Solution to the Boltzmann equation for layered systems for current perpendicular to the planes

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Present theories of giant magnetoresistance (GMR) for current perpendicular to the planes (CPP) are based on an extremely restricted solution to the Boltzmann equation that assumes a single free electron band structure for all layers and all spin channels. Within this model only the scattering rate changes from one layer to the next. This model leads to the remarkable result that the resistance of a layered material is simply the sum of the resistances of each layer. We present a solution to the Boltzmann equation for CPP for the case in which the electronic structure can be different for different layers. The problem of matching boundary conditions between layers is much more complicated than in the current in the planes (CIP) geometry because it is necessary to include the scattering-in term of the Boltzmann equation even for the case of isotropic scattering. This term couples different values of the momentum parallel to the planes. When the electronic structure is different in different layers there is an interface resistance even in the absence of intermixing of the layers. The size of this interface resistance is affected by the electronic structure, scattering rates, and thicknesses of nearby layers. For Co–Cu, the calculated interface resistance and its spin asymmetry is comparable to that measured at low temperature in sputtered samples. © *2000 American Institute of Physics.* [S0021-8979(00)71908-6]

I. INTRODUCTION

Although most studies of GMR are for the case of applied electric fields and hence net current in the plane of the film (CIP geometry), there has been considerable experimental and theoretical work on the current perpendicular to the plane (CPP) geometry. Gijs and Bauer have provided a useful review[1] of recent work on CPP GMR. Camblong, Zhang, and Levy[2] presented a simple model for the CPP conductance for a single spin channel in the case of identical free electron band structure in all layers, with the only difference between layers being possible differences in the scattering rates. Valet and Fert, in a classic paper,[3] generalized this model to include scattering processes that connect the two spin channels. The Michigan State group and co-workers[4,5] measured GMR for numerous systems for the CPP geometry, and found that many of their results could be fit with the Camblong–Levy or Valet–Fert models.

In this paper, we present a solution to the Boltzmann equation for the case in which the electronic structure can be different for different layers and different spin channels. We compare our results to the ''standard'' theory.[2,3]

II. BOLTZMANN EQUATION FOR CPP TRANSPORT

Although it is not necessary in our approach, in order to make contact with the standard approach, we shall assume that the scattering probability is isotropic. Then, within a single layer in which we can assume that $v_z^s(\mathbf{k})$ is independent of z, the Boltzmann equation can be written[3] in terms of the anisotropic function, $g_s(z,\mathbf{k})$,

$$v_z^s \frac{\partial g_s(z,\mathbf{k})}{\partial z} + \frac{g_s(z,\mathbf{k})}{\tau_s} = v_z^s \frac{\partial \bar{\mu}_s(z)}{\partial z}, \tag{1}$$

where we have defined $\bar{\mu}_s(z) = \mu(z) - eV(z)$. The ''standard'' treatment of CPP transport[2,3] is obtained by using this equation for all layers, thereby implicitly assuming that there is no change in electronic structure from layer to layer. The reason for this assumption, of course, is the difficulty in solving the CPP Boltzmann equation for an inhomogeneous system. This difficulty arises from the requirement that $g_s(z,\mathbf{k})$ be anisotropic, i.e., that

$$\sum_{\mathbf{k}} \frac{\partial f_0(E_{\mathbf{k}}^s - \mu_0)}{\partial E_{\mathbf{k}}^s} g_s(z,\mathbf{k}) \equiv 0. \tag{2}$$

This requirement arises from the definition of $g_s(z,\mathbf{k})$,

$$g_s(z,\mathbf{k}) = \mu_s(z) - h_s(z,\mathbf{k}), \tag{3}$$

where the chemical potential $\mu(z)$ is defined as the average of the distribution function, $\mu_s(z) = \langle h_s(z,\mathbf{k}) \rangle$, and the angular brackets indicate a Fermi surface average. The requirement that $g_s(z,\mathbf{k})$ satisfy Eq. (2) is equivalent to including the scattering-in term of the usual form of the Boltzmann equation and is necessary for current conservation.

In Eq. (1), the scattering rate, $1/\tau_s$, can be allowed to vary with z without significantly complicating the solution. Thus it is easy to show that for homogeneous electronic structure but varying scattering rate, the CPP resistance depends only on the averaged scattering rate,

$$R_s A = \frac{\int dz \frac{1}{\tau_s(z)}}{e^2 n_s \langle (v_z^s)^2 \rangle} = \int dz \rho_s(z), \tag{4}$$

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where A is the area of the film perpendicular to the direction of the current, n_s is the Fermi energy density of electronic states, $\rho_s(z)$ is a local resistivity of free electrons and the angular brackets denote an average over the Fermi surface. The second expression in Eq. (4) is often assumed to be the proper generalization of the free electron formulas to general electron dispersion. In the following we shall refer to this result as the ''standard'' expression for CPP resistance.

In order to treat a system in which the electronic structure is different in successive layers, it is necessary to match the solutions to the Boltzmann equation obtained for each layer across the interfaces between the layers. The procedure for performing this matching is relatively straightforward,[6] but involves the full distribution function, $h_s(z,\mathbf{k})$, not just the anisotropic part,

$$h_{i+1}^{+,j}(z_i^+,\mathbf{k}_\parallel)=\sum_{j',\mathbf{k}'_\parallel}^{N_R} T_i^{+-}(j\mathbf{k}_\parallel,j'\mathbf{k}'_\parallel)h_{i+1}^{-,j'}(z_i^+,\mathbf{k}'_\parallel)+\sum_{j',\mathbf{k}'_\parallel}^{N_L} T_i^{++}(j\mathbf{k}_\parallel,j'\mathbf{k}'_\parallel)h_i^{+,j'}(z_i^-,\mathbf{k}'_\parallel)$$

$$h_i^{-,j}(z_i^-,\mathbf{k}_\parallel)=\sum_{j',\mathbf{k}'_\parallel}^{N_L} T_i^{-+}(j\mathbf{k}_\parallel,j'\mathbf{k}'_\parallel)h_i^{+,j'}(z_i^-,\mathbf{k}'_\parallel)+\sum_{j',\mathbf{k}'_\parallel}^{N_R} T_i^{--}(j\mathbf{k}_\parallel,j'\mathbf{k}'_\parallel)h_{i+1}^{-,j'}(z_i^+,\mathbf{k}'_\parallel). \quad (5)$$

Here N_L and N_R denote the number of states on the left or right of the interface, respectively, for a given value of $k'_\parallel$.

In order to properly match the distribution functions at the boundaries of the layers, it is necessary to utilize the general solution to Eq. (1) and to admit exponentially varying solutions that could be omitted for the homogeneous case. Thus, it can be verified that the anisotropic distribution function for spin s in layer i can be written as

$$g_s(z,\mathbf{k})=\frac{J_s}{\sigma_{si}}ev_z^{si}(\mathbf{k})\tau_{si}-F_{si}(\mathbf{k})e^{(-z/v_z^{si}(\mathbf{k})\tau_{si})}+\left\langle \frac{F_{si}(\mathbf{k}')e^{(-z/v_z^{si}(\mathbf{k}')\tau_{si})}}{v_z^{si}(\mathbf{k})-v_z^{si}(\mathbf{k}')}\frac{v_z^{si}(\mathbf{k})}{\left\langle\frac{v_z^{si}(\mathbf{k})}{v_z^{si}(\mathbf{k})-v_z^{si}(\mathbf{k}')}\right\rangle_{\mathbf{k}}}\right\rangle_{\mathbf{k}'}, \quad (6)$$

$$\overline{\mu}(z)=\alpha_{is}J_s-\frac{J_s}{\sigma_{si}}ez+\left\langle\frac{F_{si}(\mathbf{k}')e^{(-z/v_z^{si}(\mathbf{k}')\tau_{si})}}{\left\langle\frac{v_z^{si}(\mathbf{k})}{v_z^{si}(\mathbf{k})-v_z^{si}(\mathbf{k}')}\right\rangle_{\mathbf{k}}}\right\rangle_{\mathbf{k}'}. \quad (7)$$

Here, J_s is the current density for spin-channel s and σ_{si} is the bulk conductivity for spin s of the material in layer i,

$$\sigma_{si}=-\frac{e^2}{V}\sum_{\mathbf{k}}(v_z^{si}(\mathbf{k}))^2\tau_{si}\delta(E_{\mathbf{k}}-E_F), \quad (8)$$

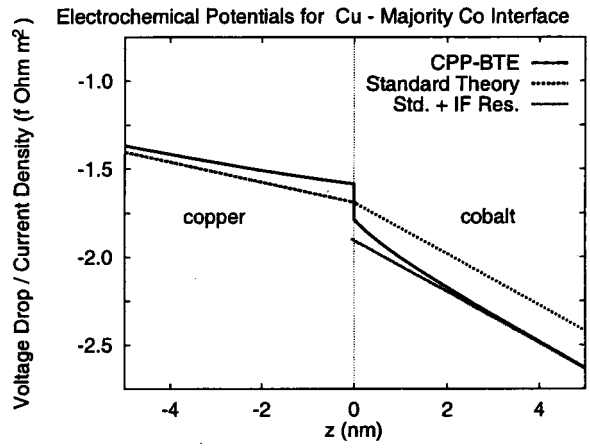

FIG. 1. Chemical potential divided by current density for copper–cobalt majority interface.

and α_{is} and $F_{si}(\mathbf{k})$ are parameters determined by the matching conditions at the boundaries, Eq. (5).

If the distribution function, Eq. (6), is used to calculate the current density, the first term yields J_s and the contributions of the other two terms cancel. The second term would have been expected from the general solution to the CIP case. The third term is made necessary by the requirement that $g(z,\mathbf{k})$ be purely anisotropic.

III. TRANSPORT FOR CURRENT PERPENDICULAR TO THE PLANES

The layer Korringa–Kohn–Rostoker approach[7] was used to calculate the self-consistent electronic structures of cobalt, copper, and cobalt–copper interfaces. These were used to evaluate the transmission (T^{++},T^{--}) and reflection probabilities (T^{+-} and T^{-+}) for Bloch electrons impinging on the interfaces. The Boltzmann equation, including the boundary matching equations, was then solved using an iterative procedure. In the calculations presented here, it was assumed that the interfaces were epitaxial and that there was no additional disorder in the vicinity of the interface.

Figures 1 and 2 show the calculated electrochemical potential, $\overline{\mu}$, for the majority and minority channels in the vi-

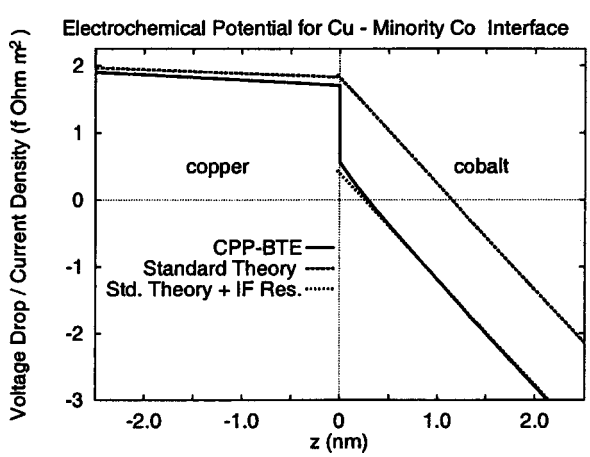

FIG. 2. Chemical potential divided by current density for copper–cobalt minority interface.

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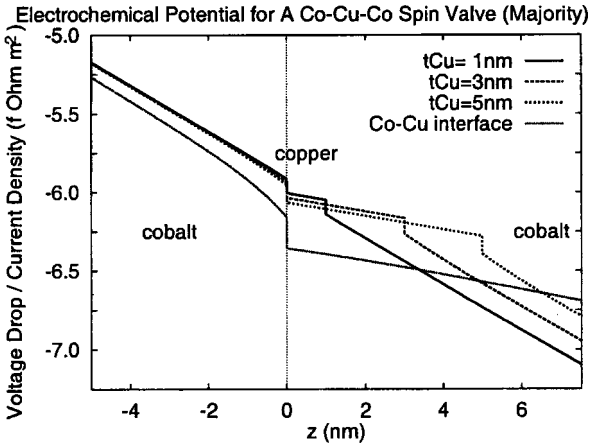

FIG. 3. Chemical potential divided by current density for the majority channel of a cobalt–copper–cobalt spin valve for various thicknesses of the copper layer.

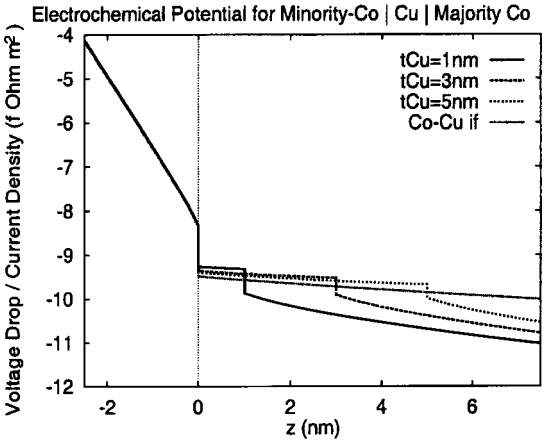

FIG. 4. Chemical potential divided by current density for a cobalt–copper spin valve with cobalt moments aligned antiparallel.

cinity of a copper–cobalt interface. The electrochemical potential has been divided by the current density so that the plots yield $\int dz \rho_s(z)$. For the standard theory this is simply a straight line for each layer. The actual solution to the Boltzmann equation differs in two ways: (1) There is a discontinuity in the chemical potential at the interface which is equivalent to an interfacial resistance. This interfacial resistance is not due to intermixing or additional scattering at the interface (although this effect can be included in the model if desired) but to the mismatch of the bands across the interface which causes some of the electrons incident on the interface to be reflected. (2) There are exponential terms in the electrochemical potential in the vicinity of the interface that decay at a rate comparable to the component of the mean free path perpendicular to the layers. The effect of these terms can be included as an additional interfacial resistance that is added to the discontinuous contribution just described, as is indicated in the dotted lines of Figs. 1 and 2. If this is done, however, it must be taken into consideration that this additional contribution depends on the environment of the interface, e.g., the proximity of other interfaces and the bulk scattering rates. The calculated interfacial resistances can be read off the figures (0.21 and 1.2 $f\Omega m^2$ for majority and minority, respectively) and are comparable to those deduced from low-temperature measurements[5] on cobalt–copper multilayers. This indicates that much of the interfacial resistance previously attributed to disorder at the interface may equally well arise from reflection.

Figures 3 and 4 show that both the discontinuous interfacial resistance and the interfacial resistance arising from the exponential terms can depend on the type and thicknesses of neighboring layers. In Fig. 3, for example, it can be seen that the discontinuous interfacial resistance on both sides of the Co–Cu–Co (majority) spin valve increase with the thickness of the copper spacer layer. The exponential contributions also increase with copper layer thickness. For the case of antiparallel alignment shown in Fig. 4, however, the discontinuous contribution increases slightly with spacer layer thickness on the minority side but *decreases* with thickness on the majority side.

Recently, Chien *et al.*[8] used a tight-binding based quantum model to calculate CPP transport through Co–Cu multilayers. They pointed out the necessity of including vertex corrections which are equivalent to the scattering-in term of the Boltzmann equation in the semiclassical limit. Very recently, Penn and Stiles[9] reported calculations of the interface resistance for free electrons incident on a model interface.

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