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ABSTRACT

The Layer Korringa Kohn Rostoker-Coherent Potential Approximation technique was used to calculate the low temperature ~~Giant~~ **Giant Magnetoresistance** from first principles for Co|Cu and permalloy|Cu superlattices. Our calculations predict large giant magnetoresistance ratios for Co|Cu and extremely large ratios for permalloy|Cu for current perpendicular to the layers. Mechanisms such as spin-orbit coupling which mix spin channels are expected to greatly reduce the GMR effect for permalloy|Cu.

Introduction

An unexpectedly large effect of an applied magnetic field on the electrical resistance has been observed in a number of ~~multilayer~~ **multilayer systems** involving transition metals. The effect consists of a dramatic decrease in the electrical resistance in the presence of an applied magnetic field and has been observed in Fe-Cr multi-layers[1, 2, 3, 4, 5, 6], in Co-Cu multilayers[3, 4, 7], in Co-Ru multilayers[3], and in bi-layers of Ni₈Fe₂ separated by a thin layer of Cu[7, 8]. The effect is seen in systems in which alternate layers of magnetic atoms are aligned anti-parallel with one another in the absence of the applied field. Application of the magnetic field brings the layers into alignment and causes a decrease in the electrical resistivity both parallel to the layers and perpendicular to them.

The resistances of bcc (100)Fe|(100)Cr[1] and fcc (111)Co|(111)Cu[4] have been observed to decrease by almost a factor of two when an applied magnetic field brings the magnetic moments on the layers into alignment. In this paper we present calculations of this giant magnetoresistance effect directly from first principles.

Previous Theory

Baibich *et. al.*[1] who first reported the effect based on their observations on Fe-Cr multi-layer systems observed that dilute Cr impurities in bulk Fe scatter majority spin electrons much more strongly than minority spin electrons. They proposed that the Cr atoms in the spacer layers might act the same way leading to a low resistance for the down spin electrons when the layers are aligned in parallel. The anti-parallel alignment would, in this picture, lead to a higher resistance by mixing the spin channels. Binasch *et. al.*[2] described the effect in terms of the necessity for electrons to undergo spin-flip scattering when traveling from one Fe layer into an adjacent one when the layers were aligned anti-parallel.

Camely and Barnas and Barnas *et. al.*[9, 10] generalized the semi-classical Boltzmann theory approach of Fuchs[11] and Sondheimer[12] to treat layered systems with different scattering properties in the two spin channels. Levy *et. al.*[13] and Zhang and Levy[14] developed a quantum mechanical treatment for spin dependent scattering in multilayer

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systems including both interfacial and bulk scattering. Both of these treatments utilize numerous adjustable parameters to account for the microscopic properties of these systems.

Calculation Technique

We have calculated the electronic structure of superlattices of copper and cobalt and of permalloy ($\text{Ni}_{80}\text{Fe}_{20}$) and Cu using the layer Korringa-Kohn-Rostoker technique[15] (LKKR) to solve the equations of density functional theory in the local spin density approximation[16, 17]. The LKKR technique is particularly well adapted for calculating the properties of layered materials. It has the advantage over most other electronic structure techniques that the time required for a calculation scales linearly with the number of layers rather than as the third power of the number of layers. The LKKR also does not require that one treat all structures as three dimensional superlattices. The properties of isolated interfaces, for example, can be calculated directly. In the work described here, however, we have modeled the systems as superlattices because this simplified the application of transport theory.

The systems which we have chosen to model in these initial calculations consist of (111) superlattices of copper and of either cobalt or permalloy. For the Co/Cu superlattices, scattering arises from the interfacial layers which we have assumed to be 1% interdiffused; i.e. the interfacial Cu layers are assumed to have 1% of the copper atoms replaced by cobalt atoms which are randomly distributed within the layer. Similarly the interfacial cobalt layers are assumed to have 1% of their atoms randomly replaced by copper atoms. For the permalloy/Cu superlattices, scattering arises from the permalloy layers which are assumed to be random solid solution alloys.

The disorder is treated in the coherent potential approximation[18, 19] which provides a means of constructing an average Green function for a disordered solid solution alloy and which has been successfully applied to the calculation of many properties of alloys[20]. A novel feature of the LKKR is the ability it provides for allowing the concentration of each species to vary from layer to layer.

The calculation of the electrical resistivity is based on the use of a CPA-like approximation to evaluate the product of two Green functions which appears in the Kubo-Greenwood expression for the conductivity[21]. For these initial calculations of the GMR it is convenient to make two approximations in addition to those implicit in the KKR-CPA theory of resistivity described in reference[21]. Firstly, we assume that the energy bands are reasonably well defined, i.e. that the mean free path is significantly greater than a typical interatomic spacing. This assumption allows the KKR-CPA theory of transport to be reduced to a Boltzmann equation in which the scattering probabilities are determined from first principles. The validity of this approximation can be checked since we calculate the mean free path for each point on the Fermi surface.

The second additional approximation that we have made in these calculations is the neglect of vertex corrections to the two particle propagator. This is equivalent to the neglect of the "scattering-in" terms in solving the Boltzmann equation. The regime of validity of this approximation is not quite so evident. It can be shown[22] that vertex corrections vanish if the individual scattering events are isotropic, or more generally, if they only connect states of the same parity, e.g. $s \rightarrow s$, $s \rightarrow d$, or $p \rightarrow p$. If the scattering is primarily in the forward direction, e.g. from a weak relatively long ranged potential (compared with the electron wavelength) the vertex corrections can be significant[23].

With these approximations the conductivity for spin i in the z -direction in response to an electric field in the z -direction can be calculated as a sum over the states, k , of the

superlattice,

$$\sigma_{zz}^i = \frac{e^2}{V} \sum_k v_z^i(k) v_z^i(k) \tau^i(k) \left(-\frac{\partial f_\mu(E)}{\partial E} \right). \quad (1)$$

Here V is the volume of the superlattice cell, $v_z^i = \hbar^{-1} \nabla_k E^i(k)$ is the electron group velocity, $\tau^i(k)$ is the Boltzmann lifetime defined below, and $f_\mu(E)$ is the Fermi function. At reasonable temperatures $(-\frac{\partial f_\mu(E)}{\partial E})$ is effectively a delta function at the Fermi energy and the conductivity can be written as

$$\sigma_{zz}^i = \frac{e^2}{\hbar(2\pi)^3} \int_\mu \frac{dS_k}{|v^i(k)|} v_z^i(k) v_z^i(k) \tau^i(k). \quad (2)$$

Using the fact that

$$\frac{dS_k}{|v^i(k)|} v_z^i(k) = dk_x dk_y, \quad (3)$$

and recognizing that $v_z^i(k) \tau^i(k)$ is simply the mean free path in the z -direction, l_z^i , we have,

$$\sigma_{zz}^i = \frac{e^2}{\hbar(2\pi)^3} \int dk_x dk_y l_z^i \quad (4)$$

where the z -component of the mean free path, $l_z^i(k_x, k_y)$ is determined by the imaginary part of the solution of the secular equation. Thus $l^i(k_x, k_y) = 1/(2\text{Im}k_z)$ where k_z is the (generally complex) solution to

$$E(k_x, k_y, k_z) = \mu \quad (5)$$

for given k_x and k_y . The detailed justification for this identification of the mean free path or the lifetime with the complex dispersion relation within KKR-CPA theory is given in reference[21] and was used to successfully calculate the electrical resistivity of Ag-Pd and other alloys[22].

Finally, in the calculations presented here, we neglect mechanisms that would mix the majority and minority scattering channels. Examples of such mechanisms which would be effective at zero temperature are spin-orbit coupling and any misalignment in the orientation of the moments of the impurities. At higher temperature, spin waves would be effective in mixing the scattering channels.

Results for Cu|Co

Table I gives the calculated conductivities, lifetimes, and resistivities for multilayers with equal thicknesses of Cu and Co. The quoted conductivities and resistivities are for a single spin channel. The $\uparrow$ symbol indicates the majority spin channel, $\downarrow$ denotes the minority spin channel, and A indicates either of the spin channels for the case in which the ferromagnetic layers alternate in moment direction (anti-ferromagnetic alignment). The calculated mean free path $\langle l_z^i \rangle$ is the average of the component of the mean free path in the z -direction defined as

$$\langle l_z^i \rangle = \frac{\int dk_x dk_y \sum_n l_z^{in}}{\int dk_x dk_y} \quad (6)$$

where the sum over n indicates that more than one sheet of the Fermi surface may have a projection on a given point in the two dimensional zone. This definition of an average mean free path may differ from other definitions and the appropriate definition for use in comparison to experiments on realistic systems may depend on the experiment and on the details of the Fermi surface.

Table I: Calculated mean free paths, single channel resistivities, parallel and anti-parallel resistivities and GMR ratios for Cu|Co superlattices. Currents are assumed to be perpendicular to the layers. Cu6Co6, for example, is a superlattice with 6 layers of Cu alternating with 6 layers of Co.

system	$\langle l_z^I \rangle$	$\langle l_z^{\downarrow} \rangle$	$\langle l_z^{AP} \rangle$	ρ^I	$\rho^{\downarrow}$	ρ^{AP}	ρ^P	ρ^{AP}/ρ^P
units	nm	nm	nm	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	
Cu1Co1	9353	280	334	0.588	19.66	8.24	0.639	12.90
Cu2Co2	6341	199	310	0.867	27.59	8.86	0.903	9.80
Cu3Co3	14279	221	377	0.385	24.87	7.30	0.425	17.17
Cu4Co4	16259	228	341	0.338	24.12	8.06	0.379	21.23
Cu5Co5	15014	356	480	0.366	15.45	5.72	0.431	13.28
Cu6Co6	32754	469	633	0.168	11.73	4.34	0.253	17.14

The column labeled ρ^{AP} is the calculated resistivity for anti-parallel arrangement of the magnetic moments in neighboring Co layers for both spin channels. The resistivity for the two spin channels is identical in this case so the total resistance for both spin channels will be half of the single channel value. The column labeled ρ^P is the net resistance (both channels) when the Co moments on all layers are parallel.

The magnitudes of the resistances depend on the amount of assumed interfacial interdiffusion, but we expect that the GMR ratio would not be affected if the amount of interdiffusion were increased under the assumption used here that all of the moments are aligned. The magnitude of the GMR effect would be reduced by scattering mechanisms such as phonons, vacancies, or grain boundaries that scatter the majority and minority spins more democratically and it would be greatly reduced by scattering mechanisms such as misaligned moments, e.g. in the interfacial regions, that cause a mixing of the spin channels and by spin waves at higher temperatures.

For reference, the calculated single channel resistivities (in $\mu\Omega\text{cm}$) of the dilute bulk alloys were Cu(1%Co): $\rho^{\uparrow} = 1.6$, $\rho^{\downarrow} = 19.2$ and Co(1%Cu): $\rho^{\uparrow} = 0.42$, $\rho^{\downarrow} = 4.92$. These are in reasonable agreement with the experimental values of the total resistance of 5.8 for Cu(Co)[24] and 0.89 for Co(Cu)[25] if it is remembered that the interpretation of the resistance of dilute Co in Cu is complicated by spin orientation and Kondo effects.

Results for Permalloy|Cu

Table II gives the calculated results for permalloy|Cu superlattices for equal thicknesses of the Ni₈Fe₂ layers and the copper layers. The calculations are for currents perpendicular to the layers. The remarkable feature of the results is that the calculated mean free paths are extremely long for the majority channel and extremely short for the minority channel. This leads to extremely large values of the predicted GMR ratio. Values of the resistivity in excess of $200\mu\Omega\text{cm}$ in the minority channel are unrealistic and result from a breakdown in the assumption that the bands are well defined. However, very strong scattering and high resistivities (on the order of $100\mu\Omega\text{cm}$) in the down spin channel should be expected since the potentials of Cu, Ni, and Fe are very different for minority electrons.

The long mean free paths and low resistivities calculated for the majority electrons result from the fact that the calculated majority Ni and Fe potentials have almost identical scattering properties at the Fermi energy. The scattering properties of the Cu atoms are almost as close but do not match quite as well. This should not be surprising since Cu has 11, valence electrons per atom, Ni has 10 and Fe has 9. Since Fe forms a moment of about $2.6\mu_B$ and Ni a moment of about $0.6\mu_B$, the number of electrons per atom for the

Table II: Calculated mean free paths, single channel resistivities, parallel and anti-parallel resistivities and GMR ratios for permalloy(P)|Cu superlattices. Currents are assumed to be perpendicular to the layers.

system	$\langle l_z^I \rangle$	$\langle l_z^I \rangle$	$\langle l_z^{AP} \rangle$	ρ^I	ρ^I	ρ^{AP}	ρ^P	ρ^{AP}/ρ^P
units	nm	nm	nm	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	$\mu\Omega\text{cm}$	
P1Cu1	707	0.782	1.291	0.202	183	55.5	0.202	274
P2Cu2	681	1.118	1.668	0.210	128	43.0	0.210	204
P3Cu3	662	0.557	1.062	0.216	256	67.5	0.216	312
P4Cu4	528	0.286	0.540	0.271	500	132.5	0.271	489
P5Cu5	623	0.191	0.468	0.230	750	152.5	0.230	664
P6Cu6	794	0.119	0.243	0.180	1206	294.1	0.180	1633

majority spins is 5.5 for Cu, 5.3 for Ni, and 5.3 for Fe. According to our calculations the difference in the number of electrons per atom in the self-consistent majority potentials for Ni and Fe is approximately 0.03. In contrast, the numbers of minority electrons per atom on the Cu, Ni, and Fe atoms is approximately, 5.5, 4.7, and 3.2. It should be remembered that the scattering rates scale as the square of the potential difference.

It is clear, however, that the calculation omits a scattering mechanism that significantly affects the majority electrons. The calculated resistivity of bulk permalloy is $0.038 \mu\Omega\text{cm}$, approximately 100 times smaller than the experimental value[26]. It is interesting to note that Mertig *et. al.* [27] obtained a calculated resistivity that is also two orders of magnitude too small in a very thorough study of the single impurity limit for Fe in Ni. The resistance of very dilute alloys of Fe in Ni is reported to be[28] $0.39 \mu\Omega\text{cm/at.}\%$. If these calculations are correct, the implication is that most of the resistance in Ni(Fe) alloys is due to mechanisms outside the standard model. One obvious omission is the neglect of spin-orbit coupling.

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