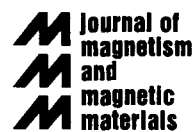




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Spin-dependent scattering and giant magnetoresistance

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Abstract

We consider the origins of the spin-dependent scattering which is believed to be responsible for the giant magnetoresistance effect. We argue on the basis of first-principles calculations of the electronic structure, magnetic moments, and electrical resistivities that this spin-dependent scattering originates largely from the tendency of spin-dependent atomic potentials to 'match' in one of the spin channels of magnetic alloys or multilayers. We also argue that the matched channel will tend to have a lower density of states at the Fermi energy. Both of these effects will contribute to the GMR. We argue that there is the potential for a very large GMR in an ideal system, but that spin-independent scattering possibly coming from misaligned spins near the interfaces prevents its observation.

1. Introduction

Recently there has been great interest in the transport properties of magnetic materials which are inhomogeneous on the scale of an electronic mean free path. This interest has arisen because of the discovery of a new form of magnetoresistance called the giant magnetoresistance (GMR). GMR is a change (usually a pronounced decrease) in the electrical resistance of an inhomogeneous system that is observed when an applied magnetic field causes an alignment of the magnetic moments in different parts of the material. GMR has been observed in several geometries. It was first observed in artificially layered systems [1,2]. Later, it was observed in systems consisting of magnetic inclusions in a non-magnetic matrix [3,4]. It has also been recognized that numer-

ous antiferromagnetic compounds exist in a natural layered structure and show a large decrease in resistivity (GMR) in the presence of a magnetic field strong enough to align their moments [5,6].

The GMR is generally considered to arise from spin-dependent scattering, that is, electrons of one spin are believed to be scattered more strongly than those of the other. Consider, for example, a hypothetical layered system consisting of layers of ferromagnetic metal, F, alternating with layers of normal metal N, and with current flowing perpendicular to the layers. Suppose, further that the majority spin electrons are hardly scattered in the ferromagnetic material whereas the minority spin electrons are very strongly scattered. Suppose further that the potentials seen by the majority electrons hardly differ between the F and N layers while the atomic potentials seen by the minority spin electrons in the F and N layers are quite different. We would expect that such a system would show a much larger conductivity when the F layers are aligned parallel than when neighbor-

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ing F layers are aligned antiparallel because in the case of parallel alignment the majority spin electrons experience an effective short-circuit.

We shall show that magnetic materials exist such that this hypothetical situation should be realizable if ideal interfaces could be constructed and that the existence of such materials is a natural and expected consequence of transition metal ferromagnetism. Unfortunately, the very large values of magnetoresistance of our hypothetical system have not been found in practice. Presumably the reason for this lies in the existence of strong spin-independent scattering both in the bulk and at the interfaces.

2. Potential matching and transition metal magnetism

Electrons can avoid one another in space and thereby lower their Coulomb energy by occupying the same spin state, thus assuring that their spatial wave functions are anti-symmetric with respect to the exchange of the labels on the electrons. In most metals this costs too much in kinetic energy and the net spin is zero, but in iron, cobalt and nickel the d-bands are sufficiently narrow that the reduction in the exchange energy exceeds the increase in kinetic energy when the metal acquires a net spin magnetic moment.

The net moment can be determined reasonably well by a model in which the ‘up’ and ‘down’ spin bands are shifted rigidly relative to one another until the gain in exchange energy just balances the cost in band energy [7–9]. To a good approximation the exchange interaction lowers the energy of the majority electron states relative to the minority states by an amount proportional to the magnetization, $m = n^\uparrow - n^\downarrow$. The constant of proportionality, I , is called the Stoner parameter and is on the order of 1 eV for iron, cobalt and nickel [10]. Thus

$$Im = \epsilon_{kn}^\downarrow - \epsilon_{kn}^\uparrow, \quad (1)$$

and the Fermi energies for the two spin systems will be shifted so that their chemical potentials will be given by

$$\mu^\uparrow = \epsilon_F^\uparrow(n^\uparrow) - \frac{1}{2}Im, \quad \mu^\downarrow = \epsilon_F^\downarrow(n^\downarrow) + \frac{1}{2}Im. \quad (2)$$

The functions $\epsilon_F^{\uparrow(\downarrow)}(n^{\uparrow(\downarrow)})$ are the energies required to contain $n^{\uparrow(\downarrow)}$ electrons, defined in terms of the density of states $N(\epsilon)$ (which we assume for the purposes of this simple argument to be the same for both spins) by

$$\epsilon_F^{\uparrow(\downarrow)}(n^{\uparrow(\downarrow)}) = \int_0^{n^{\uparrow(\downarrow)}} \frac{dn'}{N[\epsilon(n')]} \quad (3)$$

The moment will be determined by the requirement that the chemical potentials are the same,

$$I(n^\uparrow - n^\downarrow) = \int_{n^\downarrow}^{n^\uparrow} \frac{dn'}{N[\epsilon(n')]} \quad (4)$$

and will be quite sensitive to structure in the density of states.

The moment will usually adjust itself so that at least one of the Fermi energies falls at a low point in the density of states. Thus for fcc cobalt and nickel the majority d-bands adjust so that the d-bands are completely filled and ϵ_F^\uparrow falls in the low density of states region above the d-bands. Thus the majority band density of states for fcc cobalt or nickel [10] is very similar to the density of states of copper except that there are slightly fewer electrons per atom. Similarly, for bcc iron, the moment adjusts itself so that the Fermi energy for the minority electrons falls at the deep minimum in the bcc density of states near half filling which makes the minority spin density of states look very similar to that of chromium.

An examination of the density of states curves for fcc cobalt, nickel, and copper plotted with a common Fermi energy reveals that they are nearly indistinguishable. One might expect therefore, that majority spin electrons at the Fermi energy would see little difference between an atomic potential of cobalt, nickel or copper, and that similarly a minority spin electron would see little difference between the atomic potentials of bcc iron and chromium. It does not, of course, follow without proof that this matching of the density of states curves calculated for separate bulk materials implies potential matching for multilayers and alloys. We have, however, performed first-principles calculations of the electronic structure, magnetic moments, scattering rates and electrical conductivity of several systems which show GMR. The most striking feature of all of these systems is the matching of the atomic potentials in either the majority or minority channel so that Fermi

energy electrons in the matched channel experience weak reflections from interfaces, weak scattering at interdiffused interfaces and in the case of alloys such as permalloy, weak scattering within the ferromagnetic layers. We believe that for most systems which show large GMR, the primary contributor is potential matching. There will of course be other factors such as the Fermi energy density of states and the Fermi velocities which must be considered.

Our calculations are based on the local spin density approximation to density functional theory which has been shown to be reliable for calculating cohesive energies and magnetic moments of transition metals [10]. The effects of chemical disorder on the electronic structure were treated using the coherent potential approximation (CPA). The CPA replaces the random disordered system by an effective periodic one. The CPA, when implemented within the Korringa–Kohn–Rostoker technique for performing first-principles electronic structure calculations can be used to calculate cohesive energies and ground state properties of random disordered alloys [11] and has been extended to allow the calculation of the conductivities of random alloys [12]. More recently it has been extended to allow the calculation of the conductivity of systems in which the composition can vary from layer to layer [13].

Fig. 1 shows the number of majority and minority electrons per atom calculated for each atomic plane of a permalloy–copper trilayer. The layer Kor-

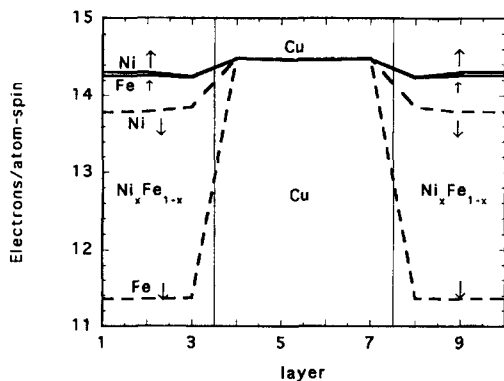


Fig. 1. Calculated number of electrons per atom for a trilayer system consisting of four atomic layers of copper embedded in permalloy. The atomic layers are fcc {111} layers. Note matching in majority channel.

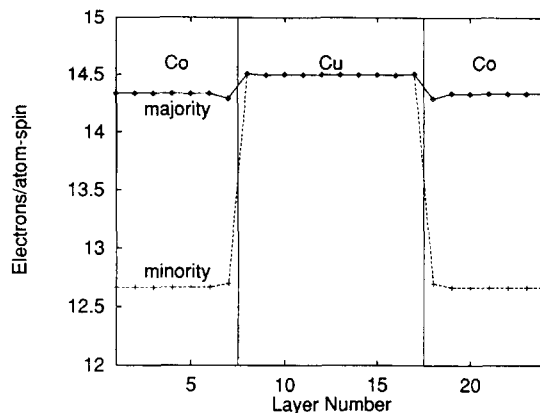


Fig. 2. Calculated number of electrons per atom for a trilayer system consisting of 10 atomic layers of copper embedded in cobalt. The atomic layers are fcc {111} planes. Note matching in majority channel.

ringa–Kohn–Rostoker coherent potential approximation [14] was used to treat the disordered atomic planes containing permalloy ($\text{Ni}_{0.8}\text{Fe}_{0.2}$) as random alloys. Note that there is a three-way matching of the potentials in the majority channel. The number of iron majority electrons matches very closely the number of nickel majority electrons and both of these match rather well to the number of copper majority electrons. Fig. 2 shows a similar plot for a cobalt–copper trilayer. Both of these calculations were performed self-consistently assuming fcc {111} planes of copper embedded in permalloy or in cobalt.

The matching can also occur in the minority channel. Fig. 3 shows the number of valence electrons in the majority and minority channels for an iron–chromium trilayer. This system consists of 8 bcc {100} atomic layers of chromium embedded in an infinite matrix of bcc {100} atomic layers of iron. In contrast to the systems consisting of fcc iron, cobalt, nickel and copper, which match in the majority spin channel, it is clear that the iron–chromium system matches in the minority spin channel. Incidentally, the small oscillations seen in the number of electrons per atom per spin in the chromium are the well known ‘almost commensurate’ spin wave, which originates from the same Fermi surface nesting as the short-period oscillations in the magnetic coupling of the the iron layers in iron–chromium multilayers.

Of course the number of electrons per atom in the majority and minority channels is only suggestive of

the scattering experienced by the electrons at the Fermi energy. Consider scattering by impurities. In the simplest model, the average scattering rate due to impurities can be shown to be approximated by

$$\left\langle \frac{1}{\tau_s^i} \right\rangle = \frac{2\pi}{\hbar} c N_s(\epsilon_F) \langle |\Delta V_s|^2 \rangle, \quad (5)$$

where $N_s(\epsilon_F)$ is the Fermi energy density of states for electrons of spin s , and ΔV_s is the difference between the impurity and host potentials for electrons of spin s . This expression is valid only in the limit of vanishing ΔV , but it can be shown [12] that the quantity which plays the role of ΔV in a realistic theory is proportional to the square of the sine of the differences of the phase shifts of the host and impurity potentials.

Fig. 4 shows the calculated phase shifts as a function of layer for the cobalt–copper trilayer of Fig. 2. If we assume that the scattering is caused by impurities resulting from interdiffusion between the copper and the cobalt at the interfaces and ignore complications due to canted or loose spins we can see that the scattering rate should be much lower in the majority than in the minority channel. The s and p phase shifts are relatively small (especially the p) and match somewhat better in the majority channel than in the minority, but it is the d -channel that is most important and for that channel the matching for the majority spins is quite good.

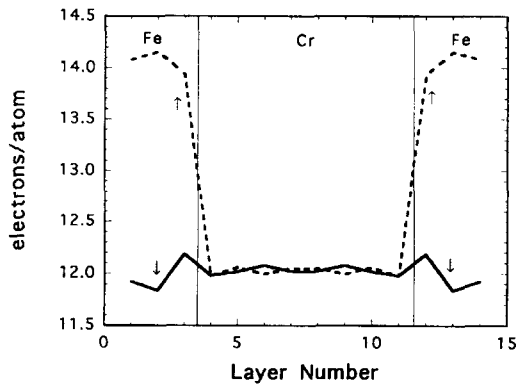


Fig. 3. Calculated number of electrons per atom for a trilayer system consisting of 8 atomic layers of chromium embedded in iron. The atomic layers are bcc {100} planes. Note matching in minority channel.

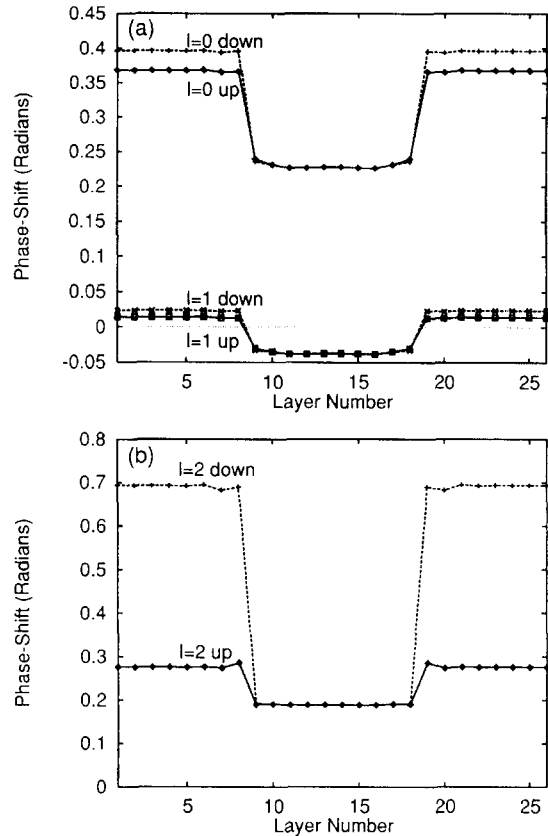


Fig. 4. Calculated phase shifts for cobalt copper trilayer. (a) s and p phase shifts for each layer, (b) d phase shifts for each layer.

Fig. 5 shows $\sin^2(\delta_d^{\text{Ni}} - \delta_d^{\text{Fe}})$, $\sin^2(\delta_d^{\text{Ni}} - \delta_d^{\text{Cu}})$, and $\sin^2(\delta_d^{\text{Fe}} - \delta_d^{\text{Cu}})$ as functions of energy for interfacial layers of permalloy and copper calculated for the permalloy–copper trilayer of Fig. 1. It shows that the scattering due to the iron in the nickel and the scattering between iron and copper is extremely weak in the majority channel. The scattering between copper and nickel is also relatively weak in the majority channel. By contrast there is extremely strong scattering in the minority channel due to iron in nickel and between iron and copper. There is also relatively strong scattering between nickel and copper in the minority channel.

Thus potential matching may lead to weak scattering in one of the spin channels in several ways. If one of the ferromagnetic layers is an alloy (e.g. permalloy) one should see a difference in the scatter-

ing rates and hence of the mean free paths between the majority and minority channels. If there is interdiffusion of the species at the interfaces and if the magnetic species maintain their moments and spin alignments there should be a large asymmetry in interfacial scattering between the majority and minority channels. Finally, even in the absence of interfacial diffusion, there will be an asymmetry in the number of electrons reflected at the interface. Since the ‘matched’ channel electrons see essentially the same potential on both sides of the interface, their transmission probability will be much higher than for the ‘unmatched’ channel.

Calculated electrical resistivities of random magnetic alloys dramatically illustrate the effects of potential matching. Fig. 6 shows the calculated residual electrical resistivity of nickel–cobalt alloys for each spin channel. Fig. 7 shows the calculated residual

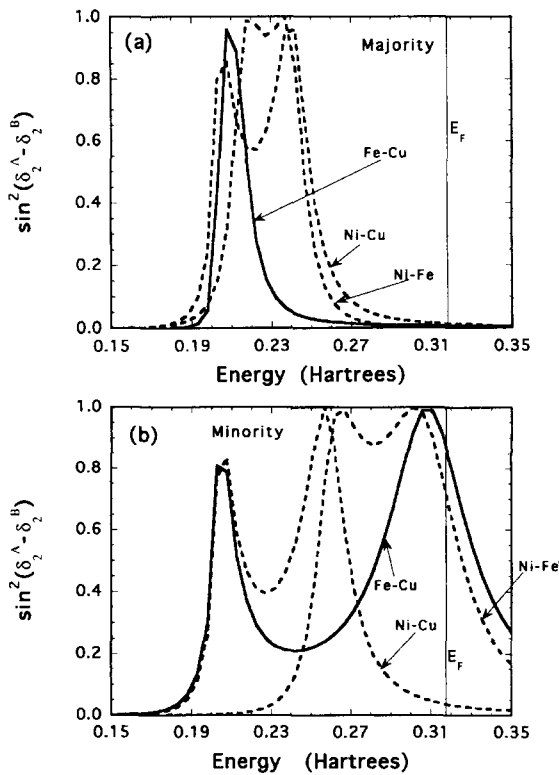


Fig. 5. Calculated squared sine of difference of phase shifts for d-channel as a function of energy for permalloy–copper trilayer. Phase shifts were calculated for potentials on interfacial layers. (a) Majority spin channel, (b) minority spin channel.

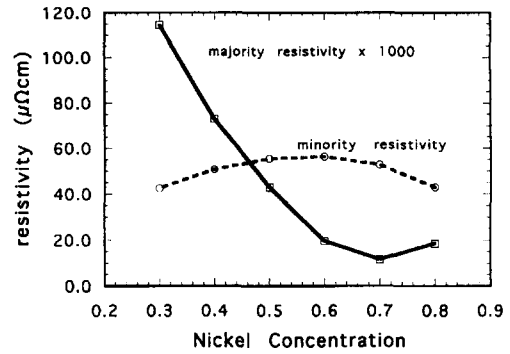


Fig. 6. Calculated electrical resistivity of Ni–Co alloys.

electrical resistivity of fcc nickel–iron alloys. For both alloys the calculations were performed using potentials calculated self-consistently using the KKR-CPA and the local spin density approximation to density functional theory. According to the calculations, the conductivity of these alloys is dominated by the majority spin electrons. A similar picture is obtained from calculations of the electrical resistivity in the dilute limit for iron and cobalt impurities in nickel [15]. Iron and cobalt impurities in nickel hardly scatter. These large asymmetries in the scattering rates between the majority and minority channels lead directly to large asymmetries in the current and hence to a very large GMR for an ideal model in which the only scattering is due to alloying or to interdiffusion at the interfaces [16,17].

The total electrical resistivities of these alloys have been measured [18,19] and although they are anomalously small for random alloys, they are not as small as these calculations predict. The inclusion of

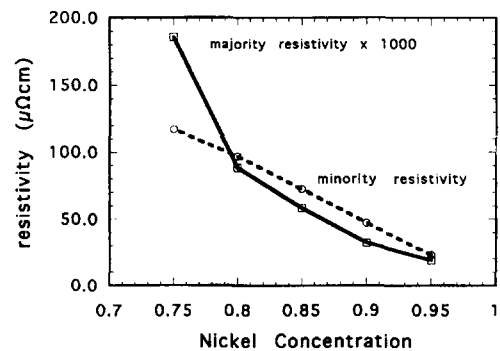


Fig. 7. Calculated electrical resistivity of Ni–Fe alloys.

spin-orbit coupling [20] increases the calculated resistivity by an order of magnitude, but not quite enough to agree with experiment. Experiments on dilute ternary alloys [21] allow one to infer ratios of resistivities in the minority and majority spin channels to be around 20 for iron in nickel and about 30 for cobalt in nickel. Our calculations predict that these ratios should remain large and may even increase for the more concentrated alloys.

The calculated electrical resistivities of chromium-iron alloys are quite interesting. For fcc alloys of iron and cobalt with nickel, the moments of the iron, cobalt and nickel are relatively independent of concentration. The situation is quite different for bcc iron-chromium alloys as is shown in Fig. 8. The calculated chromium moment is large and negative at low concentrations of chromium but it rapidly drops to zero as the chromium content is increased (in reasonable agreement with measurements from neutron scattering [22]). Associated with this decrease in the moment we calculate a large decrease in the electrical resistivity in the minority spin channel. This calculated decrease occurs because of potential matching. Since the iron moment stays relatively constant at approximately $2\mu_B$, it has approximately 3 minority valence electrons. Thus its potential will match that of Cr when Cr has zero moment. We have not been able to find low-temperature measurements of the electrical resistivity of concentrated bcc iron-chromium alloys. A decrease in the electrical resistivity of the type and magnitude predicted here would be quite extraordinary. Data for dilute alloys [23] indicate that the actual resistivity is

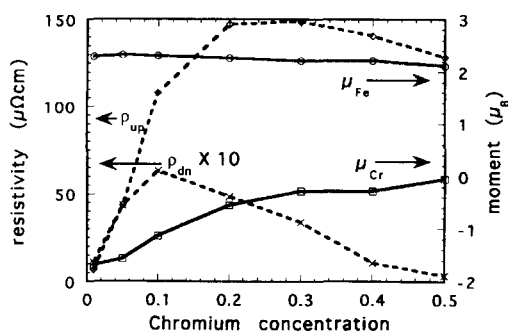


Fig. 8. Calculated magnetic moments and electrical resistivity of iron-chromium alloys as a function of chromium composition.

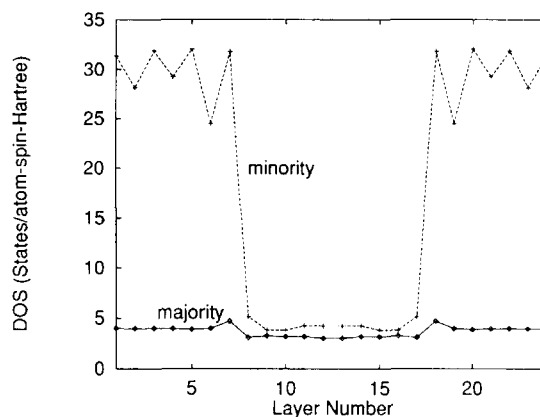


Fig. 9. Fermi energy density of states for a cobalt-copper trilayer. The trilayer consists of 10 atomic layers of copper embedded in cobalt. The layers consist of fcc {111} planes of atoms.

about twice that calculated here for the most dilute alloys.

3. Density of states

In Section 2 we argued that ‘potential matching’ is a natural, common, and expected consequence of transition metal magnetism. Another common consequence is that the density of states will be low in the channel which shows the matching effect. This is because the bands shift to minimize the energy by finding a low point in the DOS in which to place the Fermi energy. Thus the matching occurs when similar systems find the same low point for their Fermi energies. Fig. 9 shows the calculated Fermi energy density of states for each atomic layer in a trilayer consisting of 10 atomic layers of copper in a cobalt matrix. The density of states in the minority (non-matching) channel is seen to be approximately seven times that in majority channel. According to Eq. (5), the scattering rate for impurities is proportional to the density of states at the Fermi energy. This density of states factor arises because the scattering probability is proportional to the number of states available for an electron to scatter into. Thus in addition to the potential matching effect there will often be an additional contribution to the asymmetry in the scattering rates between the spin channels due to the Fermi energy density of states being substan-

tially lower for this channel. It should be remembered however that Eq. (5) is a significantly oversimplified and that the scattering rate asymmetry will in fact depend very strongly on the kinds of defects that are present.

Electron–phonon scattering is an important contributor to the resistivity at higher temperatures in relatively clean systems. This kind of scattering also has a $N_s(\epsilon_F)$ factor,

$$\left\langle \frac{1}{\tau_s^{\text{ep}}} \right\rangle = \frac{2\pi}{\hbar} c N_s(\epsilon_F) \frac{\langle I_s^2 \rangle}{M \langle \omega^2 \rangle} k_B T. \quad (6)$$

Here M is an atomic mass, $\langle \omega^2 \rangle$ is a mean square phonon frequency, and $\langle I^2 \rangle$ is the square of the electronic part of the electron–phonon matrix element which can be calculated by averaging the square gradient of the atomic potentials over the Fermi surface [24]. $\langle I^2 \rangle$ is generally spin-dependent and its variation may either enhance or partially cancel the $N_s(\epsilon_F)$ effect [24]. Magnons are the other and often more important contributor to resistivity at higher temperatures. They will usually act to counter large asymmetries between the conductivities of the spin channels because they provide a mechanism for electrons to scatter between the channels [21,25].

4. Intralayer exchange

So far we have modeled multilayers as atomically perfect planes of atoms. This is unlikely to be an accurate representation of practical systems, especially near interfaces. In addition to defects such as impurities, vacancies, dislocations, etc., which might

be expected to show some spin asymmetry due to the density of states effect, one particularly detrimental class of defects should be considered; those that are associated with a loss of the magnetic moment or with a change in its orientation.

We have investigated nickel–copper and permalloy–copper interfaces because experiments have detected magnetically dead layers near the interfaces in these systems [26]. We consider it likely that nickel and copper will interdiffuse near the interfaces in permalloy–copper and nickel–copper multilayers and spin valves. This can be particularly detrimental to the GMR because the moment on the nickel is expected to decrease if it is mixed with copper. Furthermore the interatomic exchange coupling may be decreased so that the iron atoms which maintain their moments when surrounded by copper atoms may not maintain the proper alignment.

In order to investigate these possibilities we have calculated the energy required to disorder the moments of permalloy ($\text{Ni}_{0.8}\text{Fe}_{0.2}$), permalloy diluted 50% with copper ($\text{Ni}_{0.4}\text{Fe}_{0.1}\text{Cu}_{0.5}$), and cobalt diluted 50% with copper ($\text{Co}_{0.5}\text{Cu}_{0.5}$). For the Disordered Local Moment (dlm) calculation we assume that the moments are equally likely to be up or down and treat all of the components using the KKR-CPA to calculate the moments, total energy, etc., self-consistently. Thus $\text{Co}_{0.5}\text{Cu}_{0.5}$ is treated in the dlm state as a four component alloy, $\text{Co}\uparrow$, $\text{Co}\downarrow$, $\text{Cu}\uparrow$, $\text{Cu}\downarrow$, similarly $\text{Ni}_{0.4}\text{Fe}_{0.1}\text{Cu}_{0.5}$ is treated in the disordered local moment state as a six-component alloy. In all of the calculations we found the moment on the copper site to be less than $0.01\mu_B$. All of these calculations are for the fcc phase. In reality, we

Table 1

Calculated energy differences, moments and resistivities for ferromagnetic and disordered local moment permalloy, permalloy_{0.5}Cu_{0.5}, and Co_{0.5}Cu_{0.5}.

System	Relative energy (mHa)	Ni moment (μ_B)	Fe or Co moment (μ_B)	ρ_{\uparrow} ($\mu\Omega\text{cm}$)	ρ_{\downarrow} ($\mu\Omega\text{cm}$)
ferro $\text{Ni}_{0.8}\text{Fe}_{0.2}$	0.00	0.570	2.59		
dlm $\text{Ni}_{0.8}\text{Fe}_{0.2}$	1.70	0.050	2.55		
ferro $\text{Ni}_{0.4}\text{Fe}_{0.1}\text{Cu}_{0.5}$	0.00	0.292	2.54	9	115
dlm $\text{Ni}_{0.4}\text{Fe}_{0.1}\text{Cu}_{0.5}$	0.33	0.023	2.51	83	83
ferro $\text{Co}_{0.5}\text{Cu}_{0.5}$	0.00		1.48	5	80
dlm $\text{Co}_{0.5}\text{Cu}_{0.5}$	2.13		1.20	77	77

expect that the spin disorder in the vicinity of interfaces will be much more complicated than we have assumed, although we hope to obtain qualitative insight into what may be happening.

The results are shown in Table 1. We see that dilution with copper reduces the nickel moment in permalloy and also reduces the moment in cobalt (to 1.48 from approximately 1.6 in fcc Co). Disordering the moments nearly quenches the nickel moments and further reduces the cobalt moment (to $1.2\mu_B$). We believe the relative energies of the ferromagnetic and dlm states are instructive. According to the calculations 1.7 mHa are required to disorder the spins of permalloy, but only 0.33 mHa to disorder the spins of permalloy after it has been diluted by copper; 1 mHa is 0.0272 eV and thus corresponds roughly to room temperature. Thus we predict that permalloy diluted with copper, as is likely to be found near the permalloy–copper interface in spin-valves and multilayers, is susceptible to local spin disordering. This spin disordering may arise from local structural and chemical imperfections as well as from temperature.

It is known [27] that small amounts of cobalt placed at the interface between the permalloy and the copper in a permalloy–copper spin valve will significantly increase its GMR. Our calculations show that cobalt maintains its exchange coupling much better than permalloy when diluted with copper. In fact, we find that cobalt diluted with copper has a greater resistance to spin disordering than pure permalloy (2.1 versus 1.7 mHa). Thus cobalt may act to enhance the GMR when it is placed near interfaces through strengthening the intralayer exchange coupling near the interface rather than through a direct effect on the spin-dependent scattering. This suggestion has been made previously [28]. Coehoorn [29] has shown that cobalt at a nickel–copper interface may help the nickel to maintain its moment. A second possible beneficial effect of cobalt at the interface is the inhibition of interdiffusion.

5. Discussion

From the results of first principles calculations using the local spin density approximation to density

functional theory, potential matching in the majority spin channel is predicted for fcc iron, fcc cobalt, nickel and copper. Matching is predicted for the minority spin channel for bcc iron and chromium. Resistivities for these magnetic alloys were calculated using the Kubo formula. The predicted resistivities are generally much lower than seen in experiments. This disagreement can arise from several factors. Spin–orbit coupling increases the resistivity by mixing the spin channels in permalloy. Additionally, lattice relaxation due to disorder was neglected in all of our calculations, although it is unclear what effect if any it will have on the resistivity. Vertex corrections have also been neglected in our calculations to date, but we expect that vertex corrections would actually *increase* the asymmetry in spin-channel conductivities. This is based on our experience with silver–palladium alloys [30] which showed that the vertex corrections are important and increase significantly the conductivity when the Fermi surface is above the d-band. It would probably affect the majority channel in the Ni alloys, but the effects in other systems should be small.

Due to the large ratio of the resistivities between the two spin channels, we predict a large GMR ratio for the multilayers. Although including the effects of spin–orbit coupling and lattice relaxation may reduce this ratio, we believe it should still be much larger than has been observed experimentally. We believe that the most likely reason for the observed small GMR ratio is moments near the interface which are misaligned due to weak exchange coupling. This can cause significant spin-independent scattering which can dominate the resistivity in the potential-matched spin channel.

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