Effects of interface disorder on transmission probability in magnetic multilayer

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We present a study of conductance through disordered Fe-Cr[100] and Co-Cu[100] interfaces within a realistic tight-binding model. In our model, the specular and diffuse parts of the conductance are treated on an equal footing. We observe a substantial *increase* in conductance due to disorder in the channels that are strongly reflected by pure interfaces. We also show how this phenomenon affects the giant magnetoresistance. In addition, we find that the series resistor model may significantly overestimate the resistance if the thickness of the disordered layer is less than several times the electron mean free path.

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I. INTRODUCTION

The decade and a half following the discovery of the giant magnetoresistance (GMR) in Fe-Cr multilayers,[1,2] has witnessed a continuing growth of interest in spin-dependent electron transport.[3–7] There have been numerous calculations of GMR. Some of these have been based on a rigorous quantum treatment of transport. Some have also taken into account the band structure of the materials comprising the multilayer.[8] Direct comparison between calculations and experiment, however, has been difficult because a number of factors that are important in determining the experimental resistance and magnetoresistance are difficult to take into account in model calculations. These factors may roughly be split in two groups: (a) finite temperature effects that lead to inelastic scattering, most importantly phonon and magnon scattering, and (b) effects of static disorder that lead to elastic scattering.

In this paper, we are concerned with what we believe to be an important subset of these factors, those involved with substitutional disorder at the interfaces between different materials in magnetic multilayers. The study of the interfaces is motivated by the fact that the effects of interfacial disorder have been particularly difficult to understand and the fact that interfaces can dramatically influence GMR.[9] In some cases, interfacial disorder is the primary source of electron scattering. The limitation to substitutional disorder is justified as a first step by the fact that atomic scale studies[10] of interfaces of typical sputtered films produced for GMR devices often show sufficiently strong texture that over an electron mean free path the films are well ordered crystals, the crystal structure being maintained across the interfaces between the layers.

We study the effect of interfacial disorder by calculating the effect of a random substitutional distribution of the atomic species on one or more atomic layers at the interface on transmission and reflection. We demonstrate that the supercell can be made large enough to suppress artifacts associated with the artificial periodicity imposed by the supercell. We also demonstrate that one or only a few configurations are needed in order to represent the disorder.

We report both the specular ($\mathbf{k}_\parallel$ conserving) and diffuse ($\mathbf{k}_\parallel$ nonconserving) parts of the transmission and reflectance because these help us to understand some novel effects caused by interfacial disorder. A similar approach, based on an *ab initio* LMTO code[11] was used in two recent papers.[12] In the first, the conductance of a Co-Cu-Co trilayer was studied in the presence of disorder in the bulk and close to the interfaces. The second study attempted to recover the simple resistor model in order to compare with experiment. The authors postulated that the scattering from bulk is completely diffuse, and with this condition they were able to recover a series resistor model and an explicit expression for the interface resistance. In a very recent paper,[13] the same group calculated the specular and diffuse part of the conductance separately and managed to study the validity of the resistor model used earlier. The LMTO code however, scales poorly with the system size which limits their study to a few systems in just one disorder configuration.

Our code is based on a realistic tight-binding model fitted to *ab initio* band structures which gives us more flexibility with comparable precision. The fitting parameters consist of on-site energies and interatomic matrix elements. These are transferred to the alloy by assuming that the onsite energies are not changed by the local environment and that the interatomic matrix elements between species *A* and *B* is the average of that between *A* and *A* and between *B* and *B*. Clearly this approach is limited to pairs of atoms of similar size and electronegativity such as Fe-Cr and Co-Cu. We believe, however, that our approach is particularly well suited for exploring certain questions of principle that are more difficult to explore with fully *ab initio* techniques. We study the transmission through Fe-Cr[100] and Co-Cu[100] interfaces and GMR of Fe-Cr multilayers over the full range of substitutional disorder.

II. MODEL

In this paper we employ the two current model which neglects effects such as spin-orbit coupling or noncollinear moments that might mix the spin channels and electron-magnon scattering which may lead to spin-flip scattering. The method we use to calculate the conductance was originally developed to study the conductance of nanowires.[14] For

a sample sandwiched between two leads at zero temperature, the conductance for a given spin channel is proportional to the total transmission probability through the sample

$$\Gamma = \frac{e^2}{h} \sum_{\mathbf{k}_\parallel, i, \mathbf{k}'_\parallel, j} T_{\mathbf{k}_\parallel, i; \mathbf{k}'_\parallel, j}(E_F), \tag{1}$$

where $(\mathbf{k}_\parallel, i)$ labels an incident Bloch state with transverse wave vector $\mathbf{k}_\parallel$ in one lead and $(\mathbf{k}'_\parallel, j)$ labels a transmitted Bloch state in the other. The additional integer quantum numbers i and j are needed because each of the leads may have several Bloch states for a given value of transverse momentum. The transmission probability can be written in a basis of planar orbitals using the Caroli formula[15] as

$$\Gamma = \frac{e^2}{h} \mathrm{Tr}[\tilde{\Sigma}_L G^R_{LR} \tilde{\Sigma}_R G^A_{RL}], \tag{2}$$

where $G^{R/A}_{LR}$ is the retarded/advanced Green's function (GF) matrix element between the first principal layer of the left and right lead and $\tilde{\Sigma} = i(\Sigma^R - \Sigma^A)$ is the imaginary part of the self-energy associated with the ends of the semi-infinite leads. In the calculation of the conductance, all GF and self-energies are evaluated at the Fermi energy.

We model the interface disorder by considering large supercells in the interfacial layers. In every supercell, we choose a random distribution of the species. The supercell is repeated periodically in the plane. The superlattice obtained in this way has a square lattice with lattice constant $L = Na$, where a is the bulk lattice constant and N is an integer, which indicates the size of the supercell. We use a semi-empirical tight-binding Hamiltonian constructed by fitting to *ab initio* band structures.[16] The matrix elements between different species are obtained by averaging the corresponding matrix elements of the compound species.

The transmission probability is first obtained in the supercell basis $|\mathbf{q}_{||}, i, \alpha, R_z\rangle$ where $\mathbf{q}_{||} = (q_x, q_y)$ $[|q_x|, |q_y| < (\pi/L)]$ denotes a two-dimensional (2D) wave vector within the superlattice surface Brillouin zone (BZ), α labels the symmetry type for the sp^3d^5 orbitals, R_z labels the layer, and i labels the atom coordinates in the supercell. The conductance is then transformed to the basis of the reciprocal lattice vectors of the superlattice $|\mathbf{q}_{||} + \mathbf{g}_n, \alpha, R_z\rangle$ where $\mathbf{g}_n = (2\pi/L)(n_1, n_2)$ denotes the reciprocal lattice vectors of the superlattice that fall in the first bulk Brillouin zone $(0 \leq n_1, n_2 \leq N)$. Finally, after integration over the supercell BZ we obtain the conductance in the form

$$\Gamma = \sum_n \Gamma_{spec}(\mathbf{g}_n, \mathbf{g}_n) + \sum_{n \neq m} \Gamma_{diff}(\mathbf{g}_n, \mathbf{g}_m), \tag{3}$$

where Γ_{spec} labels the specular ($\mathbf{k}_\parallel$ conserving) part of the conductance and Γ_{diff} labels the diffuse part. Here the labels α have been summed over. In the case of perfectly ordered interfaces, the layer orbitals associated with different wave vectors $\mathbf{g}_n$ are decoupled and the conductance becomes purely specular.

It is important to be aware of effects that are not included within our model. As mentioned previously, we use the two current model and neglect effects that mix the spin channels. Spin-flip scattering may be a significant effect at disordered interfaces especially if atoms near the interfaces retain their local moment but are not strongly exchange coupled to the other local moments in the magnetic layer.[17] In addition, the Cr and Cu atoms are treated as nonmagnetic, thus the small local moments that may form on these atoms in specific environments are neglected.

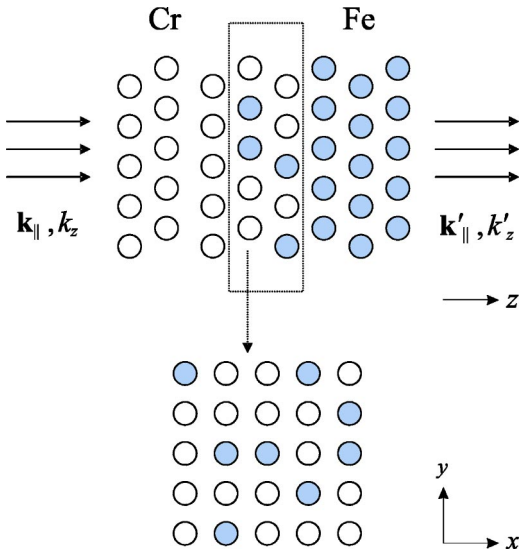

FIG. 1. Cr-Fe disordered interface. The lower part of the figure shows a plane view of the supercell. 10×10 random supercells were used in the actual calculations.

III. RESULTS AND DISCUSSIONS

We have studied two important but qualitatively different GMR systems, Fe-Cr[100] and Co-Cu[100]. The first system, bcc Fe-Cr, was the first to show GMR.[1] In this system, GMR arises from the matching of the Fe minority electronic structure with that of Cr. In our calculation, we treat Cr as nonmagnetic. In the second system, fcc Co-Cu, the electronic structure matching occurs in the majority channel. The Co-Cu system has great technological importance largely because the majority electronic structure of Co matches to the majority electronic structure of magnetically soft alloys such as permalloy ($Ni_{0.8}Fe_{0.2}$ which allows the fabrication of extremely small and sensitive magnetic-field sensors.

In order to study the specular and diffuse conductance through disordered interfaces we have calculated the conductance through a disordered region sandwiched between semi-infinite Cr on one side and semi-infinite Fe on the other or between semi-infinite Co on one side and semi-infinite Cu on the other. In one or more atomic layers at the interface between the layers we put Cr and Fe (or Cu and Co) atoms randomly. We typically use a 10×10 supercell in the plane of the layers. This is repeated periodically, as illustrated in Fig. 1.

The probabilities for majority and minority electrons to be transmitted through a disordered Cr-Fe (Cu-Co) interface with a single intermixed atomic layer are shown in Fig. 2(a) [Fig. 2(b)] for the entire range of Cr (Cu) concentrations at

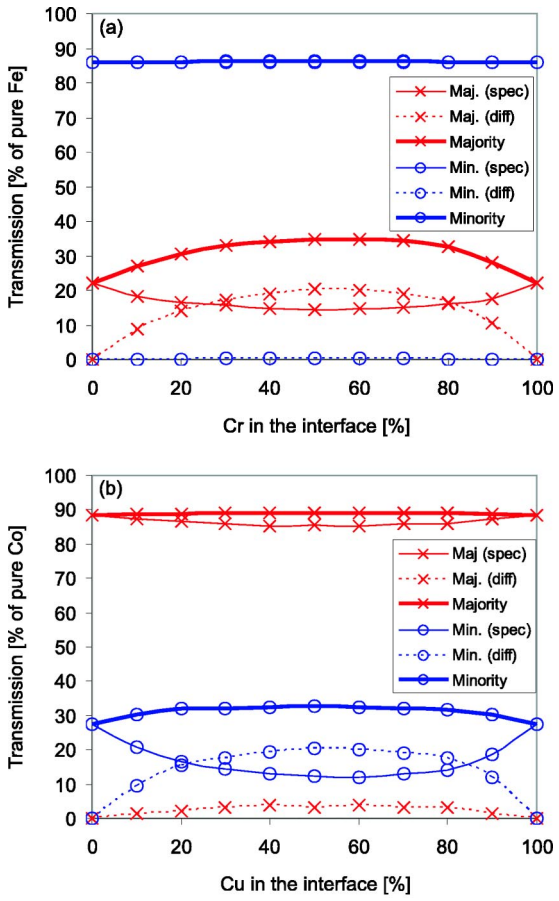

FIG. 2. Majority and minority channel transmission probability for (a) disordered Cr-Fe interface and (b) disordered Cu-Co interface. The conductance in each channel is normalized to the conductance of pure Fe (Co). Disorder is limited to one layer at the interface.

the interface. The graphs are normalized to the conductance per unit area of pure Fe or pure Co. The ballistic conductance per 2D unit cell (in units of e^2/h) of pure Cr is 1.31 for each spin and of pure Fe is 2.08 and 0.83 for the majority and minority channels respectively. The corresponding ballistic conductance of pure Cu is 0.89 per spin and of pure Co is 0.68 and 1.85. These numbers represent the average number of propagating states in the (100) direction per $\mathbf{k}_{||}$. The ballistic transmission can be readily obtained from the data for the propagating states given in Fig. 3.

In the case of Fe-Cr, the transmission of the minority channel remains specular and almost constant throughout the concentration range because there is a very good match between the bands of minority Fe and Cr. As the graph shows, the conductance per unit area in the minority channel is approximately 86% of the conductance per unit area of Fe in the minority channel. The conductance per unit area of the majority channel, on the other hand, is relatively low, about 22% of the conductance per unit area of majority Fe, and strongly dependent on the disorder. As expected, the specular part of the conductance decreases with disorder. Some of the incident states are reflected or are transmitted diffusely.

Surprisingly, however, the total transmission in the majority channel for Fe-Cr and the total transmission in the minority channel for Co-Cu both increase with disorder. This happens because the diffuse transmission increases with disorder in both cases fast enough to more than compensate for the decrease in specular transmission. For the majority channel in Fe-Cr the conductance of the interface in the absence of disorder is 22% of the conductance of majority Fe. When the interface is disordered the specular conductance drops by as much as 8% while the diffuse increases by about 20% giving

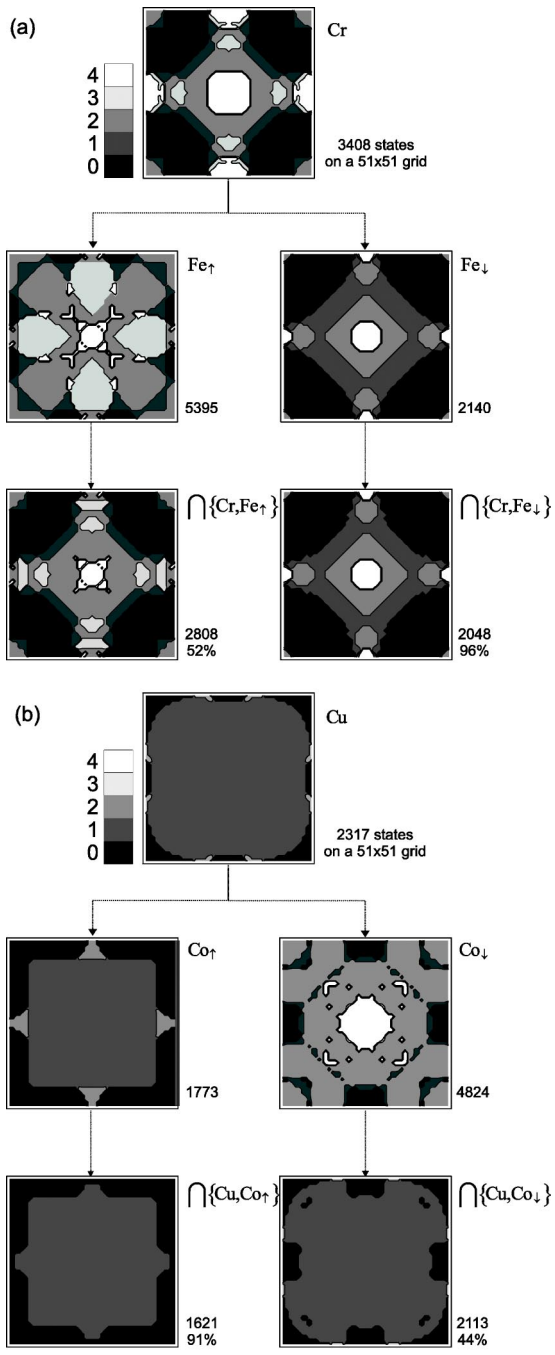

FIG. 3. Matching of the ballistic states in (a) Cr and Fe (b) Cu and Co. The intersection of the Fe majority Fermi surface and the Cr Fermi surface has only 52% of the states of Fe majority whereas the intersection of the Fe minority Fermi surface and the Cr Fermi surface includes 96% of the states of Fe minority.

an overall rise of about 12%. These percentages are given in terms of the conductance of pure Fe. In terms of the conductance of a perfect Fe-Cr interface the conductance of the disordered interface increases by 55%, which is a significant effect.

In the case of Co-Cu, the roles of minority and majority are reversed, but otherwise the picture is very similar: the majority channel conductance per unit area is about 89% of the conductance per unit area of the majority channel in pure Co and there is very little diffuse conductance. In the minority channel, on the other hand, the conductance in the presence of the interface is only about 27% of the conductance of the pure Co. Again, however, disorder *increases* the conductance. For the minority channel in Co-Cu, the specular conductance drops by 15% while the diffuse increases by about 20% giving an overall rise of about 5% measured in terms of the conductance of pure Co. Again, with respect to the conductance of pure Co-Cu interface the conductance of the disordered interface increases by 19%.

Strictly speaking, one needs to perform an average over all possible configurations of the atoms at the interface. This is impractical because of the very large number of configurations. However, the smoothness of the graph indicates that the dependence of the transmission on the actual random configuration is small. We performed an average over several random configurations at the same concentration of the materials. In the case of the minority channel of Fe-Cr, the standard deviation was essentially zero. In the case of the majority channel of Fe-Cr, the standard deviation is of order of one percent. We conclude that in the case for which the intermixing occurs between chemically similar materials and the supercell is large enough, the results for one random configuration are representative of the configuration average.

One (initially) counterintuitive aspect of our results is the prediction that disorder increases the transmission of majority electrons for the Fe-Cr interface and of minority electrons for the Co-Cu interface. This effect is the result of disorder allowing transmission of channels that are blocked for an ordered interface. In order to better understand how this mechanism works, we plotted on a grid in the surface Brillouin zone the number of propagating (Bloch) states on both sides of the interface and their overlap, see Fig. 3(a). It is important to remember that in the absence of disorder, $\mathbf{k}_\parallel$ is conserved. We shall describe $\mathbf{k}_\parallel$-conserving transmission as ''specular'' and transmission which does not conserve $\mathbf{k}_\parallel$ as ''diffuse.'' Only specular transmission can occur at an ordered interface. Thus one could imagine two semi-infinite leads made of perfect metals but with different band structures such that the projections of their Fermi surfaces in the plane of the interface had no points in common. In this hypothetical, but in principle, possible, case one would have the strange result of two perfectly conducting leads joined at a perfect interface that yields zero transmission, i.e., infinite resistance because all of the conduction channels are ''blocked'' by the requirement of $\mathbf{k}_\parallel$ conservation. Introduction of interfacial disorder relaxes this requirement and allows conduction.

For the Fe-Cr minority case, the conductance is limited by the number of states in Fe. The Fermi surface of minority Fe is almost a subset of the Fermi surface of Cr. Thus there are very few blocked channels. In the majority case, there is large band mismatch producing many states for which specular transmission is blocked. In the presence of disorder, however, these electrons can be scattered diffusely. If all of the available channels in the Cr were transmitted this could produce a maximum increase of up to 11% in the conductance of the majority channel (relative to the majority conductance of pure Fe). In fact, if we look at the total majority conductance plot in Fig. 2(a) we see that the maximum contribution is very close to this number which means that virtually all blocked states are now transmitted. The large diffuse transmission is composed partly of blocked states that are transmitted thanks to the disorder and partly of well-matched states transmitted diffusely.

In the case of Co-Cu, the majority channel, shown in Fig. 3(b), has a relatively small number of blocked states. Conversely, the minority channel has many blocked states. If all blocked states in Cu were to be allowed through, this would give a maximum increase of 4% in the conductance of the minority channel. The maximum minority conductance increase seen in Fig. 2(b) is of that magnitude implying that in Co-Cu as well as Fe-Cr the disorder is capable of transmitting nearly all blocked states. In fact, for both sets of materials, the maximum increase of the conductance is nearly equal to the lesser of the number of blocked states in material *A* and the number of blocked states in *B*. The diffuse conductance of the minority channel [Fig. 2(b)] increases with disorder to more than 20% of the conductance per unit area of the minority channel of pure Co.

What happens if there are more disordered layers at the interface? In Fig. 4(a), the conductance and the diffuse part of the majority conductance through an Fe-Cr interface are shown as a function of the interface thickness for four different concentrations of Cr. There is a clear maximum in the conductance as a function of thickness which decreases in value and shifts to higher thickness as the concentration of Cr decreases. The maximum increase in conductance for 50-50 Fe-Cr is 12% of the conductance of pure Fe at 1 monolayer (ML) thickness, while it is less than 2% at 3 ML thickness for 99-1 Fe-Cr.

The diffuse conductance for majority Fe-Cr peaks at about 4 ML for 50-50 and above 20 ML for 99-1 Fe-Cr. This can be said to be the critical thickness D_c up to which specular transmission is dominant. Above D_c, the conductance is predominantly diffuse and we observe Ohmic behavior, i.e., the conductance is inversely proportional to the thickness. A linear dependence is clearly seen if the inverse of the conductance is plotted as a function of thickness. This implies that the resistor in series model[12] can be a very good approximation for the strongly scattered channels if the thicknesses of the individual slabs exceeds 2–3 nm at 50-50 disorder. The conductance, for example, is 99% diffuse at 20 ML for majority Fe-Cr.

However, if the impurity concentration is low, one may argue that specular conductance would be present even at much larger thicknesses at low temperature implying that the series resistor model would not apply. Moreover, applicability of the resistor model would appear to require very large

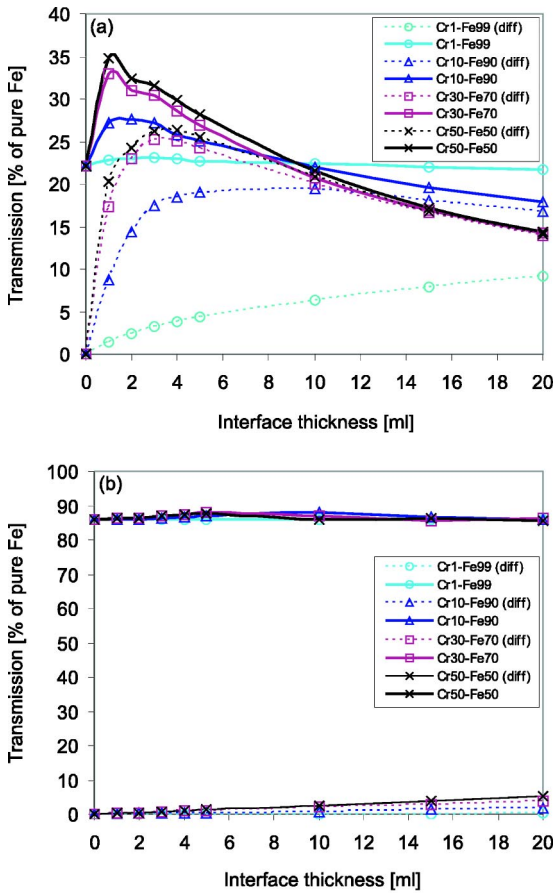

FIG. 4. Conductance and the diffuse part of the conductance as functions of the size of the disordered region at the Cr-Fe interface for (a) majority and (b) minority channel.

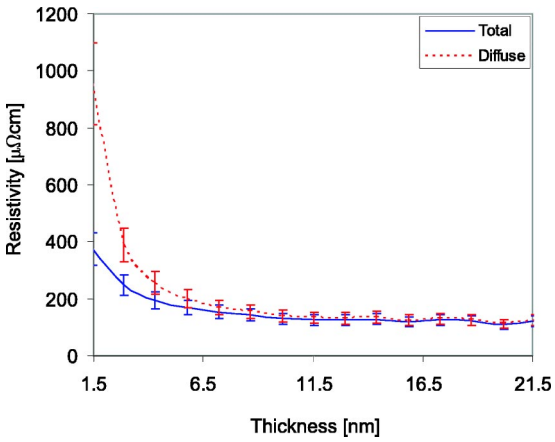

FIG. 5. Resistivity of a slab of a hypothetical single band metallic system as a function of thickness. The material was generated as described in the text. Electrons are scattered by a random Gaussian distribution of 0.5 Ry half-width on-site disorder.

thickness in the case of the well-matched channels at low temperature, as seen in Fig. 4(b) for the case of Fe-Cr minority. For all concentrations and all thicknesses for which we calculated the conductance, it remained largely specular.

As an illustration, we set up a trilayer consisting of: a semi-infinite Cr lead, a disordered "bulk" slab of 10 ML $Cr_{90}Fe_{10}$, a disordered interface 2 ML thick of $Fe_{50}Cr_{50}$, another disordered bulk slab of 10 ML $Fe_{90}Cr_{10}$, and finally a semi-infinite Fe lead. The size of 10 ML of the bulk layers is the typical size used in Ref. 12. Then we calculated the resistance of each of the three layers separately (between the Cr and Fe leads) and as a unit. The resistance of the trilayer predicted from the resistor model for the majority channel was 1.44 kΩ and the actual resistance was 0.59 kΩ, a difference of 144%. The overestimation of the resistance was naturally worse for the minority channel with the resistor model giving a resistance of 1.07 kΩ while the calculated resistance was 0.35 kΩ, a difference of 205%. In the light of the results shown in Fig. 4 and the example given above, we argue that the resistor in series model is not valid for substitutional disorder at low temperatures except for relatively large thickness. In order to demonstrate how difficult it is to get into a completely diffuse regime, we calculated the resistivity of a simple one-band material generated by removing the *p* and *d* states of the model for Cr between leads made of the same material. We added random on-site energies to simulate disorder and increased the thickness of the slab between 10 and 150 ML. The random on-site energies were obtained using a uniform distribution of width 0.05 Ry. The resistivity is shown in Fig. 5. The error bars show our estimate of the statistical error in our calculation due to limited sampling of the configuration. Even with the unphysically large disorder of this example the calculated resistance is not Ohmic below 60–70 ML thickness.

We attempted to estimate the mean free path for the systems that we calculated in order to relate the regime of validity of the resistor in series model to a well-defined physical parameter. Our estimate was based on the expectation that the specular current should decay exponentially as $\exp(-z/\lambda)$, where λ is the mean free path. For the majority channel in Fe-Cr, the mean free path estimated in this way decreases from approximately 33 ML to approximately 4 ML as the concentration increases from 1% Fe to 50% Fe in Cr. For the minority channel, the estimate is much less precise, but qualitatively the mean free path is larger than 400 ML for all concentrations. Based on these results, we estimate that the series resistor model is valid if the thickness of the disordered layer exceeds several times the mean free path.

If disorder produces increased transmission for the case in which there is strong band mismatch at the interfaces it should be detrimental to the GMR, because one major contribution to GMR is the suppression of the conductance of one of the spin channels by reflection at the interface with the spacer layer. To study the effect of interface disorder on GMR we considered a Fe(4 ML)/int(x)/Cr(3 ML)/int(x)/Fe(4 ML) trilayer between Cr leads with x intermixed layers at both interfaces where x is either 1 ML or 15 ML. In Fig. 6(a), GMR is shown as a function of the interface disorder normalized to the GMR of a multilayer with pure interfaces. Figure 6(b) shows the contributions to the conductance in parallel and antiparallel orientation of the magnetization of the Fe layers.

We considered two very different interface sizes: for 1 ML interface thickness the majority transmission is maxi-

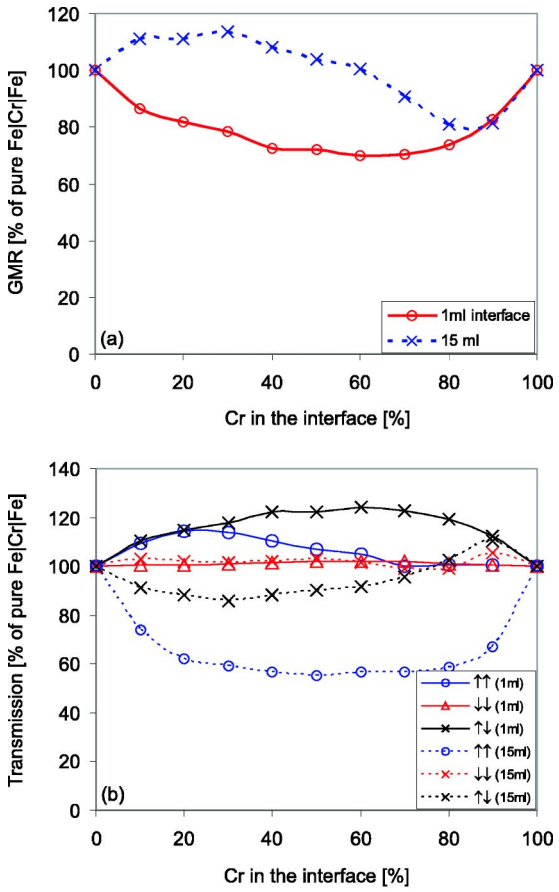

FIG. 6. GMR in an Fe(4 ML)/int$_x$/Cr(3 ML)/int$_x$/Fe(4 ML) trilayer: (a) GMR and (b) transmission in parallel and antiparallel configuration for $x=1$ ML and $x=15$ ML. All values are normalized to the corresponding values of the same multilayer with pure interfaces.

mized, while for 15 ML the majority transmission falls below the value obtained for pure interfaces. In the first case, the conductance of the strongly scattered channels increases up to 20% while GMR decreases proportionally because the conductance in parallel is dominated by the minority channel which stays the same. In the second case, when the interfaces are diffused over 15 ML, we obtain larger GMR than the GMR of a multilayer with perfect interfaces because the conductance of the mismatched channels decreases while the conductance of the well-matched channel remains the same. This may be the explanation of some experimental reports that disorder helps GMR. Interface intermixing in the 1-2 ML at the interface is what is most probable to happen in real samples and at the same time is the worst range for GMR. Pure interfaces and highly interdiffused interfaces should both give larger GMR ratios. It is clear from the study of thin interfaces that the Fe-Cr system is more sensitive to the disorder due to the larger number of blocked states. Therefore, the GMR decrease for 1–2 ML interfaces should be more pronounced for Fe-Cr and less noticeable for Co-Cu. Overall, the predicted change in GMR is not dramatic at least for the practically important cases of Fe-Cr and Co-Cu and reasonable interface roughness.

IV. CONCLUSION

We have developed a method to study the specular and diffuse conductance through disordered interfaces and applied it to interfaces between Fe[100] and Cr[100] and interfaces between Co[100] and Cu[100]. We found that up to a certain thickness of the disordered region the conductance of the strongly scattered channels increases with disorder due to diffuse transmission of states normally blocked. Above that thickness the conduction becomes Ohmic. On the other hand, the conductance of the weakly scattered channels is insensitive to disorder and the conductance is largely specular due to almost identical Fermi surfaces. GMR can be diminished or enhanced depending on the amount of disorder.

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