CONF-950412--61

Calculation of Electrical Conductivity and Giant Magnetoresistance within the Free Electron Model

X.-G. Zhang* and W. H. Butler *
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ABSTRACT

We use the model of free electrons with random point scatterers (FERPS) to calculate the electrical conductivity and giant magnetoresistance (GMR) for FeCr multilayer systems and compare our results with the experimental values. Our analysis suggests that the primary cause of the GMR in FeCr systems is regions of interdiffusion near the interfaces. We find that in the samples analyzed, these regions of interdiffusion occupy about 8.5Å of the magnetic layer near each interface.

Introduction

Previous calculations of the conductivity and Giant Magnetoresistance in magnetic multilayers have generally employed the model of Free Electrons with Random Point Scatterers (FERPS) and have approximated the conductivity within this model by using either a semi-classical approximation[1, 2, 3] or an approximate solution[4] to the Kubo formula[5, 6]. In a previous study[7] we evaluated the Kubo formula exactly within the FERPS model with a local self-energy, and compared it with the other methods. We investigated the relationships among the various approaches and found that under most circumstances the semi-classical approach agrees surprisingly well with the numerical solution, while the solution of Zhang, Levy and Fert[4] (ZLF) generally yields a conductivity which is lower than the numerical solution when the mean free path is comparable to the layer thicknesses[8].

In light of these results, the question arises as to whether the past analyses of experimental data using ZLF and the conclusions based on them should be re-examined. Specifically, since ZLF theory tends to give results that are closer to the thin limit, it usually over-emphasizes the effects of regions with strong scattering, e.g., interface regions. Therefore, one needs to reconsider the conclusion drawn from these studies that the dominant effect in these GMR systems is the interfacial scattering.

In this paper we calculate the conductivity and GMR exactly within the FERPS model for FeCr multilayer systems, and compare the results with previous studies[9]. Our study suggests that although interface roughness can be important, there may also be a region of interdiffusion that is larger than the rough regions near the interfaces, and this interdiffusion may be an important contributor to GMR. We further speculate that GMR may be significantly increased if this interdiffusion region can be increased while maintaining spin alignment.

Conductivity in the Free Electron Model

Our model of the multilayer is described by a complex local self-energy $\Sigma(z)$ that is constant in the xy directions (parallel to the layers), and is assumed to be constant in the thickness of the interdiffusion region on each side of the Fe layer, t^{int}, and three parameters from λ_ℓ^{Fe}, p_ℓ^{Fe}, $\lambda_\ell^{\text{int}}$, and p_ℓ^{int}, where the mean free paths for each spin channels can be obtained from,

$$\lambda_\sigma = \frac{\lambda_\ell}{(1+p_\ell\sigma)^2}, \tag{7}$$

with $\sigma = \pm 1$ for up (down) spins.

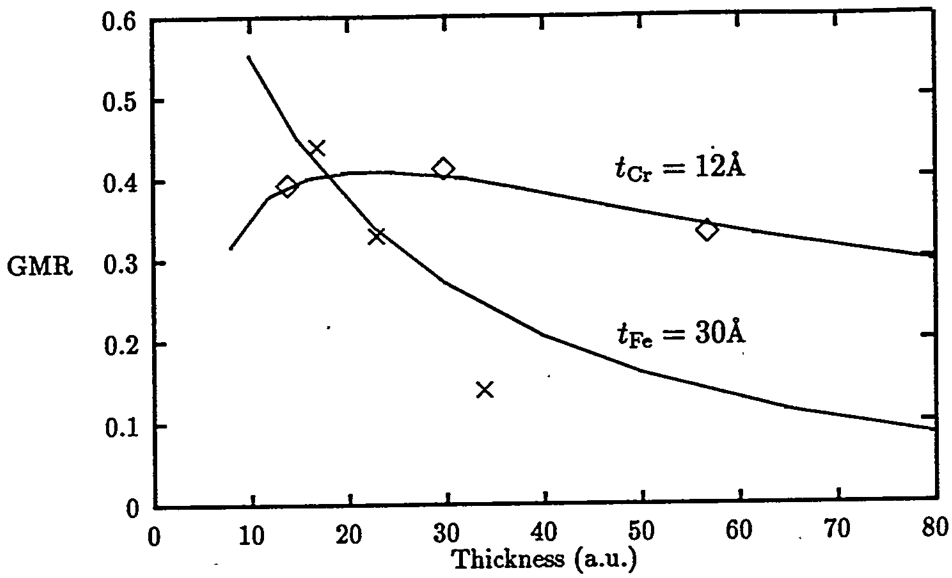
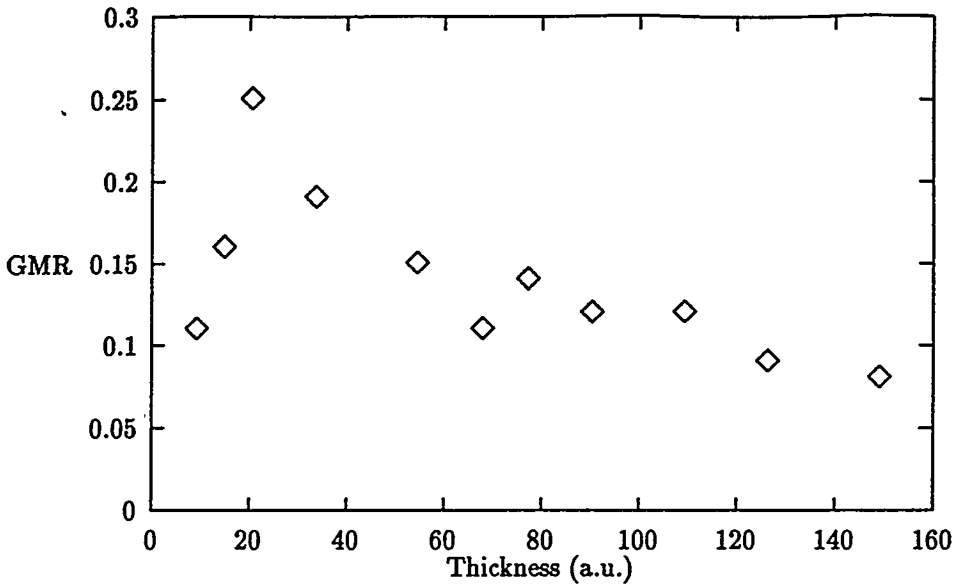


Figure 2: The GMR ratio of FeCr multilayers as a function of Fe layer thicknesses with $t_{\text{Cr}} = 12\text{Å}$ ($\diamond$), and as a function of Cr layer thicknesses with $t_{\text{Fe}} = 30\text{Å}$ ($\times$). The solid lines are calculations with the FERPS model.

We were able to fit both curves with $t^{\text{int}} = 8.5\text{Å}$, $\lambda_\ell^{\text{Fe}} = 33\text{Å}$, $p_\ell^{\text{Fe}} = 0.44$, $\lambda_\ell^{\text{int}} = 11\text{Å}$, and $p_\ell^{\text{int}} = 0.68$. The zero field resistivity calculated from these parameters is about $45\mu\Omega$cm, in good agreement with the measured residual resistivity $37\mu\Omega$cm. The existence of the rather thick interdiffusion regions has important consequences. If the scattering rates in these regions are made the same as those in the Fe layers, the GMR ratio is reduced significantly. This is consistent with the experimental result that samples with sharper interfaces yielded smaller GMR ratios.

Although it seems that we have many parameters to fit only a few data points, we believe the results are significant for the following reasons. First, several parameters, such as the Fermi energy, the mean free path in the Cr layers, and the mean free path of the majority channel in the Fe layers, have little effect on the general trend of the GMR, although they may affect the resistivities significantly. Second, the decrease of the GMR as a function of the Fe layer thickness for thick Fe layers determines quite unambiguously the ratio of bulk scattering versus interfacial scattering in the Fe layers. Lastly, the reduction of the GMR ratio for very thin Fe layers gives a good estimate of the thickness of the interfacial regions where there is a strong spin dependent scattering. Most experimental data on multilayers show a sharp downturn of the GMR ratio for a magnetic layer thickness near 10Å to 20Å. This thickness is much greater than a typical interfacial roughness of about 2Å to 4Å which suggests the existence of relatively thick magnetic regions where there is a significant concentration of nonmagnetic impurities due to diffusion in these multilayer systems. This is illustrated by

Figure 3 which shows the GMR ratio for a typical CuCo multilayer system[12]. A careful study of this system will be presented in a future publication.



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Our results are differ from those obtained by Zhang, Levy and Fert from the same data[4] in several aspects. First, they approximated the interfacial regions with a δ function type scattering potential. This leads to the unphysical consequence that the GMR extrapolates to a finite constant as the thickness of the magnetic layers goes to zero. Our analysis indicates that interfacial interdiffusion region is actually rather thick, about 8.5Å on each side of the Fe layer (17Å for every Fe layer). Secondly, their calculated zero field resistivity is too high, ($83\mu\Omega$cm). Although the resistivities tend to fluctuate from sample to sample, it is important that a theory give the correct resistivity as well as the GMR ratio for the same sample. This difference in the resistivity is due to the fact that the ZLF theory over-emphasizes the strong scattering regions compared to the exact solution of the FERPS model.

Conclusions

We have analyzed the experimental data on FeCr multilayers using the FERPS model. We found that there may exist rather thick interdiffusion regions in the magnetic layers, and these regions with very strong spin dependent scatterings are the primary contributors to the GMR. Petroff *et al*[9] found that FeCr multilayers with sharp interfaces and small residual resistivities exhibit significantly reduced GMR. Annealing these samples usually increasase the GMR ratio. These observations are consistent with our results. Other experiments on FeCr or CuCo multilayers showed similar trends.

Our results suggest that the GMR may be increased significantly in these multilayer systems by increasing the interdiffusion regions, either by annealing or impurity doping. It is important, however, that these regions should maintain their magnetic moment, which is the source of spin dependence in the scattering rates according to our first-principles studies[13, 14].

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Conductivity in the Free Electron Model

Our model of the multilayer is described by a complex local self-energy $\Sigma(z)$ that is constant in the xy directions (parallel to the layers), and is assumed to be constant in the

z direction within each layer. It can be shown that variations of the real part of the self-energy contribute very little to the GMR. Therefore we assume that the real part of $\Sigma(z)$ is a constant throughout space. The imaginary part of $\Sigma(z)$ is determined by the mean free path within each layer,

$$\mathrm{Im}\Sigma_I = -\frac{k_F}{2\ell_I}, \tag{1}$$

where k_F is the Fermi momentum, and the subscript I denotes the layer I.

The quantum solution to such a multilayer cannot be obtained analytically. To obtain a numerical solution we embed a finite number of multilayers (about 1000Å thick) into an infinite square well, and calculate the Green function using[3]

$$G(k_{||}; z, z') = \frac{\psi_L(z_<)\psi_R(z_>)}{W}, \tag{2}$$

where $k_{||}$ is the parallel component of the wave vector, and ψ_L and ψ_R are solutions to the differential equation,

$$[E + \frac{\hbar^2}{2m}(\frac{\partial^2}{\partial z^2} - k_{||}^2) - \Sigma(z)]\psi(z) = 0, \tag{3}$$

and satisfy the boundary conditions on the left and right sides of the system, respectively. For a multilayer system of total thickness d we used the boundary conditions, $\psi_L(0) = 0$ and $\psi_R(d) = 0$. W is the Wronskian of ψ_L and ψ_R.

The conductivity for current-in-plane (CIP) can be calculated from the Kubo formula which gives,

$$\sigma = -\frac{1}{8\pi^3}\frac{e^2\hbar^3}{m^2 d}\int_0^d dz \int_0^d dz' \int d^2\mathrm{k}_{||} k_{||}^2 \mathrm{Im}G(k_{||}; z, z')\mathrm{Im}G(k_{||}; z', z). \tag{4}$$

We first use this to calculate the conductivity of a simple multilayer system and compare with the semi-classical results and those obtained using the theory of ZLF. The comparison is shown in Fig. 1, as a function of the thickness of one period. In these calculations it is assumed that the scattering rates for the two layers correspond to bulk mean free paths of 36.0555 and 360.555 atomic units (1 a.u.=0.529Å) and that the thickness of the dirty layers is twice that of the clean layers. No additional scattering at the interfaces is included. In all of the multilayer calculations we used a sufficient number of periods of the multilayer to avoid the physical quantum size effects for the exact results and the large unphysical size effects that occur for the semi-classical and ZLF theories.

There are two limits that all theories approach correctly: The thin limit in which the layer thicknesses are small compared to the mean free path, and the thick limit in which the layer thicknesses are much larger than the mean free path. In the thin limit the conductivity is determined by the average of the scattering rate, which gives,

$$\frac{1}{\ell_{\text{thin}}} = \sum_I \frac{d_I}{d}\frac{1}{\ell_I}. \tag{5}$$

In the thick limit, the mean free paths are averaged,

$$\ell_{\text{thick}} = \sum_I \frac{d_I}{d}\ell_I. \tag{6}$$

There is a surprisingly good agreement between the semi-classical theory and the FERPS model. On the other hand, the ZLF theory seems to approach the thin limit too fast.

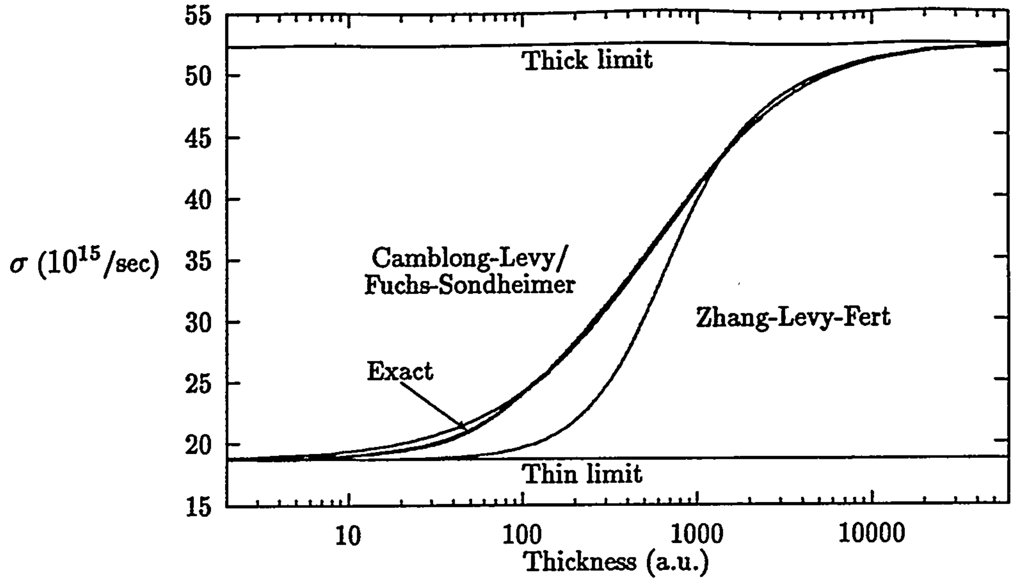

Figure 1: Conductivity as a function of the total thickness of a period of a multilayer system. The period contains two layers, with thicknesses 2/3 and 1/3 of the period, and mean free paths 36.0555a.u. and 360.555a.u., respectively.

Because in most multilayer systems the layer thicknesses are less than 100Å(about 189a.u.), this deviation would cause the ZLF theory to over-emphasize the effects of strong scattering regions, e.g., the interfacial regions.

Application to Multilayer Systems

We have applied our FERPS model to the FeCr multilayer system, and compared the results with the experiment of Baibich *et al*[10, 11] results of which are shown in Fig. 2. Like most of the data on GMR as a function of the layer thicknesses it has three qualitative features:(1)For fixed thickness of the magnetic layer the GMR ($\Delta R/R$) decreases with spacer layer thickness. (2)For sufficiently large magnetic layer thickness GMR decreases with magnetic layer thickness. (3) As the magnetic layer thickness decreases the GMR reaches a maximum and then falls rapidly to zero for zero magnetic layer thickness. In relating the experimental data to the FERPS model we find that feature (1) gives information concerning the mean free path in the spacer layer, feature (2) is related to the relative strength of the bulk scattering (asymmetry between the majority and minority scattering rates in the ferromagnetic layer) and the interfacial scattering. The thickness at which feature (3) occurs indicates the thickness of the region which contributes most strongly to the GMR.

In order to fit the data using the FERPS model we chose (somewhat arbitrarily) $E_F =$ 0.1Ha. With this value of E_F a value of the spacer layer mean free path of approximately $\lambda^{Cr} = 79$Åwas necessary to fit the decrease in GMR with spacer layer thickness. In order to fit the dependence of the GMR on the ferromagnetic layer thickness we found it necessary to assume that there is a region in the Fe layers where there is a significant amount of Cr impurities. From our experience with the bandstructure of FeCr alloys, we made an assumption that the mean free path for the minority spin channel in the interdiffusion region is the same as that of the Fe layer. Therefore there are four free parameters to fit, the thickness of the interdiffusion region on each side of the Fe layer, t^{int}, and three parameters from λ_ℓ^{Fe}, p_ℓ^{Fe}, $\lambda_\ell^{\text{int}}$, and p_ℓ^{int}, where the mean free paths for each spin channels can be obtained from,

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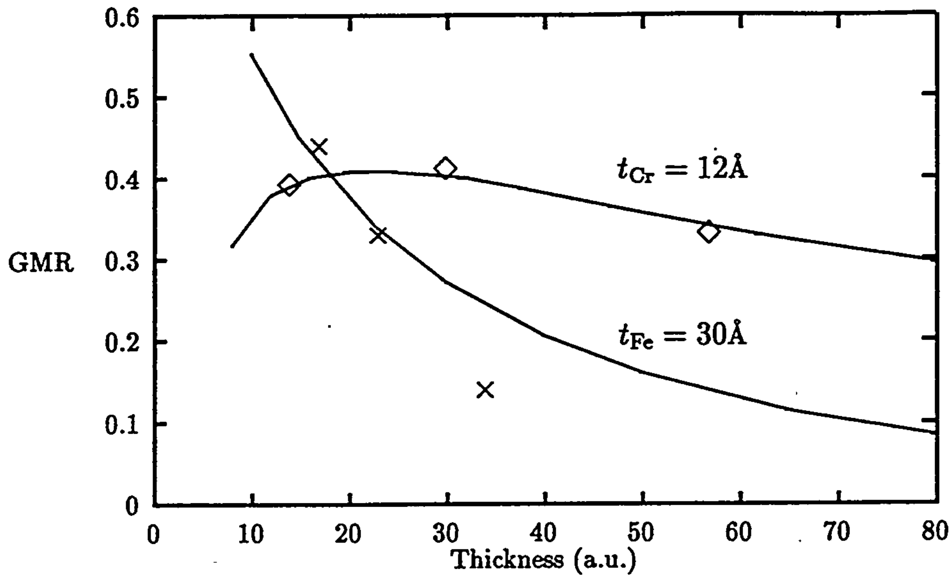

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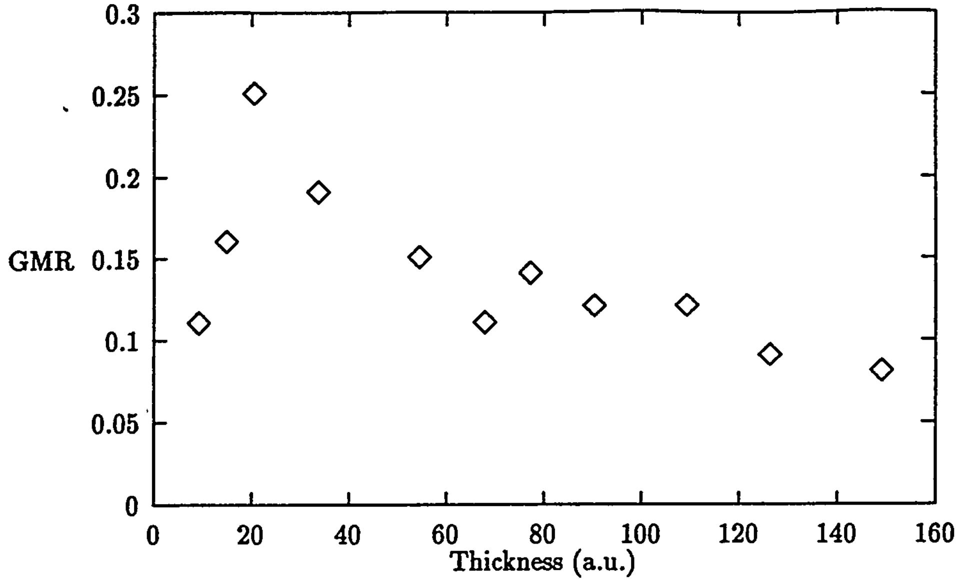

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