Calculation of spin-dependent interface resistance

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A simple expression for the interface resistance between two materials has been derived by Schep *et al.* [J. Magn. Magn. Mater. **177**, 1166 (1998)] in terms of the transmission probability for electrons at the interface. This approximation is tested for a simple model interface and good agreement is found with solutions of the Boltzmann equation. Previously calculated values of the transmission probability are used with this simple expression to evaluate the spin-dependent interface resistances of a number of ferromagnetic-normal metal interfaces. The agreement between the calculated results and the results extracted from experiments on Cu/Co argue that the interface resistance may not be dominated by defect scattering as is often assumed.

Giant magnetoresistance¹ is the change of resistance when the magnetic alignment of adjacent ferromagnetic layers separated by nonmagnetic material is changed. The case in which the current is perpendicular to the planes is referred to as current-perpendicular-to-plane giant magnetoresistance and has been reviewed by Bass and Pratt.² The semiclassical theory for this case has been developed by Valet and Fert.³ In this limit, the interfaces are sufficiently separated that quantum interference effects due to reflection from the interfaces can be neglected. If the interfaces are separated by more than a bulk mean free path, the theory shows that the total resistance can be broken into contributions from the bulk regions and to resistances associated with each interface. The theory also shows how these interface resistances can be extracted from experiment. Generally, it is assumed that the interface resistance results from defects at the interface (interfacial roughness) or interdiffused atoms. However, there is also an interface resistance for defect-free interfaces due to the nonzero reflection coefficients at the interface.⁴

Schep *et al.*⁵ derived a simple form for the resistance of a single, defect-free interface between materials A and B. To derive this form from the linearized Boltzmann equation in the relaxation time approximation, they treat the bulk transport with an approximation based on random matrix theory. The form they derive is

$$AR = \frac{h}{e^2} \left[\frac{1}{T_{\text{tot}}} - \frac{1}{2} \left(\frac{1}{S_A} + \frac{1}{S_B} \right) \right], \tag{1}$$

in terms of the areas of the Fermi surfaces (FS) projected in the direction of the interface

$$S_i = \frac{1}{(2\pi)^2} \int_{FS_i} d^2 K,$$
 (2)

for i = A,B and the transmission probability integrated over the Fermi surface

$$T_{\text{tot}} = \frac{1}{(2\pi)^2} \int_{\text{FS}_A} d^2 K T_{A \leftarrow B}(\mathbf{k}). \tag{3}$$

The wave vector \mathbf{k} is on the Fermi surface of material B and has a components perpendicular to the interface \mathbf{K} , which is the integration variable for the projection in the direction of

the interface. The resistance of an interface R is inversely proportional to the area of the interface A, so the product AR is independent of the detailed geometry of the interface. The definition of $T_{\rm tot}$ appears asymmetric because it only involves the transmission in one direction, but because of microscopic reversibility, $T_{\rm tot}$ is the same for transmission in either direction. Even though the existence of a meaningful interface resistance depends on there being enough bulk scattering to eliminate quantum interference effects, the interface resistance in this approximation, Eq. (1), is independent of the details of the bulk scattering.

Schep *et al.* applied Eq. (1) to interfaces between Co and Cu in the (111) and (110) directions. However, they were not able to test its validity. In this paper, we test Eq. (1) in a model system for which exact results are known, and then apply it to a series of interfaces.

We test Eq. (1) by considering a model interface inserted in an infinite free-electron material. A stacking fault would be an example of this type of interface. The transmission probability across this interface is modeled by a simple expression in terms of two parameters. In a previous paper, 6 we described a method to numerically solve the linearized Boltzmann equation, and used that method to compute the interface resistance for this model interface as a function of the parameters that describe the transmission probability. Here we compare those "exact" solutions with approximate solutions of the same model using Eq. (1).

For a sheetlike δ -function potential inserted in a free-electron material, the transmission probability depends on the perpendicular component of the electron wave vector, k_z as

$$T_{A \leftarrow B}(\mathbf{k}) = \frac{k_z^n}{\alpha k_F^n + k_z^n},\tag{4}$$

with exponent n=2. The dimensionless parameter α is proportional to the square root of the strength of the δ -function potential. It determines the strength of the reflection. In Ref. 6, we considered a generalized model for the transmission probability with n allowed to take on other values and α parametrizing the strength of the reflection. These generalizations are useful for testing the validity of various approximations, such as the approximation discussed in this paper.

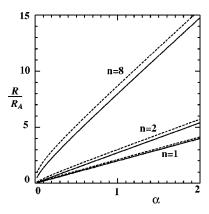


FIG. 1. Interface resistances. For the model interface described around Eq. (4), parametrized by the variables n and α the solid lines give the interface resistance from a numerical solution of the Boltzmann equation and the dashed lines give the approximate results based on Eq. (1).

The choice n=1 is analytically soluble. For this choice, the approximation of Schep *et al.*, Eq. (1), gives

$$AR = \left[2\alpha \frac{3\pi h}{k_{\rm F}^2 e^2}\right] \left[\frac{1}{3\alpha} \left(\frac{1}{2} - \alpha + \alpha^2 \log \frac{1+\alpha}{\alpha}\right)^{-1} - \frac{2}{3\alpha}\right]. \tag{5}$$

The first factor in square brackets is the result obtained by solving the linearized Boltzmann equation in the relaxation time approximation (analytically for this case). The second factor can be expanded in a Taylor series for small $1/\alpha$ as

$$1 + \frac{1}{12\alpha} - \frac{3}{80\alpha^2} + \dots$$
 (6)

In the limit of large interface resistance, small $1/\alpha$, the result becomes quite good. The exact result and the approximate result are compared in Fig. 1. Also shown in that figure are a comparison for n=2 and n=8 between numerical solutions

of the Boltzmann equation⁶ and analytic solutions of Eq. (1). This figure shows that for high-resistance interfaces, the approximation gives reasonable results. For low-resistance interfaces, the absolute error decreases, but the relative error increases.

The approximation Eq. (1) is related to the relaxation time approximation because the details of the bulk scattering do not enter into the interface resistance. As we showed in Ref. 6, when the bulk scattering is treated without invoking the relaxation time approximation, there are deviations of up about 10% in the interface resistance. We expect there to be similar deviations from Eq. (1) whenever the relaxation time approximation breaks down.

In Table I, we use Eq. (1) and previously published results for the transmission probability, 12,13 to compute values of the spin-dependent interface resistance for a series of interfaces. We report the resistivities for the minority and majority electrons, AR^{\downarrow} and AR^{\uparrow} , respectively, and the combinations

$$\gamma = \frac{AR^{\downarrow} - AR^{\uparrow}}{AR^{\downarrow} + AR^{\uparrow}},\tag{7}$$

and

$$AR^* = \frac{AR^{\downarrow} + AR^{\uparrow}}{4},\tag{8}$$

which are typically extracted from experiment. The results for Co/Cu(111) and Co/Cu(110) are in good agreement with the results of Schep *et al.*, which are based on the same model, but make use of independent calculations of the transmission probabilities. The transmission probabilities were calculated on uniform grids in the interface Brillouin zone using from 61 to 157 points in the irreducible wedges. These correspond to on the order of 500 points in the full interface Brillouin zone. The uncertainty due to the *k*-space integrations are smaller than the uncertainties due to the use of the approximation Eq. (1) and the local-density approxi-

TABLE I. Spin-dependent interface resistances. The relationships between R^{\downarrow} , R^{\uparrow} , γ , and R^* are given in Eqs. (7)–(8). The upper portion of the table is our theoretical results and the lower portion gives experimental results. The interface orientations are not known in the experimental systems.

	$AR^{\downarrow} (f\Omega \text{ m}^2)$	$AR^{\uparrow} (f\Omega \text{ m}^2)$	γ	$AR* (f\Omega \text{ m}^2)$
Au/Fe(100)	11.39	1.06	0.83	3.11
Ag/Fe(100)	12.86	1.07	0.85	3.48
Cr/Fe(100)	0.77	2.87	-0.58	0.91
Cr/Fe(112)	0.42	0.76	-0.28	0.30
Cr/Fe(110)	0.81	2.11	-0.44	0.73
Cu/Co(100)	2.31	0.31	0.76	0.65
Cu/Co(110)	2.54	0.55	0.64	0.77
Cu/Co(111)	1.95	0.43	0.64	0.60
Cu/Ni(100)	1.20	0.43	0.47	0.41
Cu/Ni(110)	1.52	1.08	0.17	0.65
Cu/Ni(111)	0.93	0.56	0.25	0.37
Co/Cu (Ref. 8)			0.77±0.04	0.51±0.02
Co/Cu (Ref. 9)			0.3-0.6	0.3-1.1
Co/Cu (Ref. 10)			0.85 ± 0.1	0.3 ± 0.05
$Ni_{80}Fe_{20}/Cu$ (Ref. 11)			0.81 ± 0.14	0.5 ± 0.04

mation. In the local-density approximation, there are systematic errors in the shape of the Fermi surface, which can lead to unknown errors in the interface resistance.

Some trends are clear from the results. The strongest asymmetries of any of the interfaces are for the Au/Fe and Ag/Fe interfaces. For these interfaces, the strong reflection for the minority states arises in large part because the states near the center of the interface Brillouin zone have very different symmetries for the two materials. The interfaces that have the lowest symmetry, fcc(110) and bcc(112), tend to have the lowest asymmetries. The asymmetries are positive for all combinations except for Fe/Cr, where the Fermi surface of paramagnetic Cr is very similar to the minority Fermi surface of Fe, leading to weak reflection for those spins.

The experimental results in Table I are from measurements on polycrystalline samples with little information on the interface quality. The layer thicknesses are large enough that quantum interference effects can be neglected. By analyzing the dependence of the resistance on the thicknesses of the different layers, the bulk resistivities and the spin-dependent interfaces resistances can be extracted. It could be that the measured interface resistance is caused by reflection from the interface, as is assumed in the present model, or it could be caused by diffuse scattering at the interface. The

experimental values for Co/Cu are close to the theoretical values for the (111) interface, which is believed to be the predominant orientation for polycrystalline samples. Actually, the results for Co/Cu are not very sensitive to interface orientation. This agreement is at least consistent with an important contribution from the interface reflection. However, the presence of both reflection and diffuse scattering can affect the interface resistance in a complicated way. The magnitude of the interface resistance for Ni₈₀Fe₂₀/Cu is close to the theoretical results for Ni, but the asymmetry γ is quite a bit higher than the theoretical results in Table I. This discrepancy might occur because Ni₈₀Fe₂₀ is sufficiently different from Ni or because the interfaces are significantly more disordered.

In summary, we have shown that the simple approximation for interface resistance derived by Schep *et al.* works reasonably well for certain model interfaces. We have also shown that the interface resistances calculated using this approximation and transmission probabilities computed from first principles give reasonably good agreement with interface resistances determined experimentally. This agreement indicates that the measured interface resistances might not be dominated by defect scattering as is often assumed.

¹M.N. Baibich, J.M. Broto, A. Fert, F. Nguyen Van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. **61**, 2472 (1988); G. Binasch, P. Grünberg, F. Saurenbach, and W. Zinn, Phys. Rev. B **39**, 4828 (1989).

²J. Bass and W.P. Pratt, J. Magn. Magn. Mater. **200**, 274 (1999).

³T. Valet and A. Fert, Phys. Rev. B **48**, 7099 (1993).

 ⁴R.S. Sorbello, Phys. Rev. B **39**, 4984 (1989); B. Laikhtman and S. Luryi, *ibid.* **49**, 17 177 (1994); R. Landauer, *ibid.* **52**, 11 225 (1995); C. Kunze, *ibid.* **51**, 14 085 (1995).

⁵K.M. Schep, J.B.A.N. van Hoof, P.J. Kelly, G.E.W. Bauer, and J.E. Inglesfield, J. Magn. Magn. Mater. 177, 1166 (1998).

⁶D.R. Penn and M.D. Stiles, Phys. Rev. B **59**, 13 338 (1999).

⁷In Ref. 6 a factor of $v_{\rm F}$ was omitted from the expression for R_A , Eq. (34).

⁸P. Holody, Ph.D. thesis, Michigan State University, 1996.

⁹B. Doudin, A. Blondel, and J.P. Ansermet, J. Appl. Phys. **79**, 6090 (1996).

¹⁰L. Piraux, S. Dubois, C. Marchal, J.M. Beuken, L. Filipozzi, J.F. Despres, K. Ounadjela, and A. Fert, J. Magn. Magn. Mater. **156**, 317 (1996); L. Piraux, S. Dubois, and A. Fert, *ibid*. **159**, L287 (1996).

¹¹Q. Yang, P. Holody, R. Loloee, L.L. Henry, W.P. Pratt, P.A. Schroeder, and J. Bass, Phys. Rev. B 51, 3226 (1995).

¹²M.D. Stiles, J. Appl. Phys. **79**, 5805 (1996).

¹³M.D. Stiles, Phys. Rev. B **54**, 14 679 (1996).

¹⁴S. Zhang and P.M. Levy, Phys. Rev. B **57**, 5336 (1998).