Interface resistance for perpendicular transport in layered magnetic structures

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The spin-dependent interface resistance due to electron reflections and refractions at an interface potential step between ferromagnetic and nonmagnetic metals and due to impurities located at the interface is calculated within the Landauer approach for a current perpendicular to the interface. We show that experimental values of the interface resistance in Co/Ag and Co/Cu multilayers can be accounted for by assuming reasonable values of the potential steps and impurity concentrations.

Recent experiments on transport properties of magnetic multilayers with current perpendicular to the sublayers have raised several fundamental questions. One of them is the role of spin accumulation at the interface between ferromagnetic and nonmagnetic materials and the role of spin-flip electron scattering. Another important problem is the resistance due to electron scattering by interface roughness and potential steps. In the first theoretical treatment of the perpendicular transport based on the Kubo formalism[1] the spin-flip scattering was neglected so that not only the total current but also the currents for each spin direction were supposed to be constant, i.e., position independent. The role of the spin accumulation layer and spin-flip electron scattering was discussed by Johnson and Silsbee[2] and van Son, van Kempen, and Wyder[3] for a single interface between ferromagnetic and nonmagnetic metals and by Johnson[4] and Valet and Fert[5] for multilayers.

In a recent paper Valet and Fert[5] developed a model in which the current density j_σ is related to the spin-dependent electrochemical potential $\bar{\mu}_\sigma$ by simple macroscopic relations. Within this model the electron scattering at the interface, placed say at $x=0$, is included via the boundary condition[5]

$$\bar{\mu}_\sigma(x=0^+)-\bar{\mu}_\sigma(x=0^-)=r_\sigma j_\sigma(x=0)/e\ , \tag{1}$$

with $j_\sigma(x=0^+)=j_\sigma(x=0^-)\equiv j_\sigma(x=0)$. In Eq. (1), r_σ is the spin-dependent interface resistance of a unit square, which includes contributions from the electron reflections by the potential step and from the diffuse scattering by the roughness or chemical disorder of the interface. The model assumes incoherent scattering by successive interfaces. It has been used successfully to account for recent experimental data obtained on Co/Cu and Co/Ag multilayers.[6] The analysis of Pratt and co-workers[6] shows a relatively large spin asymmetry factor for the interface resistances, $r_-/r_+\simeq 12$ in Ag/Co for example, and a definitely smaller corresponding factor for the bulk resistivities of Co, $\rho_-/\rho_+\simeq 2.9$. The objective of this paper is to calculate the interface resistance and, by comparison with the experimental data of Ref. 6, to draw some conclusions about the possible origin of the interface resistance in Co/Ag or Co/Cu, i.e., if it is mainly due to the potential steps or to the diffuse scattering. The calculations are performed within the multichannel Landauer formalism.[7] A similar formalism has also been used in the theory of Bauer,[8] but in a different way. In our approach, related directly to the macroscopic theory of Valet and Fert,[5] we apply the Landauer formalism to describe the coherent transport across a single interface. The important parameters of our calculations are the potential steps. The objective of the calculation is to determine whether the experimental interface resistances can be accounted for by introducing plausible values of the potential steps or whether a significant contribution is due to diffuse scattering by interface roughness.

According to the above we consider an interface between nonmagnetic ($x<0$) and magnetic ($x>0$) metals and assume an electric current flowing perpendicularly to the interface, say in the positive x direction. Consider first the case of ideal interface, i.e., no interface roughness. The potential step at the interface is caused by the difference in the bottom energy of the conduction bands in the two metals. Since one of the metals is ferromagnetic, the potential step depends on the electron spin and consequently its contribution to the interface resistance is also spin dependent. Due to the potential steps the electrons suffer partial or total reflection from the interface with spin-dependent reflection and transmission coefficients. The wave-vector component parallel to the interface, $\mathbf{k}_\parallel$, is however conserved. The potential step may be different for each spin channel. For clarity of notation the spin index is suppressed here and will be restored when necessary. Assume the potential step to be of the form

$$U(x)=\begin{cases}0 & \text{for } x<0\ ,\\ U & \text{for } x>0\ ,\end{cases} \tag{2}$$

where U ($U>0$) is a constant. In the framework of the Landauer approach we considered two perfect leads—

one of the nonmagnetic material and the other one of the magnetic material—which are connected to two electron reservoirs described by the chemical potentials $\mu^<$ (on the left) and $\mu^>$ (on the right). The electron scattering at the interface is represented by an elastic scatterer placed between the leads. The resistance of the scatterer is defined as the ratio of a difference of chemical potentials in the leads and the electric current flowing through the resistor. As we consider here two independent spin currents (no spin-flip scattering at the interface), the local chemical potentials in the leads are different for the two currents (and also different from $\mu^<$ and $\mu^>$). Following Ref. 7, the resistance R due to scattering by a potential step is given by the asymmetric multichannel Landauer formula

$$R=\frac{h}{2e^2}\frac{1+(g^<)^{-1}\sum_i (V_i^<)^{-1}R_i-(g^>)^{-1}\sum_j (v_j^>)^{-1}T_j}{\sum_j T_j}, \tag{3}$$

where

$$g^<=\sum_i (v_i^<)^{-1}, \tag{4a}$$

$$g^>=\sum_j (v_j^>)^{-1}. \tag{4b}$$

In Eq. (3) T_j (R_i) is the total transmission (reflection) probability into the jth channel on the right (ith channel on the left)

$$T_j=\sum_i T_{ji};\quad R_i=\sum_{i'} R_{ii'} \tag{5}$$

where T_{ji} ($R_{ii'}$) is the transmission coefficient into the jth channel on the right (reflection coefficient into the ith channel on the left) for electrons incident in the ith (i'th) channel of the left lead. Finally, $v_i^<$ and $v_j^>$ are the electron velocities normal to the interface, whereas the summations over i and j in Eqs. (3)–(5) are the summations over all channels in the left and right leads. All parameters in Eq. (3) are calculated at the Fermi energy. For periodic boundary conditions in the plane of the interface the different channels correspond to different wave vectors $\mathbf{k}_\parallel$. For an ideal interface one can write $T_{ji}\equiv T(\mathbf{k}_\parallel^j,\mathbf{k}_\parallel^i)=T(\mathbf{k}_\parallel^j)\delta_{ij}=T_j\delta_{ij}$. Similar relations hold also for the reflection coefficients. Apart from this, the relation $T_i+R_i=1$ is fulfilled. In a quantum description the transmission coefficients can be written in the form used, for example, by Hood and Falicov,[9]

$$T_i=\frac{4k_i^>k_i^<}{(k_i^>+k_i^<)^2}, \tag{6}$$

when $k_i^>$ is real. Consequently

$$R_i=\frac{(k_i^>-k_i^<)^2}{(k_i^>+k_i^<)^2} \tag{7a}$$

for $k_i^>$ real, whereas

$$R_i=1 \tag{7b}$$

when the corresponding $k_i^>$ is imaginary. In the above equations, $k_i^>$ and $k_i^<$ are normal components of the wave vectors in the ith channel for $x>0$ and $x<0$, respectively.

For sufficiently thick leads one may change all sums in Eqs. (3) and (4) into the corresponding integrals over $\mathbf{k}_\parallel$. It is also convenient to transform the integrals over $\mathbf{k}_\parallel$ to integrals over the angle θ between the electron wave vector and the normal to the interface. The interface resistance R can then be written in the form

$$R=\frac{\pi h}{2e^2}\frac{1}{Sk_F^2}\frac{1-2[J_3+J_2(1-x_c^2)^{-1/2}]}{J_1}, \tag{8}$$

where k_F is the Fermi wave vector in the material on the left side ($E_F=\hbar^2k_F^2/2m$, with E_F being the Fermi energy), S is the lead cross section and J_1, J_2, and J_3 are defined as follows,

$$J_1=\int_{x_c}^1 dx\frac{x^2(x^2-x_c^2)^{1/2}}{[x+(x^2-x_c^2)^{1/2}]^2}, \tag{9a}$$

$$J_2=\int_{x_c}^1 dx\frac{x^2}{[x+(x^2-x_c^2)^{1/2}]^2}, \tag{9b}$$

$$J_3=\int_{x_c}^1 dx\frac{x(x^2-x_c^2)^{1/2}}{[x+(x^2-x_c^2)^{1/2}]^2}, \tag{9c}$$

where x_c is defined as

$$x_c=\cos(\theta_c)=(U/E_F)^{1/2}. \tag{10}$$

For $\theta>\theta_c$ the kinetic energy of perpendicular motion is lower than the potential step and the electrons are totally reflected [Eq. (7b)].

On calculating the above integrals one can write the interface resistance per unit area, $r=SR$, in the form

$$r=\frac{2\pi h}{e^2}\frac{1}{k_F^2}\frac{\Phi_1}{\Phi_2}, \tag{11}$$

where

$$\Phi_1=\tan(\varphi_c)[\tfrac{4}{15}-\tfrac{1}{6}\tan^3(\varphi_c/2)-\tfrac{1}{10}\tan^5(\varphi_c/2)]+\sin(\varphi_c)[\tfrac{16}{15}-\tfrac{1}{6}\tan^3(\varphi_c/2)+\tfrac{1}{10}\tan^5(\varphi_c/2)] \tag{12a}$$

and

$$\Phi_2=\cos^2(\varphi_c)-\tfrac{1}{3}\cos^2(\varphi_c)\sin^2(\varphi_c)\frac{3+\cos(\varphi_c)}{[1+\cos(\varphi_c)]^3}. \tag{12b}$$

In the above equations the parameter φ_c is defined as

$$\sin(\varphi_c)=x_c, \tag{13}$$

or, equivalently, $\varphi_c=\pi/2-\theta_c$. Equations (11) and (12) determine the interface resistance in the case of perfect potential steps. The formulas are valid for currents flowing in both directions normal to the interface. After slight changes they apply also to the case of $U<0$.

Consider now the interface resistance for some typical situations shown schematically in Fig. 1, where the spin subbands for minority (−) and majority (+) electrons in a magnetic metal are shifted respectively up and down

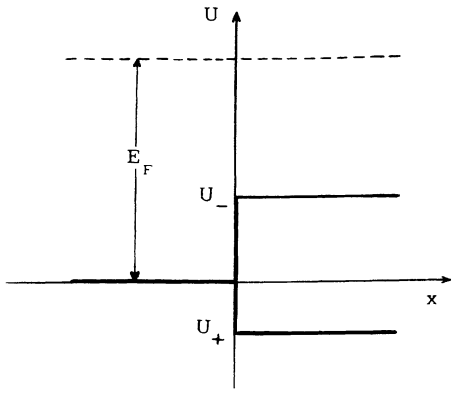

FIG. 1. Potentials for minority U_- and majority U_+ electrons at the interface between normal and ferromagnetic metals.

with respect to the electronic band in the nonmagnetic metal. Dependence of the resistance r_σ upon the parameter U_σ/E_F is shown in Fig. 2 for a typical Fermi wave vector in a nonmagnetic metal, $k_F=1.3\times10^{-10}$ m^{-1}. The resistance r_- increases from $r_-=0$ at $U_-=0$ to about 5.0 fΩ m^2 (f=femto=10^{-15}) at $U_-/E_F\cong0.7$. As U_- approaches E_F the resistance r_- increases rapidly to infinity. The dependence of r_+ on U_+/E_F is similar. The resistance r_+ increases from $r_+=0$ at $U_+=0$ to about 1.1 fΩ m^2 at $U_+/E_F=-1.0$ and increases further with increasing $|U_+|/E_F$. For small U_-/E_F and $|U_+|/E_F$ the resistances r_- and r_+ are approximately the same.

Figure 2 also applies to the situation when both spin subbands in the ferromagnetic metal are shifted up (or down) with respect to the electronic band of the nonmagnetic metal. In that case both interface resistances can be found from Fig. 2(a) [or Fig. 2(b)].

In the general case the potential step for majority electrons is different from the one for minority electrons. Consequently, the resistances r_+ and r_- are also different. Any value of the asymmetry factor r_-/r_+ can be obtained. Let us compare the predicted values with those found experimentally. The experimental data are $r_-=2.08$ fΩ m^2 and $r_+=0.17$ fΩ m^2 for Co/Ag and $r_-=1.76$ fΩ m^2 and $r_+=0.24$ fΩ m^2 for Co/Cu multilayers.[6] As can be seen from Fig. 2, the higher resistances, $r_-=2.08$ fΩ m^2 in Co/Ag and $r_-=1.76$ fΩ m^2 in Co/Cu, can be accounted for by assuming reasonable values of U_-/E_F around 0.4 [in the free-electron model for s electrons in Co, Cu, and Ag, $U_-/E_F=0.4$ means k_F^-(Co)/k_F (Cu or Ag)$=\sqrt{0.6}$, or alternatively 0.23 minority-spin s electrons per atom in Co if one assumes 0.5 s electrons per atom and spin direction in Cu or Ag]. The smaller values for r_+ correspond to $|U_+|/E_F$ of the order of only 0.03, i.e., to a not very different number of s electrons in Co, Cu, and Ag for this spin direction. Qualitatively, the high value of the ratio r_-/r_+ can be supposed to follow from the contrast between a good fit of the s bands of Co, Cu, and Ag for one spin direction [n_+(Co)$\approx n$(Cu)/2$\approx n$(Ag)/2] and bad mismatch of the bands for the other spin direction [n_-(Co) is definitely smaller than n(Cu)/2 or n(Ag)/2].

An additional contribution to the interface resistance arises from diffuse scattering by interface disorder. As a model situation we consider impurities concentrated at the interface ($x=0$) with the areal concentration n. The impurities introduce some mixing between different quantum channels, i.e., the in-plane wave vector is not conserved at the transition through the interface. The in-plane translational symmetry is, however, restored by averaging over the impurity distribution. To find effective coefficients T_i and R_i we use a method similar to that developed by Cahay, McLennan, and Datta.[10] In the simplest approximation, i.e., neglecting the vertex corrections, one finds

$$T_i=\frac{4k_i^>k_i^<}{(k_i^>+k_i^<)^2\left|1+\mathcal{T}\frac{\Gamma}{4}\frac{2}{k_i^>+k_i^<}\right|^2} \tag{14}$$

for $k_i^>$ real. Consequently, $R_i=1-T_i$ for $k_i^>$ real and $R_i=1$ for $k_i^>$ imaginary. In Eq. (14) $\mathcal{T}$ is defined as

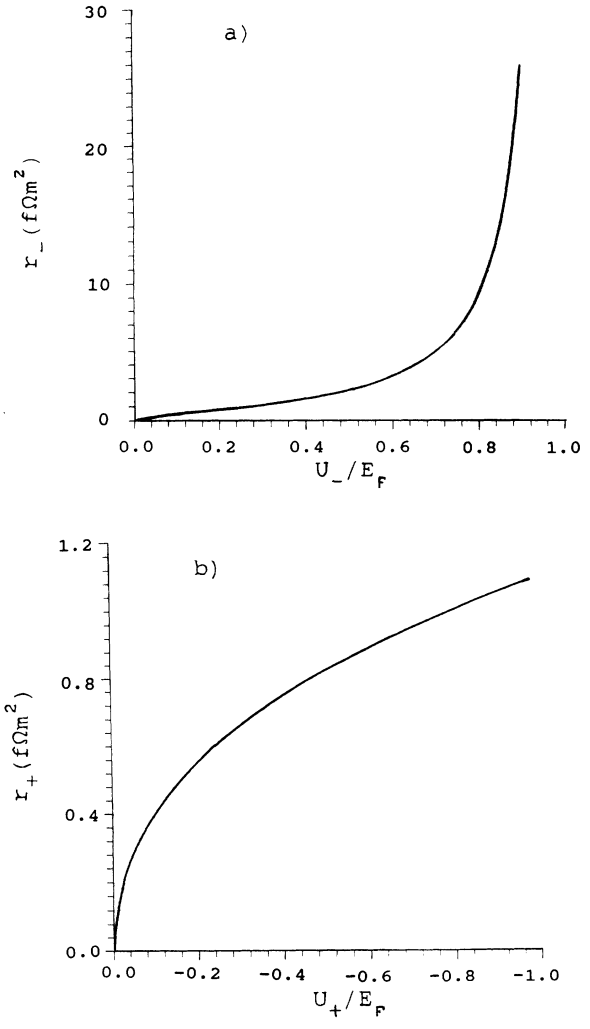

FIG. 2. Dependence of the interface resistances on the potential steps shown in Fig. 1 for $k_F=1.3\times10^{-10}$ m^{-1}. (a) Interface resistance for minority electrons and (b) interface resistance for majority electrons.

$$\mathcal{J}=\frac{1}{S}\sum_i \frac{2}{k_i^{>}+k_i^{<}} , \tag{15}$$

and

$$\Gamma=\left[\frac{2m}{\hbar^2}V\right]^2 n , \tag{16}$$

where V is the impurity scattering potential.

The transmission coefficient (14) differs from that used in Ref. 8. In the limit of a clean interface (no impurities), Eq. (14) becomes the formula used, for example, by Hood and Falicov,[9] whereas the Bauer[8] form is not consistent with those formulas.

It is easy to find the following explicit expression for the parameter $\mathcal{J}$,

$$\mathcal{J}/k_F=f=\frac{1}{3\pi x_c^2}[1-(1-x_c^2)^{3/2}-ix_c^3] . \tag{17}$$

The interface resistance is then given by Eq. (8) with the integrals J_1, J_2, and J_3 given by Eqs. (9a)–(9c), in which the denominators are multiplied by an additional factor $A(x)$

$$A(x)=1+\frac{\Gamma \mathrm{Re}\{f\}}{x+(x^2-x_c^2)^{1/2}}+\frac{\Gamma^2|f|}{4[x+(x^2-x_c^2)^{1/2}]^2} . \tag{18}$$

The integrals have been calculated numerically and some results are shown in Fig. 3 for several values of Γ. For small values of U_-/E_F, the interface resistances due to the potential step and the interface roughness are approximately additive. This is not true for larger values of U_-/E_F. The basic task now is to estimate the relative importance of the two contributions. We have seen above that even the highest experimental values of the interface resistance can be accounted for by reasonable values of U/E_F. On the other hand, the contribution due to electron scattering by interface defects, for reasonable values of Γ, is also comparable with the experimental data. One can find that $\Gamma=3$ corresponds to plausible values of the impurity concentration and the phase shift associated with the scattering potential V.

There is also another argument supporting the conclusion that both contributions are comparable. Let us consider a disordered interfacial layer of thickness 4 Å with the typical high resistivity of an amorphous alloy of 4 $\mu\Omega$ m in each spin channel (2 $\mu\Omega$ m is a typical value of the resistivity for amorphous alloys containing transition metals, which gives 4 $\mu\Omega$ m for each spin channel). Writing $r_\sigma=\rho_\sigma l$ with $l=4\times10^{-10}$ m and $\rho_\sigma=4$ $\mu\Omega$ m one obtains $r_\sigma=1.6$ fΩ m^2. We thus find that scattering by interface roughness can also contribute significantly to the interface resistance. A balanced contribution from potential steps and disorder cannot be ruled out. Experiments on samples prepared in different ways and having the same intrinsic steps but different interface roughness could be helpful in separating the two contributions.

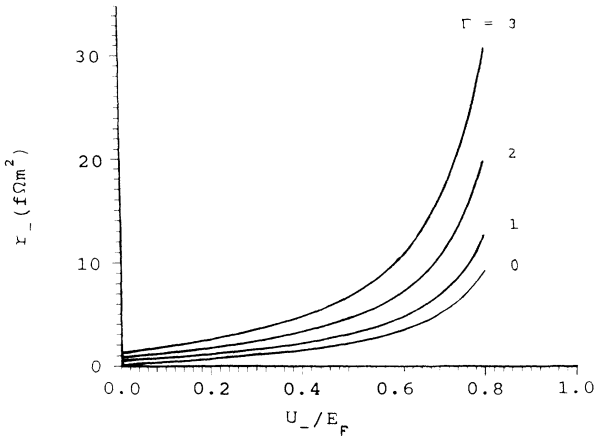

FIG. 3. Dependence of the interface resistance on the potential step shown for several different values of the parameter Γ. The other parameters are as in Fig. 2.

In conclusion, we have calculated the spin-dependent interface resistance caused by electron reflections from the potential steps as well as by impurities located at the interface between magnetic and nonmagnetic metals. The results can be applied to magnetic multilayers in the macroscopic limit, when the electron scattering by successive interfaces is incoherent. We have found that both contributions are comparable with the experimental data.

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