

tials are written as

$$V(\hat{\sigma}) \equiv v + j\hat{\mathbf{M}}_{\mathrm{Fe}} \cdot \hat{\sigma} , \tag{2}$$

where the operator $\hat{\sigma}$ represents the Pauli spin matrix, and $\hat{\mathbf{M}}_{\mathrm{Fe}}$ is a unit vector in the direction of the magnetization of an iron layer. The chromium layers are nominally nonmagnetic; therefore we set $j_{\mathrm{Cr}}=0$ in these layers.

The conduction electrons are subject to different potentials in the iron and chromium layers, and in principle, one should determine their wave functions for a Kronig-Penney-like potential representing the Fe/Cr superlattice. However, when the Fermi level is far from the bottom of the potential and if there are no gaps at the Fermi level, e.g., in the chromium layers due to spin-density waves, it is reasonable to use plane waves to represent conduction electrons in calculating the transport properties of Fe/Cr superlattices. Therefore, to the lowest order in the scattering, the t matrix near the Fermi surface is

$$t_{\bar{\nu}}(k\omega,\hat{\sigma})|_{\omega\approx\epsilon_F} \equiv -i\pi\left[\sum_l \Delta_l^b(\hat{\sigma}) e^{-i\bar{\nu}z_l} + \sum_l \Delta_l^s(\hat{\sigma}) e^{-i\bar{\nu}z_l}\right] , \tag{3}$$

where

$$\begin{aligned} \Delta_l^b(\hat{\sigma}) &= \rho(\epsilon_F)\langle V_l^b(\hat{\sigma})^2\rangle_t , \\ \Delta_l^s(\hat{\sigma}) &= \rho(\epsilon_F)[V_l^s(\hat{\sigma})]^2\langle f_l^2\rangle , \end{aligned} \tag{4}$$

$\mathbf{k}\equiv(k,\nu)$ has been used (i.e., $k\equiv k_x,k_y$ are the directions in reciprocal space parallel to the layers, $\nu\equiv k_z$ is normal to the layers, $\bar{\nu}\equiv\nu-\nu'$), and $\rho(\epsilon_F)$ is the density of states of conduction electrons at the Fermi surface. To arrive at this form we averaged the bulk scattering potential $V_l^b(\hat{\sigma})$ over a random distribution of impurities in a plane t parallel to the layers, and we used a "white noise" surface profile for the uncorrelated atomically rough Fe/Cr interface; i.e., we take $\langle|f_l(k)|^2\rangle$ a constant independent of k.[8] For the matrix elements of the *scattering* potential to exist for all vectors $\bar{\nu}$, and not just those of the reciprocal lattice of the superlattice, it is necessary that the parameters Δ_l^s (Δ_l^b) are random. As the real parts of these parameters have the periodicity of the superlattice we must make these parameters complex and take their imaginary parts to be random. In addition we make the assumption that the Δ's are independent of ν near the Fermi surface. In normal metals, i.e., no Kondo effect or resonant scattering at the Fermi surface, this is an entirely reasonable approximation.

The loss of translational invariance requires us to calculate the current at finite $\mathbf{q}$ even though we apply a *uniform* electric field. Our discussion of the transport properties of superlattices is limited to currents parallel to the layers, i.e., the longitudinal conductivity; this is the case that has been experimentally studied.[1-4] When a uniform electric field E_x is applied in the x direction, the position-dependent current in the x direction is

$$j_x(z) = \sigma(z) E_x , \tag{5}$$

where $\sigma(z)$ is the position-dependent conductivity due to the inhomogeneous nature of the problem.

We calculate the conductivity $\sigma(z)$ by using the Kubo formalism[8,9] in which the current response is given in terms of Matsubara Green's functions. We separate the Green's functions into *diagonal* and *off-diagonal* parts,

$$\begin{aligned} G_{\nu\nu'}^{\sigma\sigma'}(k,\omega) &= G_\nu^\sigma(k,\omega)\delta_{\nu\nu'}\delta_{\sigma,\sigma'} \\ &\quad + G_\nu^\sigma(k,\omega) T_{\nu\nu'}^{\sigma\sigma'}(k,\omega) G_{\nu'}^{\sigma'}(k,\omega)(1-\delta_{\nu\nu'}) , \end{aligned} \tag{6}$$

where

$$T_{\nu\nu'}^{\sigma\sigma'} = t_{\nu\nu'}^{\sigma\sigma'} + \sum_{\nu_1\sigma_1,\nu_2\sigma_2} t_{\nu\nu_1}^{\sigma\sigma_1} G_{\nu_1\nu_2}^{\sigma_1\sigma_2} T_{\nu_2\nu'}^{\sigma_2\sigma'} , \tag{7}$$

and $t_{\nu\nu'}^{\sigma\sigma'}$ is the spin matrix element of the t matrix, Eq. (3), which is an operator in spin space. The G_ν^σ is the *diagonal* part of the Green's function which is written as

$$G_\nu^\sigma = 1/(\omega - \epsilon_{k\nu} + i\Delta^\sigma) ,$$

where

$$\Delta^\sigma \equiv -\pi^{-1}\,\mathrm{Im} T_{\nu\nu}^{\sigma\sigma(*)}(k_F,\epsilon_F) , \tag{8}$$

and $T_{\nu\nu'}^{\sigma\sigma(*)}$ is the irreducible self-energy, which to leading order is the diagonal part of the t matrix, Eq. (3). In adopting the integral equation (7) we are neglecting interference terms from scatterings at different sites (these are usually quite small). By placing Eq. (6) in Eq. (7) we find an integral equation for T which cannot be solved exactly. Nonetheless, we can solve for the Fourier transform of the product $G_\nu T_{\nu\nu'}$ which enters the expression for the conductivity. Upon placing Eq. (6) into Eq. (7) and taking the transform of the product GT we are able to uncouple the ensuing expressions by using the property that our t matrix Eq. (3) is of the form

$$t_{\nu\nu'} = -i\pi\sum_l e^{i(\nu'-\nu)z_l}\Delta_l , \tag{9}$$

where the Δ_l are independent of ν and ν' near the Fermi surface. We find the position-dependent conductivity at zero temperature is given as

$$\sigma(z) = \frac{ne^2}{2m^2}\sum_\sigma \frac{1+a^{-\sigma}(z)}{[1+a^\sigma(z)][1+a^{-\sigma}(z)] - b^\sigma(z)b^{-\sigma}(z)} , \tag{10}$$

where

$$1+a^\sigma(z) = \frac{1}{\lambda^\sigma}\left[\sum_t \mathrm{Re}\Delta_t^{\sigma\sigma} e^{-|z-z_t|/\lambda^\sigma} + \sum_l \mathrm{Re}\Delta_l^{\sigma\sigma} e^{-|z-z_l|/\lambda^\sigma}\right] ,$$

$$b^\sigma(z) = \frac{1}{\lambda^\sigma}\left[\sum_t \mathrm{Re}\Delta_t^{\sigma\,-\sigma} e^{-|z-z_t|/\lambda^\sigma} + \sum_l \mathrm{Re}\Delta_l^{\sigma\,-\sigma} e^{-|z-z_l|/\lambda^\sigma}\right] ,$$

$h \equiv 1$, and $\Delta^{\sigma\sigma'}$ is a spin matrix element of the scattering potential Eq. (4). The mean free path is derived from the *diagonal* part of the Green's function

$$\lambda^{\sigma} \equiv k_F / m \Delta^{\sigma}(\epsilon_{kv} = \epsilon_F) , \tag{11}$$

where

$$\Delta^{\sigma} = \frac{1}{T} \left(\sum_{l \in T} \mathrm{Re} \Delta_l^{\sigma\sigma} + \sum_{l \in T} \mathrm{Re} \Delta_l^{\bar{\sigma}\sigma} \right) \equiv \Delta_b^{\sigma} + \Delta_s^{\sigma} , \tag{12}$$

and $k_F = (3\pi^2 n)^{1/3}$. Finally, the *average* conductivity is obtained by averaging $\sigma(z)$ over a period T. In the limiting cases of the mean free paths much greater and much smaller than the period T our result reduces to the correct forms. We have also confirmed that the conductivity is independent of the direction of the spin quantization.

We have applied these results to determine the *magnetoresistance* of a metallic superlattice, e.g., Fe/Cr. The *amplitude* of the magnetoresistance is defined as the difference of the resistivity in the antiferromagnetic and ferromagnetic ordered states,

$$R \equiv \frac{\rho(H=0) - \rho(H_s)}{\rho(H=0)} = \frac{\sigma_{H_s} - \sigma_{H=0}}{\sigma_{H_s}} , \tag{13}$$

where σ_H is the average of the conductivity Eq. (10) over the period T.

The spin dependence of the interface scattering comes from placing $V(\hat{\sigma})$, Eq. (2), in $\Delta_l^{\sigma}(\hat{\sigma})$, Eqs. (3) and (4). The ensuing expression for the conductivity Eq. (10) can be written in terms of the coefficients entering Eq. (2), i.e., v and $p \equiv j/v$. To keep our adjustable parameters to a minimum we set $\langle v_{\mathrm{Fe}}^2 \rangle = \langle v_{\mathrm{Cr}}^2 \rangle \equiv \langle v_{\mathrm{bulk}}^2 \rangle$, $p_{\mathrm{Fe}} = p_{\mathrm{int}} \equiv p$ (int means interface), and $p_{\mathrm{Cr}} = 0$. In this way we find *three* parameters enter our model for $\sigma(z)$, i.e.,

$$\lambda_b = a_0 k_F / m \langle v_b^2 \rangle \rho(\epsilon_F) ,$$

$$\lambda_s' \equiv 2\lambda_s/(a+b) = k_F / m v_{\mathrm{int}}^2 \langle f_{\mathrm{int}}^2 \rangle \rho(\epsilon_F) ,$$

and p; a and b are the thickness of the iron and chromium layers and $a_0 = b_0$ is the common lattice constant for iron and chromium. The mean free path λ^{σ}, Eq. (11), depends on the angle between the iron moments in *adjacent* layers. For Fe/Cr superlattices they are antiparallel in zero magnetic field. As a function of field the angle between the Fe moments decreases until "saturation" H_s when they are parallel. The origin of the magnetoresistance is a short circuit for which $\lambda_F^{\downarrow} \gg \lambda_F^{\uparrow}$, so that $\lambda_F = \lambda_F^{\downarrow} + \lambda_F^{\uparrow} > \lambda_{AF} = 2\lambda_{AF}^{\uparrow}$ ($\lambda_{AF}^{\downarrow} = \lambda_{AF}^{\uparrow}$).

To calculate the magnetoresistance we specify the thickness of the layers a and b, and we must choose values of λ_b, λ_s', and p which best fit the data. The bulk scattering λ_b determines the length scale for the dependence of the magnetoresistance on t_{Cr}; therefore we start by fitting λ_b to the data on $R(t_{\mathrm{Cr}})$. Then, as bulk and interface scattering produce very different dependences for $R(t_{\mathrm{Fe}})$ we fix the ratio λ_s'/λ_b to fit that data. Finally, we choose p to obtain the experimental magnitude of the magnetoresistance. From our knowledge of the scattering of chromium impurities in iron[10] we know that $p \approx 0.42$–0.55. With this *restriction* we have fitted Eq. (13) to the data on epitaxially grown Fe(001)/Cr(001) multilayers at $T = 4.2$ K,[1] and we find reasonable fits with $\lambda_b = 19$ Å, $\lambda_s' = 1.1$, and $p = 0.55$. For a superlattice with $a = 30$ Å and $B = 12$ Å, this yields $\lambda = 23$ Å, so that the ratio of the interfacial to bulk resistivity is 0.83. A further check is that of the absolute value of the resistivity. For the above parameters we find $\rho(H=0,\ T=0\ \mathrm{K}) = 83\ \mu\Omega\,\mathrm{cm}$ which is well within the scatter of the values found for Fe/Cr superlattices. In Fig. 1, we show the variation of the amplitude of the magnetoresistance, Eq. (13), as a function of thickness of the iron layers $t_{\mathrm{Fe}} = a$ for $b = 12$ Å, and as a function of chromium layer thickness $t_{\mathrm{Cr}} = b$ for $a = 30$ Å. While the variation with a is very gradual, it is much stronger with b. This is in agreement with the experimental data available to date on Fe/Cr superlattices.[1,4] While the data from Ref. 1 give the impression that there is a sharper decrease around $b = 18$ Å, there may be other effects that contribute to this decrease, e.g., a change in sign of the interlayer coupling in this range of thickness.[4] By varying the values of λ_b, λ_s', and p we *gradually* worsen the fits to the experimental data; nothing drastic happens.

It is of interest to compare our quantum-mechanical model to the semiclassical approach of the Fuchs-Sondheimer (FS) type.[5,7] This approach treats interface scattering phenomenologically by introducing the pro-

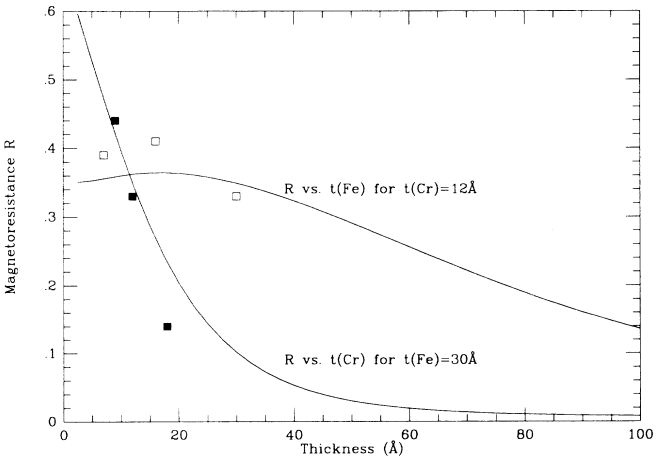

FIG. 1. The magnetoresistance R, Eq. (13), of Fe/Cr superlattices as a function of the thickness of iron layers for $b = 12$ Å, and for variable thickness of the chromium layer for $a = 30$ Å. The parameters used for these curves are $p = 0.55$, $\lambda_b = 19$ Å, and $\lambda_s' = 1.1$; the calculation is for $T = 0$ K. The solid squares refer to data at $T = 4.2$ K on R vs t_{Cr} and the open ones to R vs t_{Fe} taken from Ref. 1, except for the point $t_{\mathrm{Fe}} = 7$ Å and $t_{\mathrm{Cr}} = 12$ Å which comes from recent (unpublished) data of the same group.

portion of electrons transmitted T_σ and those scattered $1-T_\sigma$; in our approach bulk and interfacial scattering are treated in the same way by introducing bulk and interface scattering potentials. While there is a large degree of overlap in the *qualitative* results of the two models, the *proportion* of interface to bulk scattering cannot be as freely tuned in the FS approach as in our model. While this does not seem to present problems for the small resistivities of the sandwich structures discussed by Camley and Barnaś,[7] difficulties show up when we have attempted quantitative fits to data on Fe/Cr superlattices with large resistivities.[11] A second advantage of our approach is that we can relate the magnetoresistance to the interface roughness, see Eq. (4); from λ_s' and by assuming, in first approximation, the values of $V_i^s(\sigma)$ corresponding to Cr impurities in Fe,[10] we find the rms roughness of the interfaces in the Fe/Cr superlattices $(\langle f_{\rm int}^2\rangle)^{1/2}$ is about $a_0/5$. This is reasonable as it represents a rms deviation of only 40% of the distance between atomic planes. Finally, our approach avoids the well-known drawbacks of the semiclassical models in the limit when the mean free path is much larger than the layer thickness.[8]

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[11]The low-temperature resistivity of the superlattices studied in Ref. 1 are scattered around 60 $\mu\Omega$ cm; however, for some samples [F. Petroff and A. Fert (private communication)] it can be as large as 80 $\mu\Omega$ cm or more.