

Theoretical evaluation of magnetotransport properties in Co/Cu/Co-based spin valves

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The current-in-plane resistivities and corresponding magnetoresistance ratios are calculated for realistic Co/Cu/Co-based spin-valve samples by applying the Kubo-Greenwood approach together with the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method for layered structures. We study the effects of both alloying in the spacer layers with a selection of $3d$, $4d$, and $5d$ elements as well as different profiles for interdiffusion at the Co/Cu interfaces. On comparing our results to available experimental data we find that both interdiffusion and confinement effects, due to the finite overall thickness of the spin valve, strongly influence the magnetoresistance of spin-valve structures.

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I. INTRODUCTION

The magnetotransport properties of magnetic multilayered structures, e.g., the giant magnetoresistance (GMR), have been of current interest both for their potential applications, such as the read heads of hard disk drives in computers, as well as for the basic physics of electrical transport in magnetically inhomogeneous materials. In particular it has been a challenge to do *ab initio* calculations of these properties that can be compared with experimental data. The primary difficulties lie both in using an appropriate algorithm to calculate the resistivities as well as gaining sufficient knowledge from experiments of the precise nature and distribution of the impurities and defects which produce the resistance and magnetoresistance in these multilayers.

As of the middle 1990s several attempts have been made to explore various effects giving rise to or controlling GMR in magnetic multilayer systems, in particular on Co/Cu-based structures.^{1,2} By means of nonlocal conductivities obtained from the Kubo-Greenwood formalism as applied to a layered Korringa-Kohn-Rostoker approach Butler *et al.*¹ shed light on the nonlocal and channeling (wave-guide) effects that contribute to the intrinsic origins of GMR. These ideas have been supported by Mertig *et al.*² in terms of a Boltzmann-type approach by using a screened Korringa-Kohn-Rostoker method; in addition they pointed out the importance of diffusive interface scattering to the GMR in repeated Co/Cu

sequences. These authors also studied dilute alloys of the Co interface layer with various $3d$ elements, as well as for $c(2 \times 2)$ interface alloys, and found remarkable variations of the GMR.

We have recently developed an *ab initio* code that is capable of including both the effects of electronic structure as well as defect scattering on the electrical resistivities of magnetic multilayered structures.^{3,4} As it is nigh impossible to know the precise nature and distribution of the defects and impurities that produce the resistance in these multilayered structures we have undertaken a study of how specific impurities and distributions of impurities affect the transport properties of multilayered structures. In large part we focused on Co/Cu/Co-based spin valves because of the experimental data available. However, the data is usually given at room temperature whereas our calculations are limited to zero temperature. Therefore, we have taken data at low temperatures on a specific spin-valve structure in the current-in-plane (CIP) geometry and present an analysis based on our modeling of this structure.

As interfaces are known to be centers of strong spin-dependent scattering we will present in this paper how different concentration profiles of interdiffused impurities about an interface between a magnetic and nonmagnetic metallic layer affect the transport properties of Co/Cu/Co-based spin valves. Scattering from impurities in the bulk of the layers is known to be a secondary source of resistivity; therefore, we

have determined the effect of alloying the bulk of the non-magnetic spacer layers with impurities. Our salient conclusions are that the transport properties are sensitive to the distribution of the interdiffused impurities as well as to the amount of impurities. When we introduce impurities which are strong spin-orbit scatterers in the bulk of the nonmagnetic spacer layer we find that the magnetoresistance drops precipitately; e.g., as little as 1% Ti in Cu reduces the GMR by a factor of 2, and at 5% Ti the GMR is nearly completely destroyed.

II. METHOD OF CALCULATION

Applying the Kubo-Greenwood approach the CIP resistivity (ρ^C) and conductivity (σ^C) for disordered layered systems with growth direction along the surface normal (z axis) are given by⁵

$$\begin{aligned}\rho^C &\equiv \rho_{xx}(n; \mathbf{c}; \mathcal{C}), & \sigma^C &\equiv \sigma_{xx}(n; \mathbf{c}; \mathcal{C}), \\ \rho_{\mu\mu}(n; \mathbf{c}; \mathcal{C}) &= 1/\sigma_{\mu\mu}(n; \mathbf{c}; \mathcal{C}), & \mu &\in \{x, y\}, \\ \sigma_{\mu\mu}(n; \mathbf{c}; \mathcal{C}) &= \sum_{i,j=1}^n \sigma_{\mu\mu}^{ij}(\mathbf{c}; \mathcal{C}), & \mu &\in \{x, y\}, \\ \sigma_{\mu\mu}^{ij} &= \frac{\hbar}{\pi N_0 \Omega_{\text{at}}} \text{Tr} \langle J_{\mu}^i \text{Im} G^+(\epsilon_F) J_{\mu}^j \text{Im} G^+(\epsilon_F) \rangle.\end{aligned}\quad (1)$$

Here, n denotes the number of layers considered, \mathbf{c} gives the layerwise compositions, and \mathcal{C} denotes a particular magnetic configuration. $\sigma_{\mu\mu}^{ij}$ is the conductivity that describes the current in layer i caused by an electric field in layer j , N_0 is the number of atoms per plane of atoms, Ω_{at} is the atomic volume, $\langle \dots \rangle$ denotes an average over configurations, J_{μ}^i is the μ th component of the current operator referenced to the i th plane, and G^+ is the electron propagator (one-particle Green's function) from planes i to j at the Fermi energy ϵ_F . The expressions given in Eq. (1) are restricted to CIP [for currents perpendicular to the planes of layers the resistivity for a finite layered structure cannot be written in this way (see Ref. 6)].

In spin-valve structures the relative change in resistivities between ‘‘antiparallel’’ (AP) and ‘‘parallel’’ (P) alignments of the magnetizations of the magnetic slabs is commonly referred to as GMR or the magnetoresistance ratio:

$$R = \frac{\rho^{\text{AP}} - \rho^{\text{P}}}{\rho^{\text{AP}}}.\quad (2)$$

We adopt this definition of the GMR, rather than the one usually used to report experimental results (in which the denominator is the resistivity of the parallel configuration), because the ratio given by Eq. (2) is bounded between zero and one. Unless stated explicitly otherwise, all numbers and figures presented in this paper refer to the choice of definition according to Eq. (2); for small values of R the difference between the two definitions appears to be a relatively constant shift of about 1%–2%.

All our calculations are done within the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker (KKR) method for layered systems; the effects of introducing impurities (interdiffused impurities about an interface or impurities inside the bulk of a layer) are incorporated by means of the single-site coherent-potential approximation (CPA). Therefore, we can calculate resistivities and GMR for magnetic multilayered structures with *no* adjustable parameters other than the lattice constant, i.e., in an *ab initio* manner. In this scheme the effects arising from the electronic structure and those coming from concentrated impurities on the magnetotransport properties are evaluated simultaneously.^{3–5}

A fully relativistic spin-polarized calculation of the resistivities is of course essential when dealing with systems that have strong spin-orbit coupling. It offers a possibility to test the mixing of the spin currents (that are assumed to be independent channels in the so-called ‘‘two current model’’⁷) due to impurities which have strong spin-orbit scattering potentials. But also for the Co/Cu/Co-based spin valves without strong spin-orbit scattering impurities the fully relativistic treatment is important to obtain realistic resistivities as it prevents the short circuit produced by the near matching of potentials for one spin channel that is usually found by applying the ‘‘two current model.’’ Unique to a fully relativistic spin-polarized approach the dependence of the resistivities on the orientation of the magnetization relative to the layers can be determined without further parameters or approximations; therefore, it allows us to determine the contributions coming from the anisotropic magnetoresistance to the GMR of magnetic multilayered structures.

However, our current implementation has a few limitations: Using the single-site approximation to the CPA to describe the electronic structure of substitutional alloys implies that all sorts of short-range order or concentration fluctuations are excluded. Furthermore, in our present use of the Kubo-Greenwood approach for layered systems no vertex corrections arising from the configurational average of the product of two Green's functions are included (however, they are usually found to be quite small for the CIP geometry; see also the discussion in Ref. 5). All interlayer distances refer to the ‘‘parent lattice’’ of the substrate, i.e., surface and interface relaxations are completely neglected, and in order to establish a well-defined Fermi level we conveniently use a semi-infinite metal as substrate (see also the discussion on outgoing boundary conditions in Sec. IV). In addition, for computational purposes a finite imaginary part to the Fermi energy (δ) has to be used in the calculation of the conductivities σ_{xx}^{ij} that in turn produces a spurious resistivity for which correction should be made.

In the present paper all calculations are based on self-consistent effective potentials and effective exchange fields as obtained by using the fully relativistic, spin-polarized, screened KKR method⁸ together with the CPA for layered systems⁵ and applying the local-density functional of Vosko *et al.*⁹ All scattering channels up to and including $l_{\text{max}}=2$ were taken into account, and all interlayer distances refer to the fcc(100) ‘‘parent lattice’’ of Co ($a_0=3.47$ Å, $d=1.73$ Å). In the self-consistency runs 45 \mathbf{k}_{\parallel} points in the irreducible wedge of the surface Brillouin zone (ISBZ) have

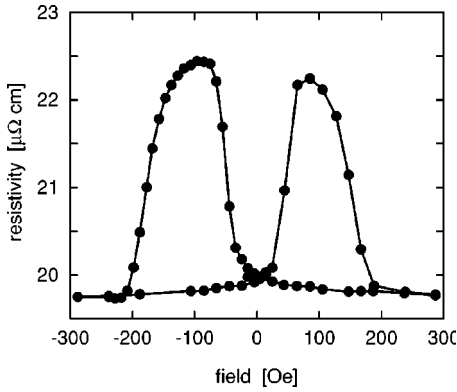


FIG. 1. Resistivity of the spin-valve sample NiO/Co(25 Å)/Cu(22 Å)/Co(40 Å)/Ta(10 Å) as a function of field measured at 4.2 K.

been used to determine the electronic structure. However, in calculating the conductivities σ_{xx}^{ij} 1830 \mathbf{k}_{\parallel} points in the ISBZ together with a finite imaginary part to the Fermi energy of $\delta=2$ mRy have been used to evaluate the surface-Brillouin-zone integrals⁵ involved. In order to speed up the computations we have “chosen” the magnetization to point uniformly perpendicular to the planes of atoms, i.e., along the z axis [with this choice the xx and yy components in Eq. (1) are identical], for most of the calculations (see also the discussion on the orientation of the magnetization in Sec. IV).

III. EXPERIMENTAL RESULTS

As a prototypical example of the magnetoresistance one can expect from a spin-valve structure we made and performed measurements on polycrystalline (no preferred orientation) NiO/Co(25 Å)/Cu(22 Å)/Co(40 Å)/Ta(10 Å) spin-valve structures. The Co/Cu/Co films were deposited onto Si substrates coated with NiO by using dc magnetron sputtering. The antiferromagnetic NiO films are polycrystalline and provide pinning to the bottom Co layer. Both the resistance and magnetoresistance were measured using the Van der Pauw method at temperatures ranging from 4.2–300 K. The absolute resistivity values were deduced from the film thickness, and the measured resistance was corrected for a small asymmetry between the two conducting paths by conventional methods. At low temperatures, as the pinning field increases, the nearly full antiparallel alignment is realized in the high-resistance state. Therefore, the quoted magnetoresistances were calculated from the resistances in the well-defined parallel and antiparallel states. In Fig. 1 we show the resistivity of this structure at 4.2 K; the measured GMR varies from 12% at 4.2 K to 5% at 300 K.

IV. MODELING

If we were to calculate the transport properties of the actual spin valve studied we would need a total of 56 monolayers; this far exceeds the present computing capabilities as we are currently limited to consider on the order of 40 monolayers. Therefore, we must judiciously transcribe the

actual structure to a model which retains the features of the original structure that are critical for magnetotransport properties.

We have chosen to do our calculations on the model spin-valve structure Co(100)/Co₁₂Cu₁₂Co₁₂/Co(100), i.e., considering 36 magnetically active monolayers. Our model spin-valve structure differs from the measured structure in three ways: (i) the thicknesses of the magnetic layers are different; the 12 monolayers correspond to a thickness of 20.8 Å; (ii) the substrate and capping layers in which the magnetically active part of the spin valve is embedded are substituted by semi-infinite Co; and (iii) we forced the magnetization to point perpendicular to the planes of atoms in our calculations instead of pointing in plane. Since the measured spin valve was polycrystalline and therefore had no preferred orientation in the spin-valve layers, we have deliberately chosen to use the fcc(100) stacking sequence in our calculations, because the computations are much faster for fcc(100) than for fcc(111). In addition, in our calculations we are constrained to use a finite imaginary part to the Fermi energy ($\delta = 2$ mRy) that produces an artificial resistivity for which corrections will have to be made.

Regarding point (i), as we focus in this paper on the role of interdiffusion at the Co/Cu interfaces and not on the impurity scattering in the Co layers themselves the thickness of the Co layers is not critical provided one considers a minimum of 8–12 monolayers of Co. As for the second point (ii), the boundary conditions on the magnetically active part of the spin valve are essential to obtain a realistic estimate of the transport properties. Our model structure places the spin valves in direct contact with semi-infinite metals; this is needed in our calculational scheme to establish a well-defined Fermi level. However, this computational aid has the drawback that it is equivalent to outgoing boundary conditions on the spin-valve structure (allowing some electrons to leak out into the semi-infinite leads) and therefore produces spurious contributions to the resistivities which are not present in the spin-valve structures embedded between NiO and Ta layers.¹⁰ To access the magnitude of this spurious resistivity we have calculated the resistivity of a companion structure vacuum/Co₁₂Cu₁₂Co₁₂/vacuum, i.e., again our model spin-valve structure but with reflecting boundary conditions.

In Fig. 2 we show the layer-resolved contributions to the conductivity for our model structure with outgoing and reflecting boundary conditions. When we look at the layer-diagonal contributions [Fig. 2(a)] we find that the major differences occur in the vicinity of the boundary; specifically the conductivities are oblivious to the boundaries when one has outgoing boundary conditions, while the reflecting boundary conditions cause a pile up of charge and concomitantly conductivity at the boundaries. Also noteworthy is the insensitivity of the layer-resolved conductivities σ_{xx}^{ij} in the interior of the spin valve especially about the Co/Cu interfaces and inside the Cu spacer layers [Figs. 2(a), 2(c), and 2(d)]. When we look at the total contribution to the conductivity coming from each layer, i.e., $\sigma_{xx}^i = \sum_{j=1}^n \sigma_{xx}^{ij}$ [Fig. 2(b)], we find that the reflecting boundary condition more or less uniformly shifts the σ_{xx}^i upwards compared to the outgoing

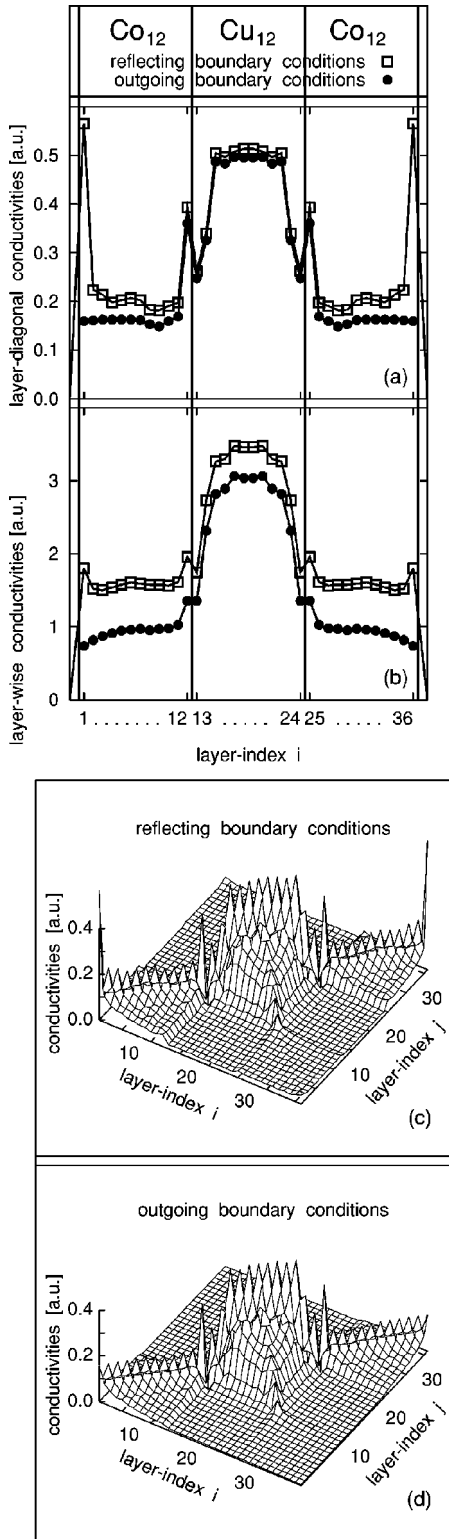


FIG. 2. Layer-resolved contributions to the conductivity with $\delta=2$ mRy for the parallel configuration of the model spin-valve structure with reflecting (vacuum/Co₁₂Cu₁₂Co₁₂/vacuum; open squares) and outgoing [Co(100)/Co₁₂Cu₁₂Co₁₂/Co(100); full circles] boundary conditions: (a) Layer-diagonal contributions σ_{xx}^{ii} , (b) layerwise conductivities $\sigma_{xx}^i = \sum_{j=1}^n \sigma_{xx}^{ij}$, and (c) and (d) layer-resolved conductivities σ_{xx}^{ij} with reflecting and outgoing boundary conditions, respectively.

boundary condition. This comes from the additional contributions to σ_{xx}^{ij} along the boundaries [see Figs. 2(c) and 2(d)] which enter the σ_{xx}^i for all layers. For our model structure we find that the outgoing boundary condition produces a spurious resistivity of $\sim 4 \mu\Omega \text{ cm}$ (independently of δ) as compared to the free-standing spin valve. Concomitantly the GMR depends on these boundary conditions; the GMR of our model structure evaluated from resistivities at $\delta = 2$ mRy is 10.1% for outgoing and 14.5% for reflecting boundary conditions.

Finally on the last point (iii), although in the Co/Cu/Co-based spin valves studied in this paper the orientation of the magnetization is in the plane of the layers (according to our calculations and confirmed by experiment), in the present study—for ease of computation—we forced the magnetization to point perpendicular to the planes of atoms. As we use a fully relativistic code we are able to determine the contribution coming from anisotropic magnetoresistance to the GMR; it is less than what one would normally expect. For our model structure with outgoing boundary conditions the GMR is 10.1% when it is evaluated from resistivities at $\delta = 2$ mRy and for magnetization perpendicular to the layers, while it is 9.7% for in-plane magnetization; therefore the anisotropic magnetoresistance, $[(\rho_{\parallel} - \rho_{\perp})3/(2\rho_{\perp} + \rho_{\parallel})]$, is 0.7% in the parallel configuration and 0.3% in the antiparallel configuration.

V. INTERDIFFUSION AT INTERFACES

The interfaces in metallic multilayered structures have two sources of scattering: the interdiffusion of atoms between layers and the geometrical roughness of the interface.¹¹ At the present time we have used only the single-site CPA to consider the effects of disorder on transport properties. In particular we neglect short-range order and are unable to consider extended defects. For this reason we will not consider interface roughness; rather we will focus on interdiffusion which can be described at some level within the single-site CPA.

There are two aspects to the interdiffusion we will consider: the amount of interdiffused atoms across the interfaces and the concentration profile of the interdiffusion. In Fig. 3 we show the different interdiffusion profiles we have considered in our calculations. We assume the same interdiffusion profile at both Co/Cu interfaces, and all profiles are symmetric about the interfaces. Interdiffusion between the two layers forming the interface (*P2*) means that the monolayer of the Co slab adjacent to the interface has a composition of Co_{100-c}Cu_c and the adjoining monolayer in the Cu spacer has a composition of Cu_{100-c}Co_c. The broader interdiffusion profiles *P4*, *P6*, *P8*, and *P10* are formed by 4, 6, 8, and 10 interdiffused monolayers around the interfaces with total interdiffusion concentrations of 15%, 20%, 25%, and 30%, respectively; the layerwise interdiffusion concentrations for these profiles can be read off from Fig. 3.

In Fig. 4 we present the resistivities and GMR we find as a function of the interdiffusion amount and profile. It is important to stress that the results quoted in this figure are for $\delta=2$ mRy and should therefore not be considered as actual

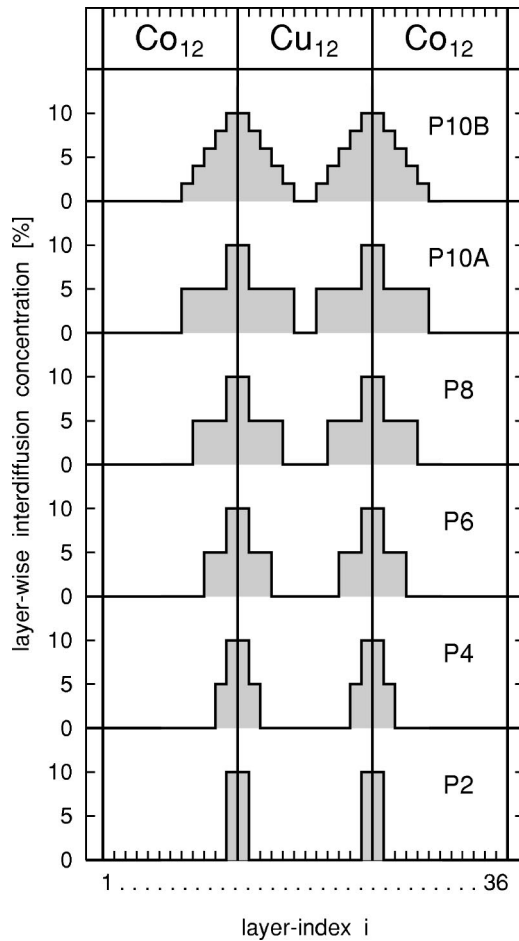


FIG. 3. Various interdiffusion profiles considered in our calculations.

resistivities. However, the general trends are as expected; the resistivities increase with the amount of interdiffusion. They saturate if we confine the interdiffusion to the two layers adjacent to the interface (*P2*, solid lines), whereas they continue to grow for broader interdiffusion profiles (*P4*–*P10*, dotted lines).

To compare our resistivities calculated for this model system to the experimental data we have to correct for both the effects of the finite imaginary part of the energy and for the outgoing boundary conditions. While we can remove the effects of the outgoing boundary by the scheme discussed in the previous section, it is computationally prohibitive to determine the resistivity in the limit $\delta \rightarrow 0$. Therefore, we have had to adopt an *ad hoc* procedure to pinpoint the effects of interdiffusion on the transport properties of these spin-valve structures. We know the resistivity is zero for the perfectly flat free-standing film vacuum/Co₁₂Cu₁₂Co₁₂/vacuum without any defects and with $\delta = 0$; indeed we have also checked this numerically for thinner slabs, e.g., vacuum/Co₂Cu₂Co₂/vacuum. Therefore, it is reasonable to identify the resistivities calculated without any interdiffusion as the spurious contributions coming from the boundary conditions and from the finite δ . For this reason, we have subtracted the resistivities found without interdiffusion from the resistivities with interdiffusion in our calculation so as to

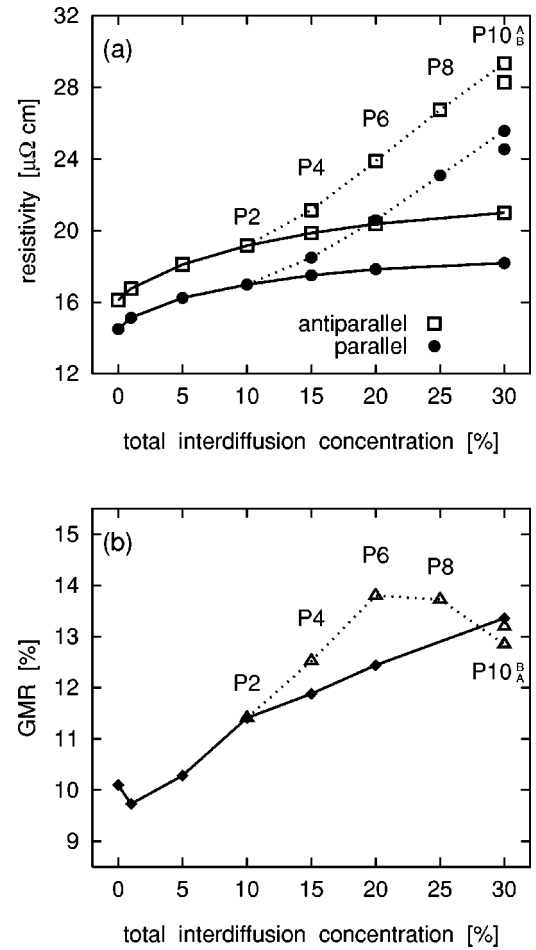


FIG. 4. (a) Raw resistivities, and (b) GMR as a function of interdiffusion amount and profile for the model spin-valve structure Co(100)/Co₁₂Cu₁₂Co₁₂/Co(100) with $\delta = 2$ mRy and with outgoing boundary conditions. Resistivities for the antiparallel configuration are displayed by open squares, resistivities for the parallel configuration by full circles. The solid lines connect the values corresponding to *P2* profiles (interdiffusion confined to the two monolayers adjacent to the interface), the dotted lines connect the various broader profiles *P4*–*P10* as illustrated in Fig. 3. The GMR values (b) correspond to the definition according to Eq. (2); the GMR values with respect to the parallel configuration, i.e., using the other kind of definition, would be higher, e.g., by about 2.2% for *P6*.

isolate the effects of interdiffusion on the transport properties. For the Co₁₂Cu₁₂Co₁₂ spin valve the outgoing boundary condition adds $\sim 4 \mu\Omega \text{ cm}$ (see previous section) whereas the finite imaginary part $\delta = 2$ mRy accounts for the remaining $\sim 10 \mu\Omega \text{ cm}$ in the parallel configuration and $\sim 12 \mu\Omega \text{ cm}$ in the antiparallel configuration.

In Fig. 5 we show the results of Fig. 4 that have been corrected by zeroing out the resistivities for the pure structure as discussed above, i.e., the resistivities for the parallel and antiparallel configurations are displaced by constant amounts; the trends as a function of interdiffusion remain the same. To the extent that the above correction is valid and that interdiffusion is the primary source of resistance the resistivities given in Fig. 5 are meaningful, i.e., we can identify the resistivity of the multilayer with a range of concentrations

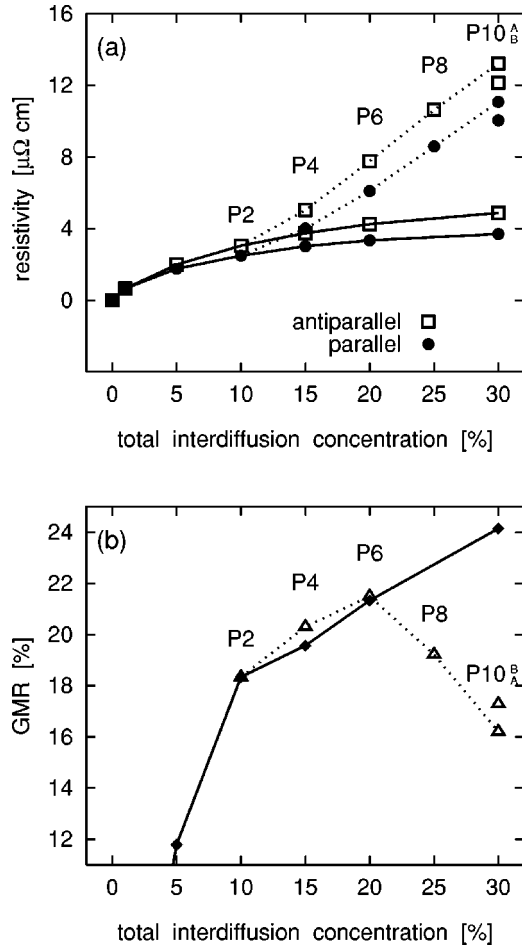


FIG. 5. (a) Corrected resistivities, and (b) GMR as a function of interdiffusion amount and profile for the model spin-valve structure $\text{Co}_{12}\text{Cu}_{12}\text{Co}_{12}$. Resistivities for the antiparallel configuration are displayed by open squares, resistivities for the parallel configuration by full circles. The solid lines connect the values corresponding to $P2$ profiles (interdiffusion confined to the two monolayers adjacent to the interface), the dotted lines connect the various broader profiles $P4$ – $P10$ as illustrated in Fig. 3. The GMR values (b) correspond to the definition according to Eq. (2); since the corrected resistivities are rather small the GMR values with respect to the parallel configuration, i.e., using the other kind of definition, would be higher, e.g., by about 6% for $P6$.

and interdiffusion profiles that produce it.

The GMR we find from the corrected resistivities is well within the experimental range of spin-valve structures. As we have zeroed out the resistivities for the pure samples it is not possible to estimate the GMR for the corrected values at small concentrations of the interdiffusion. From the raw data [see Fig. 4(b)] but also from the corrected data [see Fig. 5(b)] we can see that the GMR increases with the amount of interdiffusion. However, this increase for the $P2$ profile (interdiffusion confined to the two monolayers adjacent to the interface, solid lines) does not continue *ad infinitum*, but rather the GMR reaches a maximum (at about $c = 40\%$) and then it will drop again. In addition, we see that some dispersion in the concentration profile ($P4$, $P6$) promotes GMR (with the highest GMR value obtained for the $P6$ profile formed by six

interdiffused monolayers around the interfaces) but that too broad a distribution ($P8$, $P10$) decreases the GMR; see in particular Fig. 5(b) at $c = 30\%$.

Generally one finds that the effect of the Cu spacer is to dilute the GMR that would come from two Co slabs without any spacer aligned into a parallel and an artificial antiparallel configuration; the GMR for raw data drops from 22.2% without a spacer to the 10.1% quoted previously for the Cu_{12} spacer. By studying our results in more detail, we can state that the effect of interdiffusion onto the magnetotransport properties is a real effect due to introducing impurities around the interface; interdiffusion should not be interpreted as making the spacer effectively thinner. While the corrected resistivity for symmetric interdiffusion about the interface is just the sum of the resistivities of the corresponding asymmetric interdiffusion profiles (with impurities on only one side of the interface), in order to obtain the highest GMR value one needs to have impurities on both sides of the interface (e.g., the corrected GMR for the symmetric $P10^B$ profile is 17.3%, whereas the GMR is only 13.5% or 14.5% for the corresponding asymmetric profiles with impurities only inside the magnetic slabs or with impurities only inside the spacer, respectively).

When we compare the calculated results to the measured data on the spin-valve structure discussed in Sec. III we find that the experimental resistivities are between two and three times larger than the corrected values shown in Fig. 5(a) and that the experimental GMR is about one half of the GMR calculated from these corrected resistivities in Fig. 5(b). From this comparison we infer that there are additional sources of scattering in the actual spin valve and that they are probably nonmagnetic in origin.

VI. ALLOYING IN THE SPACER

A second source of defect scattering in magnetic multilayers comes from impurities in the bulk of the layers. The role of impurities in the magnetic Co layers was studied in a previous paper;³ here we consider the effects of impurities in the Cu spacer layer. Specifically we have considered two types of impurities: one that is isoelectronic with Cu, i.e., Ag, and others which we believe will produce strong spin-orbit and spin-dependent scattering, i.e., Pd, Pt, and Ti. In Fig. 6 we show the resistivities and GMR of the model spin-valve structure as we alloy the spacer with these impurities $\text{Co}(100)/\text{Co}_{12}(\text{Cu}_{100-c}X_c)_{12}\text{Co}_{12}/\text{Co}(100)$. It is important to stress that these are not true resistivities and should not be compared to experimental data as these values were calculated with an imaginary part to the energy $\delta = 2$ mRy. Nonetheless the overall trends are what one normally anticipates from alloying. Notably Ag produces practically no scattering when resolved in Cu, whereas Pd, Pt, and Ti produce a huge effect.

While in the previous section on interdiffusion we were able to remove the effects of the boundary condition (finite size) and δ by positing the *ad hoc* procedure of zeroing out the resistivity of the defect-free multilayer, we cannot follow this procedure for this series because the electronic structure varies too much across the entire range of concentrations we

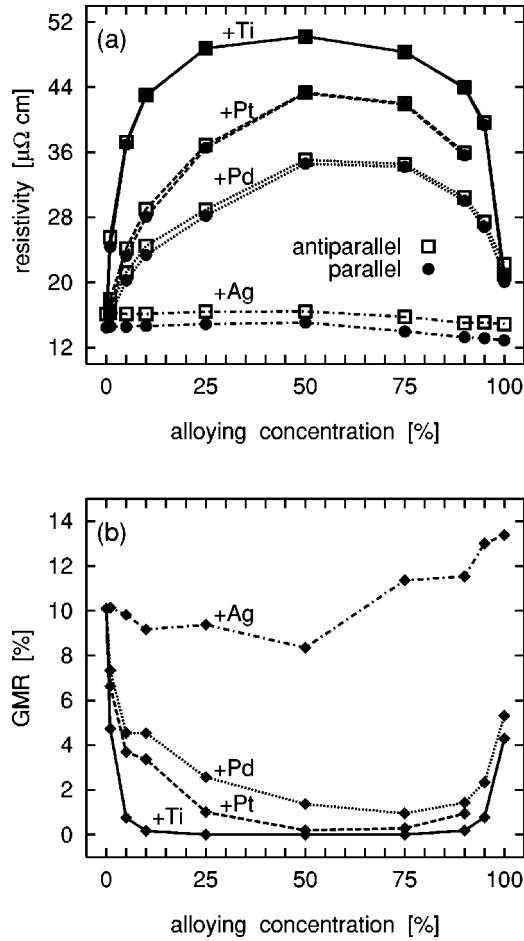


FIG. 6. (a) Raw resistivities, and (b) GMR for the model spin-valve structure with homogeneously alloying the Cu spacer layers $\text{Co}(100)/\text{Co}_{12}(\text{Cu}_{100-c}\text{X}_c)_{12}\text{Co}_{12}/\text{Co}(100)$ with $\delta=2$ mRy and with outgoing boundary conditions. $X = \text{Ag}$ (dash-dotted lines), Pd (dotted lines), Pt (dashed lines), or Ti (solid lines). Resistivities for the antiparallel configuration are displayed by open squares, resistivities for the parallel configuration by full circles. The GMR values (b) correspond to the definition according to Eq. (2); the GMR values with respect to the parallel configuration, i.e., using the other kind of definition, would be higher by about 1%–2% for alloying with Ag, whereas for alloying with Pd, Pt, or Ti they would remain unchanged.

are considering in Fig. 6. With this caveat we have taken the uncorrected raw resistivity values for the parallel and antiparallel configurations of the Co layers to determine the GMR values which are shown in Fig. 6(b). Alloying the Cu spacer with Ag has only minor effects on the GMR. However, we note that the strong spin-orbit disorder scattering of Ti in Cu causes the GMR to precipitately drop, so that by 5% Ti the GMR is close to zero. Pt and Pd have similar traits although they are not as aggressive as Ti. The origin of this decrease can be understood by referring to the “two current model” of conduction in magnetic materials⁷ although we have not in any way used this model in our calculations. In this model the current is carried by two independent spin channels. The Ti, and to a lesser extent Pt and Pd, impurities mix these independent channels and therefore remove the

short circuit effect that was there when the channels were independent, i.e., the role of the impurities is to neutralize the effects of the spin-dependent scattering on the resistivities so that the GMR goes to zero. It is important to stress that the spin-orbit scattering effects of these impurities on the resistivity can only be ascertained in a relativistic calculation such as the one we have carried out.

The above results are in line with the model calculations of Tsymbal and Pettifor¹² for a fcc(100) $\text{Co}_{10}\text{Cu}_{10}\text{Co}_{10}$ trilayer based on the Kubo-Greenwood formula within a nonrelativistic, *spd* tight-binding approximation. In their calculations a parameter γ was introduced to describe the degree of disorder; this reflects the spin-independent scattering by defects, which can thus be considered to be a monotonously increasing function of the concentration of impurities. It was found that the conductivity for the majority channel in the parallel configuration decreases much faster with increasing γ in the spacer region than that of the minority channel or for the conductivity of either channel in the antiparallel configuration; this in turn gives rise to a rapid, almost exponential decrease of the GMR.

VII. CONCLUSIONS

Our transport calculations allow us to take account of the roles of the electronic structure and of the defect scattering on the electrical resistivity and GMR. However, there are two impediments to our obtaining unambiguous values of the resistivity in all cases. They are the effects coming from the finite size of the structures we consider, i.e., we have resistivities that depend on the boundary conditions that we set on the problem, and for computational reasons we must include an imaginary part to the energy in our conductivity calculations so that it is not always clear how to extrapolate the result to $\delta \rightarrow 0$.

For these reasons the GMR coming solely from the electronic structure is difficult to estimate from our calculations. If we adopt the hypothesis that the resistivities scale uniformly with the imaginary part and therefore the δ cancels out in the GMR we obtain some idea from Fig. 4 that for the $\text{Co}_{12}\text{Cu}_{12}\text{Co}_{12}$ spin valve the GMR coming from the electronic structure is on the order of 10%. This number still includes the role of the finite size, i.e., it is for outgoing boundary conditions; when we use the calculation we described in Sec. IV on the role of outgoing versus reflecting boundary conditions we are led to a GMR on the order of about 14.5% for the reflecting boundary conditions.

To estimate the role of interdiffusion on the GMR we refer to Fig. 5. While the values for low concentrations should not be fully trusted because of our *ad hoc* zeroing out of the resistivities of the pure structure, by the time $c = 10\%$ the GMR values we find reflect the roles of interdiffusion and electronic structure on the GMR, i.e., with about $c = 15\%$ interdiffusion we can get a 20% GMR effect. The GMR is very sensitive to the distribution of impurities; it increases with the amount of interdiffusion and while some dispersion in the interdiffusion profile will promote GMR,

too broad a distribution will decrease the GMR.

From our previous work on the role of alloying the bulk of the Co slabs³ and from our present work of alloying the Cu spacer layer we see that the GMR can either be increased or decreased depending on the type of impurity. For Fe, Ni, and Cu impurities in Co as well as for Ag in Cu the GMR increases moderately with alloying; however, by introducing impurities which produce strong spin-orbit scattering of the conduction electrons, e.g., Ti, Pt, or Pd in Cu, we rapidly suppress the GMR due to the mixing of spin currents in the multilayer.

In summary, we find that the CIP conductivity of a spin-valve structure is sensitive to the boundary conditions on the active region of the spin valve, i.e., the substrate, capping layer, and their interfaces with the magnetically active region. While in general spin-dependent interface scattering, e.g., interdiffusion at interfaces, promotes GMR, the profile

of the interdiffusion is important. Finally as we made a fully relativistic calculation we were able to demonstrate that the spin-flip scattering due to impurities with sizeable spin-orbit coupling destroys GMR.

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