Influence of Intralayer Quantum-Well States on the Giant Magnetoresistance in Magnetic Multilayers

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A model which can account for the experimentally observed variations of the giant magnetoresistance in thin magnetic multilayers with mean free path, interface roughness, magnetic layer, and normal layer thickness has been developed. The model requires the existence of quantum-well states within individual layers or groups of layers, depending on the magnetic state of the film. The calculated results are obtained by the application of quantum size effect transport theory to these individual layers.

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The first report by Baibich *et al.* [1] of a very large negative magnetoresistance, the so-called giant magnetoresistance (GMR), in Fe/Cr multilayers has provoked a great deal of experimental work in sandwiches and multilayers of this system [2,3] as well as other magnetic multilayers [4]. This large decrease in resistance with applied magnetic field occurs when an originally antiparallel orientation of the magnetization of adjacent ferromagnetic layers of the film is driven parallel. The origin of the magnetic structure and behavior of these systems is closely related to that of the GMR and like it is also under intense study. Currently, experiments are exploring and finding dependence of the properties of these multilayers on the detailed electronic structure of the constituent materials [5]. In this paper only the behavior of the magnetoresistance arising from the relative orientation of the magnetization will be addressed. We will use "M" and "N" to mean the magnetic and nonmagnetic layers, respectively, of any of these films.

The goal of this paper is to define a simple and plausible mechanism which can semiquantitatively account for the large number of well-established and still puzzling features associated with these multilayered films. These include the following: a larger effect in a superlattice than in a sandwich structure; a larger effect at low temperatures than at room temperature; a clear enhancement of the GMR with interface roughness [6]; a rapid variation of the effect with N thickness [7]; a slower variation with M thickness which can have either of two characteristics [4], a monotonic decrease of the GMR with M layer thickness above some relatively small thickness (10 Å in Fe/Cr) or an increase of GMR up to large thicknesses of the magnetic layers followed by a broad maximum as the thickness is increased further; and a behavior dependence on the detailed electronic structure of the multilayer materials. The model we present here is a single mechanism which predicts the existence of all of these features in a very natural way.

The theoretical modeling has generally emphasized spin dependent scattering [2,4]. More specifically, Inoue, Oguri, and Maekawa [8] addressed the origin of the spin dependent potential responsible for the spin dependent scattering at the M/N interface. Camley and Barnas [9] and, with fewer approximations, Hood and Falicov [10] have extended Fuchs' semiclassical theory [11] of size effect to spin dependent scattering at the Fe/Cr interface. Levy, Zhang, and Fert [12] have followed the quantum mechanical theory of Tesanovic, Jaric, and Maekawa [13] to treat the Fe/Cr interface as a source of spin dependent interfacial roughness scattering. Stearns [14] has treated the spin dependent scattering as arising from the difference in the spin up and spin down density of states.

In this paper it is shown that the GMR can be largely understood in terms of (i) the vacuum-metal-like character of the interface between M and N and the consequent quantum-well-like states established within each layer or groups of layers of certain multilayer films and (ii) the application of already existing quantum mechanical size effect theories of electrical conduction. (i) has already been experimentally established in a number of different overlayers of nonmagnetic metals on other nonmagnetic metal substrates. Furthermore, Edwards and Mathon [15,16] have presented a theory of the exchange coupling of the ferromagnetic layers in magnetic multilayers based on the idea of quantum confinement of the electrons within the individual layers.

Recently, using angle-resolved photoemission Lindgren and Wallden [17] and Chiang and co-workers [18,19] have discovered and explored discrete valence electron states in thin metal overlayers on a metal substrate. These have been identified as arising from electron confinement within the overlayer and thus as quantum-well states (QWS) [18]. The degree to which the overlayer states manifest quantum-well behavior revolves around the amount of electron reflection versus electron transmission [18]. This depends on the dissimilarity of the two metals at the interface and the abruptness of the interface. Nevertheless, Ag(111) on Au(111), two very similar metals, displays strong QWS characteristics for those Ag electrons energetically below the Ag L point and above the Au L point in the Brillouin zone boundary. In this region, called by Chiang and co-workers [18] a "relative" gap, there are no energy gaps in either material, but there are no available states in Au which conserve both energy *and* the (111) component of the Ag electrons' wave vectors, k. *The reflectivity, then, can be explained in terms of band structure mismatch, and thus just the detailed electronic structure effects so actively under study in magnetic multilayers at the present time [5].*

Since the original submission of this paper a great deal of additional evidence has accumulated to support the existence of QWS within individual layers of magnetic multilayers. Using inverse photoemission techniques Himpsel and co-workers have detected QWS in magnetic multilayers of the sort under discussion here; Fe in Au and Au in Fe [20], and the Fe-Ag and Co-Cu layered systems [21]. More recently Ortega *et al.* [22] have extended the evidence in these systems and added the Cu-Fe system. In addition they have related their electronic structure findings to the magnetic properties of these films. Most recently, Suzuki and Katayama [23] have explained magneto-optical transition data in Au-Fe sandwiches by the presence of QWS in the Fe and Clarke *et al.* [23] report above saturation magnetic field effects supportive of QWS.

On this basis we suppose that N/M interfaces can give rise to metallic QWS and model the electronic structure of the individual layers of the multilayer films giving rise to GMR in the following way. We take the majority spin, $s+$, and minority spin $s-$, M electrons to be separate and distinct spin bands for the purpose of electrical conductivity as is customarily done. For N electrons, $s+$ and $s-$ distinguish only the electrons' spin direction in space (say $s+$ for up and $s-$ for down), since the two spin subbands are identical. We assume that the ratio of reflection to transmission at the M/N interfaces is substantially different for $s+$ and $s-$ electrons by virtue of the greater or lesser similarity of the two spin bands of the M electrons compared to the N electrons. If one spin band were identical to the N electron band, those M electrons would not recognize the existence of the interface.

For our purpose here of simply identifying the origin of the GMR we will carry out our calculation as if the $s-$ M electrons at the Fermi surface are perfectly transmissive at the interface and the $s+$ M electrons are perfectly reflecting; i.e., $s-$ M electrons are indistinguishable from N electrons with the same spin direction in space. This simplification will exaggerate the calculated magnetoresistance somewhat but not affect the results qualitatively. (To the extent that some electrons in thicker layers might lose phase coherence or some electrons assumed to be reflected are actually transmitted, they might best be treated separately by a classical model such as is found in Ref. [4]).

The electronic structure of a sandwich (three layers, MNM) with antiferromagnetic and ferromagnetic orientation between the M layers is illustrated in Figs. 1(a) and 1(b), respectively. In Fig. 1(a) the M layer on the left has the majority $s+$ electrons pointing up in space whereas in the M layer on the right the $s+$ electrons point down in space. Figure 1(b) illustrates ferromagnetic orientation and $s+$ electrons in both M layers are taken to point up. For convenience we take the two M layers to have the same thickness t_M with the N thickness being t_N. By virtue of the simplifications made $s-$ M electrons and the half of the N electrons with spin in the same spatial direction constitute a single conductor. In Fig. 1(a) this means two distinct parallel conducting films of thickness t_M+t_N whose electrons are confined to this thickness *and have eigenstates quantized to this thickness.* In Fig. 1(b) we again have two parallel conducting films, one with thickness $2t_M+t_N$ and the other with thickness t_N. Here each $s-$ M electron and $s-$ N electron ($s+$ N electron) is confined to the $2t_M+t_N$ (t_N) conducting film and has eigenstates quantized to *these* thicknesses. GMR arises from the difference in the conductivities associated with the differences in the effective thicknesses between the arrangements shown in Figs. 1(a) and 1(b) and should be calculated using quantum size effect theories of metallic conduction. The $s+$ M electrons in both M layers are confined to t_M for both the ferromagnetic and antiferromagnetic film states and do not change their contribution to the conductivity with magnetic orientation. We have neglected their conductivity which reduces the GMR from the results obtained here.

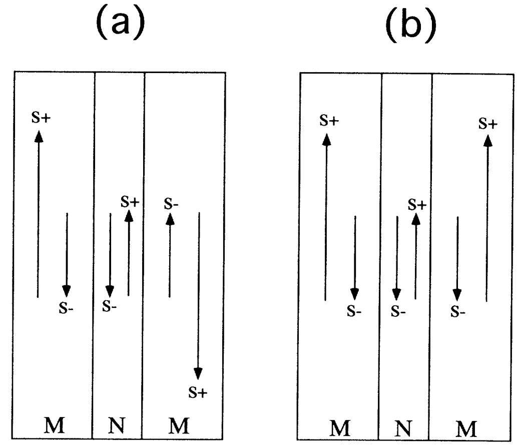

FIG. 1. The spin structure of a sandwich film with a nonmagnetic, N, layer between two identical magnetic layers, M. In M, $+$ and $-$ refer to majority and minority spin bands, respectively, and $\uparrow$ and $\downarrow$ are the spin directions in space. In N, $+\equiv\uparrow$ and $-\equiv\downarrow$. (a) and (b) illustrate antiferromagnetically and ferromagnetically oriented M layers, respectively.

An early treatment of the effects of quantum size effect on electrical transport properties was given by Sandomirskii [24]. Tesanovic, Jaric, and Maekawa [13] extended the theory for electrical conductivity to include scattering from rough surfaces. Most recently, Trivedi and Ashcroft [25] have further generalized the theory. We use the expressions they have developed for the conductivity under conditions of quantum size effect suitable for comparison with realistic experiments which is

$$\sigma_{xx}=\frac{e^2k_F}{\hbar\pi^2}\frac{1}{\kappa}\sum_{n=1}^{n_c}\left[\frac{1-n^2}{\kappa^2}\right]\Big/\left[\frac{2n_c+1}{k_Fl_0\kappa}+\left(\frac{\delta d}{d_0}\right)^2\frac{s(n_c)n^2}{3\kappa}\right], \tag{1}$$

where e is the electronic charge, $\hbar$ is the Planck's constant, k_F is the Fermi wave vector, d_0 is the quantum well (film) average thickness, δd is its root-mean-square deviation, $\kappa=k_Fd$, n_c is the integer part of κ and is equal to the number of occupied subbands arising from size quantization, l_0 is the impurity mean free path, and $s(n_c)=3S(n_c)/n_c^3$ with $S(n_c)=\sum_{n=1}^{n_c}n^2$.

This equation comes about in the following way. The thin film considered is presumed to be of a material which has a single, spherical, free electron, Fermi surface and isotropic scattering in the bulk. In the film, the wave functions are quantized in the thin, say z, (or k_z) direction and the Fermi sphere becomes a set of disks (subbands) parallel to the x-y (or k_x-k_y) plane [25]. Surface roughness on the scale of l_0 is contained in δd and results in a scattering rate that varies as n^2 where n is the subband number. Variations in d over segments of film larger than l_0 are ignored here but could be properly treated semiclassically; i.e., along the current direction the total resistance of the film would be the sum of resistances obtained from Eq. (1) for each segment.

We have carried out numerical calculations for the difference in conductivity between Figs. 1(a) and 1(b) for a variety of numerical values of the relevant parameters; bulk mean free path l_0, number of electrons/atom n, and surface roughness δd, t_M, and t_N. The lattice is taken as sc and the dimensional parameters are measured in monolayers (ML). A monolayer here is a single complete layer of atoms in the (100) direction. Space limitations dictate only a partial presentation of the results. The results presented will be for $10<t_M<70$ ML, $5<t_N<50$ ML, $\delta d=1$ and $\delta d=5$ ML, and $l_0=10$ and $l_0=70$ ML.

For films without any special fluctuations in their thickness and in the quantum size effect regime the electrical conductivity will oscillate with thickness [25]. In real metallic films the oscillations will smear out. By considering an sc lattice, varying our thicknesses in units of monolayers and assuming $n=\pi/3$ free electrons/atom (giving a Fermi wave vector of π/a) the oscillations are avoided and the underlying trends are most easily discerned.

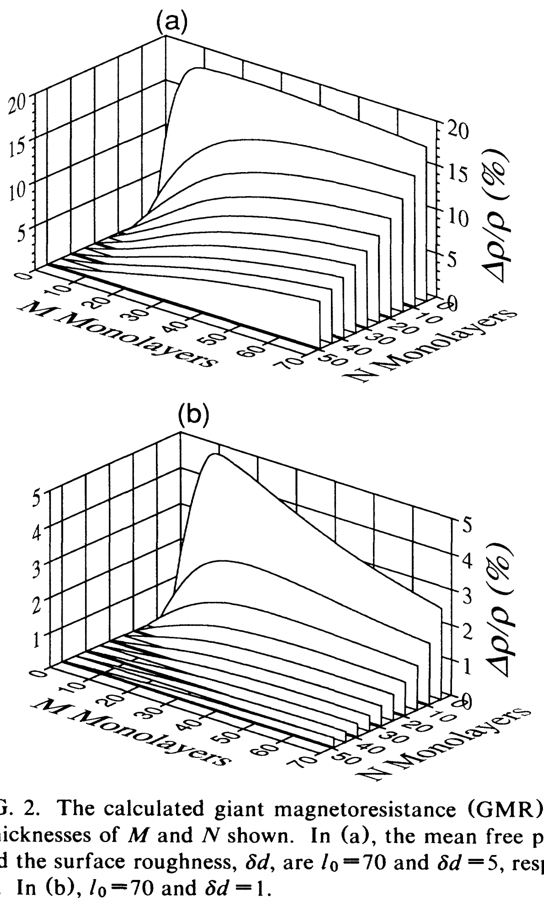

FIG. 2. The calculated giant magnetoresistance (GMR) for the thicknesses of M and N shown. In (a), the mean free path, l_0, and the surface roughness, δd, are $l_0=70$ and $\delta d=5$, respectively. In (b), $l_0=70$ and $\delta d=1$.

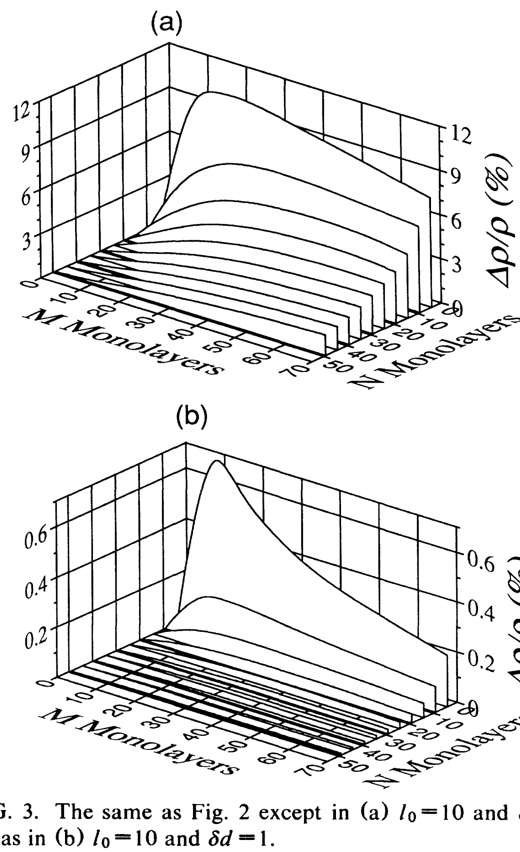

FIG. 3. The same as Fig. 2 except in (a) $l_0=10$ and $\delta d=5$ whereas in (b) $l_0=10$ and $\delta d=1$.

The results for GMR are shown in Figs. 2 and 3. The general shapes of the curves, plotted against M or N monolayers, are almost identical to those found experimentally. The rapid decrease with increasing t_N for all parameter values studied and both characteristic variations with t_M mentioned above are seen. Generally, GMR vs t_M will always have a peak, but the peak becomes progressively broader and occurs at greater t_M as any or all of l_0, δd, or t_N increase. Comparison of Figs. 2(a) with 2(b) as well as 3(a) with 3(b) shows the experimentally supported increase of GMR with increasing δd [6]. Comparison of Figs. 2(a) with 3(a) as well as 2(b) with 3(b) shows increased GMR with increased l_0 (reduced temperature or bulk crystallographic imperfection). It is also obvious from its very nature that this theoretical model yields a larger GMR for a superlattice than for a three layer sandwich. The magnitude that we calculate is also as expected. Although our calculated GMR values are somewhat large, this was to be expected since all the simplifications that we have made [perfect transmission (reflection) for $s-$ $(s+)$ electrons, neglecting current carried by $s+$ M bands] lead to overestimating the GMR.

In summary, we have demonstrated a theoretical mechanism that accounts for all the major features of GMR. Like other theoretical models that have been proposed, it is based on spin dependent electron scattering. Unlike previous theories it includes the fact that scattering at a metal-metal interface between thin films can establish quantum-well-like states within a layer and that because of spin dependent scattering these can be established preferentially for one spin compared to the other.

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