A simple treatment of the ''scattering-in'' term of the Boltzmann equation for multilayers

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We present a simple approximation for treating anisotropic scattering within the semiclassical Boltzmann equation for current in plane geometry in magnetic multilayers. This approximation can be used to qualitatively account for the forward scattering that is neglected in the lifetime approximation, and requires only one additional parameter. For the case of a bulk material its effect is a simple renormalization of the scattering rate. The simplicity of this term has allowed quick and simple solution to the Boltzmann equation for magnetic multilayers using realistic band structures. When we use the band structures for Cu|Co multilayers obtained from first-principles calculations, we find an increase in the resistance of the multilayer, compared to the solution without the scattering-in term, due to the higher scattering rates needed to fit the same bulk conductivities. The giant-magnetoresistance ratio is also changed when the vertex corrections are included. © *2000 American Institute of Physics.* [S0021-8979(00)72008-1]

Most studies of giant magnetoresistance[1] (GMR) are for the current in plane (CIP) geometry. Typically, these have been based on the Fuchs–Sondheimer solution[2,3] to the Boltzmann equation for thin films and its generalization to multilayers.[4,5] However, the Fuchs–Sondheimer approach utilizes the lifetime approximation which assumes that the scattering probability between states $\mathbf{k}$ and $\mathbf{k}'$ in the Boltzmann equation, $P_{\mathbf{kk}'}$, is isotropic, i.e., is independent of the electron wave vectors before and after the scattering. Specifically, $P_{\mathbf{kk}'}$ is assumed to have the form,

$$P_{\mathbf{kk}'}=\frac{1}{N(E_{\mathbf{k}})\tau}\delta(E_{\mathbf{k}}-E_{\mathbf{k}'}), \tag{1}$$

where τ is the lifetime and $N(E_{\mathbf{k}})$ is the density of states at $E_{\mathbf{k}}$. This isotropic scattering probability allows one to neglect the scattering-in term of the Boltzmann equation because it does not contribute to the current for bulk or CIP.

This approximation usually works rather well for bulk materials, because the effect of the scattering-in term can be included simply by scaling the lifetime. In an inhomogeneous system, however, simply scaling the lifetime would lead to an incorrect spatial distribution of the current. Therefore, the scattering-in corrections need to be included at least approximately and we need to obtain at least a qualitative understanding of their effect on the resistance, GMR, and current distribution. The effects of the scattering-in terms are sometimes referred to as vertex corrections because of the manner in which they appear as a correction to the self-energy in a quantum mechanical calculation.

One approach to including the scattering-in corrections for substitutional impurity scattering is to evaluate the Kubo formula using the coherent potential approximation with vertex corrections.[6] Another approach would be to solve the Boltzmann equation with the scattering-in term using the scattering rate calculated from the multiple scattering solutions of dilute substitutional impurities in a first-principles calculation. For example, in Fig. 1 we show the scattering rate $P_{\mathbf{kk}'}$ due to Co impurities in Cu at a fixed $\mathbf{k}$. The scattering is highly anisotropic, with the maximum occurring at about $\mathbf{k}'=\mathbf{k}$, and a smaller peak at $\mathbf{k}'=-\mathbf{k}$. Thus, the scattering is dominated by forward scattering. For the same measured resistivity, this can greatly reduce the effective lifetime and significantly change the calculated current distribution. Inclusion of such a scattering term in the Boltzmann equation and its numerical solution is straightforward.

However, substitutional impurities represent only one possible source of scattering in a GMR material. Most other defects that cause electron scattering are difficult to model from the first principles. Therefore, it is desirable to have a simple phenomenological model that can account for all forms of defect scattering and can be easily incorporated into the Boltzmann equation. In this article we present such a model that needs only one additional parameter, captures most of the qualitative features of the vertex corrections, and allows a fast solution of the Boltzmann equation.

We use g to describe the deviation of the distribution function from equilibrium, i.e.,

$$f(z,\mathbf{k}_{\parallel})=f_0(E_{\mathbf{k}})+g(z,\mathbf{k}_{\parallel})\,\delta(E_{\mathbf{k}}-E_F), \tag{2}$$

where f_0 is the equilibrium distribution function and E_F is the Fermi energy. For the CIP geometry, we assume that the layers are stacked in the z direction, and the current flows in the x direction. The Boltzmann transport equation for multilayers is

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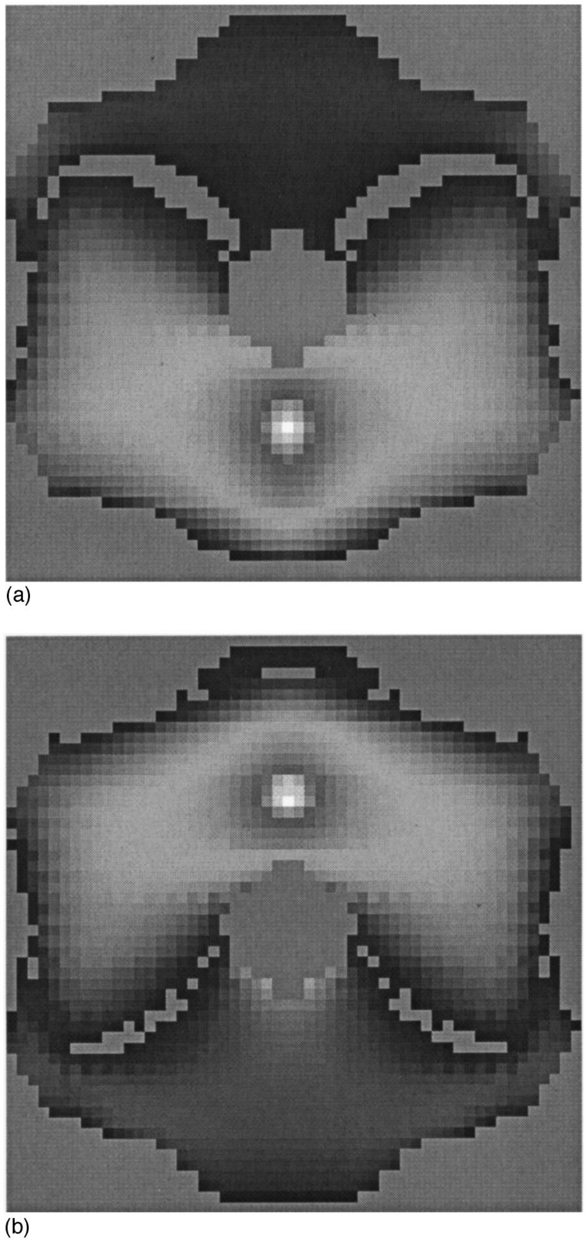

FIG. 1. Scattering rates for a Co impurity in Cu as a function of outgoing wave vector for an incoming wave vector of (0.326, −0.188, −0.561). The upper panel (a) is for negative outgoing wave vectors k_z' (forward scattering) where the highest scattering rate has the value of 0.922, and the lower panel (b) is for positive k_z' (backward scattering) where the highest scattering rate is 0.525. The calculation is for the majority spin channel with Co moment oriented parallel to spin quantization axis.

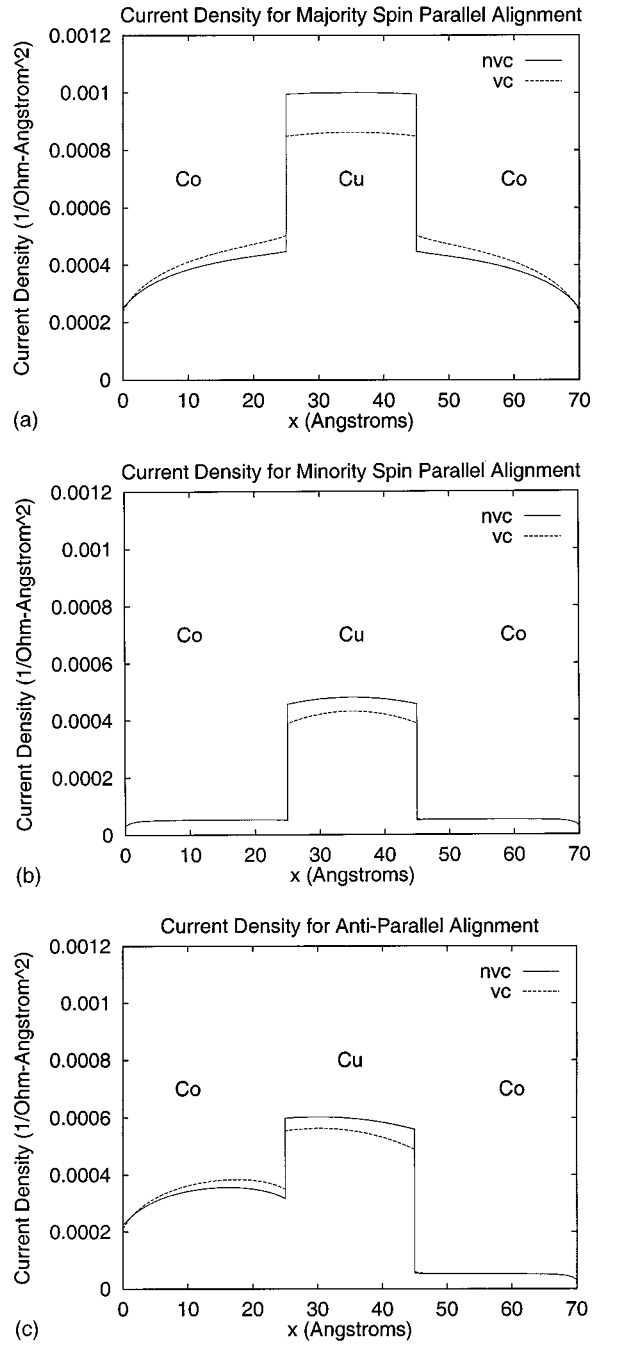

FIG. 2. Current distribution for a Co|Cu|Co trilayer with and without vertex corrections. (a) Majority spin channel for parallel alignment; (b) minority spin channel for parallel alignment; (c) one of the spin channels for antiparallel alignment. Solid lines are without the vertex corrections (nvc) and dotted lines are with the vertex corrections (vc).

$$v_z \frac{\partial g(z,\mathbf{k}_\parallel)}{\partial z} - \sum_{\mathbf{k}_\parallel'} P_{\mathbf{k}\mathbf{k}'}[g(z,\mathbf{k}_\parallel') - g(z,\mathbf{k}_\parallel)] = \frac{eE_x v_x}{m}, \quad (3)$$

where $P_{\mathbf{k}\mathbf{k}'}$ is the scattering rate between states $\mathbf{k}$ and $\mathbf{k}'$ and E_x is the external electric field. The lifetime approximation to the Boltzmann transport equation assumes that the scattering rate is isotropic, Eq. (1), so that

$$v_z \frac{\partial g(z,\mathbf{k}_\parallel)}{\partial z} + \frac{1}{\tau} g(z,\mathbf{k}_\parallel) = \frac{eE_x v_x}{m}, \quad (4)$$

using $\Sigma_{\mathbf{k}_\parallel} g(z,\mathbf{k}_\parallel) = 0$. This leads to the Fuchs–Sondheimer solution,[2,3]

$$g^{(0)}(z,\mathbf{k}_\parallel) = \frac{eE_x v_x \tau}{m}[1 + F^{(0)}(\mathbf{k}_\parallel) e^{-z/v_z\tau}], \quad (5)$$

where the coefficients $F(\mathbf{k}_\parallel)$ are determined by the continuity condition of the distribution function $g(z,\mathbf{k}_\parallel)$ at the boundaries of each layer, and the superscript (0) indicates a solution without the vertex corrections.

The condition that the scattering rate $P_{\mathbf{kk}'}$ satisfies is $P_{\mathbf{kk}'}=P_{\mathbf{k}'\mathbf{k}}$. Therefore the lowest order correction to the isotropic approximation is

$$P_{\mathbf{kk}'}=\left[\frac{1}{N(E_{\mathbf{k}})\tau}+p_x v_x v_x'+p_y v_y v_y'+p_z v_z v_z'\right]\delta(E_{\mathbf{k}}-E_{\mathbf{k}}'),\tag{6}$$

where v_i are the components of the group velocity at $\mathbf{k}$, and v_i' are those at $\mathbf{k}'$, and p_i are the coefficients of expansion, and are presumably small. Substituting back into Eq. (3), we find

$$v_z\frac{\partial g(z,\mathbf{k}_\parallel)}{\partial z}+\frac{1}{\tau}g(z,\mathbf{k}_\parallel)=\frac{eE_x v_x}{m}+p_x j_x(z)v_x,\tag{7}$$

where $j_x(z)$ is the current density at z,

$$j_x(z)=\sum_{\mathbf{k}_\parallel} v_x g(z,\mathbf{k}_\parallel).\tag{8}$$

The second term on the right-hand side represents a simple approximation to the vertex corrections. For a homogeneous bulk system, there is no z dependence of j_x and g. Thus g can be trivially solved as

$$g(\mathbf{k}_\parallel)=\frac{eE_x v_x\overline{\tau}}{m},\tag{9}$$

and

$$j_x=\frac{eE_x\overline{\tau}}{m}\sum_{\mathbf{k}_\parallel} v_x^2,\tag{10}$$

where

$$\overline{\tau}=\frac{\tau}{1-p_x\tau\Sigma_{\mathbf{k}_\parallel}v_x^2}.\tag{11}$$

This is identical to the solution without the vertex corrections, but with a renormalized lifetime.

The solution to Eq. (7) for a general multilayer system is

$$g(z,\mathbf{k}_\parallel)=g^{(0)}(z,\mathbf{k}_\parallel)+g^{(1)}(z,\mathbf{k}_\parallel),\tag{12}$$

where the extra term due to the vertex corrections can be calculated iteratively through

$$g^{(1)}(z,\mathbf{k}_\parallel)=e^{-z/v_z\tau}\left[g^{(1)}(z_0,\mathbf{k}_\parallel)+\frac{p_x v_x}{v_z}\int_{z_0}^{z}dz\ e^{z/v_z\tau}j_x(z)\right].\tag{13}$$

The term $g^{(1)}(z_0,\mathbf{k}_\parallel)$ represents the boundary condition at $z=z_0$ which is determined from the reflection and the transmission coefficients of the interfaces, which are determined using the layer-Korringa–Koha–Rostoker approach.[7]

We calculated the effect of the vertex corrections for a Co|Cu|Co trilayer system. The current distribution in the trilayer is plotted for parallel and antiparallel alignments for each spin channel in Fig. 2. The effect of the vertex correction term is compared. The scattering rates (with and without the vertex corrections) in each layer are adjusted so that they always give the same bulk resistivity as measured experimentally. Consequently, the scattering rates when the vertex corrections are included are much higher than without the vertex corrections. The size of the vertex correction term is chosen so that the scattering rates for the Cu layer and for the Co majority spin channel are changed by a factor of 2. For the Co minority spin channel the scattering is assumed to be isotropic so that the scattering-in term vanishes. The calculation shows that the vertex corrections cause a large reduction in the current in the Cu layers, but have much smaller effect in the Co layers. The combined effect is a higher resistance for the film. We also observe a small reduction in the GMR ratio, from about 20% to about 17%.

In conclusion, a simple term is added to the Boltzmann equation to account for the ''scattering-in'' term. It is demonstrated that this term can change dramatically the current distribution in the GMR systems, but has a small effect on the GMR ratio. We note that this term captures qualitatively the anisotropic feature of defect scattering, but except for a maximum in the forward direction, it is rather unlike the anisotropic impurity scattering rates one would obtain from first principles. The biggest difference is that the impurity scattering rates have a small maximum in the backward direction, while Eq. (6) gives a minimum in the backward direction. This difference, however, should have minimal effect on the change of current distribution due to vertex corrections.

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