Angular dependence of the giant magnetoresistance for a current perpendicular to the plane of the layers in a magnetic sandwich

A. V. Vedyaev, O. A. Kotel'nikova, N. G. Pugach,*) and M. G. Chshiev

M. V. Lomonosov Moscow State University, 119899 Moscow, Russia
(Submitted February 18, 1999)
Fiz. Tverd. Tela (St. Petersburg) **41**, 1814–1818 (October 1999)

A quantum-statistical model using the Kubo formalism is proposed for describing the magnetoresistance of a multilayer structure with the current perpendicular to the plane of the layers. In particular, this model describes the case of noncollinear magnetization of consecutive ferromagnetic layers of the structure. Interference between electron wave functions with different directions of the spin projections onto the magnetization axis, which arises in the noncollinear configuration, is investigated along with the role of electron scattering, not only within the bulk of the layers, but also at their interfaces. © *1999 American Institute of Physics.* [S1063-7834(99)02010-9]

Two main theoretical approaches to the description of giant magnetoresistance (GMR) have evolved since this phenomenon first began to be investigated.[1] One approach places greatest emphasis on the spin-dependent scattering of conduction electrons by the surfaces and in the bulk of the ferromagnetic layers.[2–4] The electrons of each layer are described by the model of a free electron gas.[5] Some of the models incorporate the most characteristic features of the band structure. In particular, the creation of spin-dependent potential barriers at the boundaries of the ferromagnetic layers by the different populations of the valence band in adjacent layers is taken into account, but without regard for the details of the band structure.[6–9] Transport phenomena are described by simple parameters such as the spin-dependent mean free path and the Fermi wave vector.

The second approach is concerned primarily with the influence of the band structure on transport phenomena.[10–12] The electronic structure is calculated from first principles in both the parallel and the antiparallel magnetization configuration of adjacent layers. The magnetization is calculated with allowance for the complete electronic structure of the superlattice. This approach requires complex numerical computations. It is difficult to compare the results of the latter with experimental measurements of the absolute conductivity and magnetoresistance. In particular, the nature of the scattering centers in real multilayer structures is poorly accounted for. The role of such centers can be played by surface defects, magnetic inclusions in the nonmagnetic layers, impurities in the ferromagnetic layers, and finite-temperature phonons. The exact relationship between the electronic structure and the scattering amplitude for each type of defect requires a separate numerical analysis, making it extremely difficult to perform calculations ''from first principles.''

For this reason we prefer the first approach and, while disregarding the complete electronic band structure, we nonetheless take interfacial potential barriers into account, which constitute one of the main features introduced by band-structure calculations.

It has been shown previously[9] that, regardless of whether the current is perpendicular to the plane of the layers (CPP geometry) or is parallel to this plane (in-plane or CIP geometry),[8] the main contribution to the conductivity is from *s*-like electrons, which obey the relation

$$\frac{k_F^{\uparrow}-k_F^{\downarrow}}{k_F^{\uparrow}+k_F^{\downarrow}} \ll 1, \tag{1}$$

where $k_F^{\uparrow}$ and $k_F^{\downarrow}$ are the Fermi quasi-momenta for electrons whose magnetic moments are directed (respectively) in the same and opposite directions as the magnetization. The dependence of the magnetoresistance on the angle γ between the directions of the magnetizations of adjacent layers has been investigated[8,9] with allowance for the above-mentioned potential barriers between adjacent ferromagnetic layers and also the volume scattering of conduction electrons. However, these papers ignore scattering at the layer interfaces, which has been included in a similar analysis[13] confined to strictly parallel and antiparallel magnetization configurations of the adjacent ferromagnetic layers. In such configurations the spin channels do not mix, and the potential barrier (1), which is small in comparison to the Fermi energy, does not play a significant role.

In this paper we present a quantum-statistical analysis of the angular dependence of the magnetoresistance in CPP geometry, taking all the above-indicated mechanisms into account: the spin-dependent potential barrier created by hybridized exchange between the *s* and *d* bands; the spin-dependent scattering of conduction electrons in the bulk of the layers; scattering by the interfaces as distinct from volume scattering. The interfacial type of scattering is caused by roughness of the surfaces between the layers, ''dirt,'' and various kinds of surface defects. The problem is that, when the angle γ between the magnetizations of the layer differs from either 0 or π, mixing takes place between electronic states with spin directions $\uparrow$ and $\downarrow$ as electrons pass from one layer to another, and surface scattering together with volume scattering contributes to a term that depends on the height of the po-

tential barrier, which is found to be proportional to $\sin^2\gamma$, i.e., describes the deviation of the angular dependence from linearity in $\cos\gamma$.

1. THE MODEL

We consider a sandwich consisting of two identical ferromagnetic layers of thickness a and c separated by a paramagnetic interlayer of thickness b. The electronic system of each layer is described as a gas of free electrons subjected to spin-dependent scattering both in the bulk of the layers and at the interfaces. In the case of a noncollinear configuration of the magnetizations of adjacent ferromagnetic layers it is impossible to diagonalize the electron Green's functions in spin space in both layers simultaneously by choosing the right quantization axis. We therefore choose the direction of the magnetization in one layer (c) as the axis in question. Then upon transition from one ferromagnetic layer to the other a pure electronic state with wave vector $k^{\uparrow(\downarrow)}$ goes over to a mixed state, and the electrons pass through the potential barrier, because $k_F^{\uparrow}\neq k_F^{\downarrow}$.

For the zeroth-approximation Green's functions $G_0^{\alpha\beta}(z,z')$, which describe the system with volume scattering only, we adopt the solutions of the matrix equation[9]

$$\left[\left(\frac{\partial^2}{\partial z^2}+k_F^2-k^2\right)I-\frac{2m}{\hbar^2}\Sigma_{\rm vol}^{\alpha\beta}\right]G_0^{\alpha\beta}(z,z')=\frac{2m}{\hbar^2}\,\delta(z-z')I, \tag{2}$$

where m is the effective mass of the conduction electrons, $\delta(z)$ is the Dirac delta function, α and β are the spin indices ($\alpha,\beta=\uparrow,\downarrow$), and I is the unit matrix. For sandwich calculations, i.e., for a structure with spatial inhomogeneity in one direction, we use a mixed coordinate-momentum representation for all quantities. The coordinate z describes the position of a point on the axis perpendicular to the plane of the sandwich layers, and the vector k is the projection of the quasimomentum onto this plane. The self-energy part corresponding to volume elastic scattering in layer c, where the quantization axis coincides with the direction of the magnetization, has the diagonal form

$$\Sigma_{\rm vol}^{\alpha\beta}=\begin{pmatrix}\Sigma_{\rm vol}^{\uparrow} & 0\\ 0 & \Sigma_{\rm vol}^{\downarrow}\end{pmatrix}. \tag{3}$$

Upon rotation of the quantization axis through the angle γ in layer a, this matrix is transformed according to the law

$$\Sigma_{\rm vol}^{\alpha\beta}=\frac{\Sigma_{\rm vol}^{\uparrow}+\Sigma_{\rm vol}^{\downarrow}}{2}I^{\alpha\beta}+\frac{\Sigma_{\rm vol}^{\uparrow}-\Sigma_{\rm vol}^{\downarrow}}{2}\begin{pmatrix}\cos\gamma & \sin\gamma\\ \sin\gamma & -\cos\gamma\end{pmatrix}. \tag{4}$$

The spin-dependent mean free paths of electrons in the bulk of the ferromagnetic layers are

$$l^{\uparrow(\downarrow)}=\frac{\hbar^2 k_F^{\uparrow(\downarrow)}}{m\,{\rm Im}\,\Sigma_{\rm vol}^{\uparrow(\downarrow)}}. \tag{5}$$

Note that $(\Sigma_{\rm vol}^{\uparrow}-\Sigma_{\rm vol}^{\downarrow})$ is the energy of exchange interaction between electrons of the subbands with different spin directions. We consider the case in which the potential barrier overcome by electrons crossing from one ferromagnetic layer to the other is small by virtue of relation (1), i.e., is much lower than the Fermi energy. We can therefore disregard the reflection of electrons by the potential barriers and any effects associated with such reflection, and in Eq. (2) we can set $k_F=(k_F^{\uparrow}+k_F^{\downarrow})/2$. However, the presence of a barrier between electronic states with spins $\uparrow$ and $\downarrow$ must be taken into account in expressions of the type $(k_F^{\uparrow}-k_F^{\downarrow})l^{\uparrow(\downarrow)}$, which can be much larger than unity.

Equation (2) must be augmented by the conditions of continuity of the Green's function and its derivative at the interfaces and by boundary conditions corresponding to the weakening of correlations of the electronic states at infinity.

Taking into account scattering at the interfaces in the sandwich, we find the Green's functions of our system as solutions of the Dyson equation

$$G^{\alpha\beta}(z,z')=G_0^{\alpha\beta}(z,z')+G_0^{\alpha\beta}(z,a)\Sigma_{\rm int}^{\alpha\beta}(a)G^{\alpha\beta}(a,z')+G_0^{\alpha\beta}(z,a+b)\Sigma_{\rm int}^{\alpha\beta}(a+b)G^{\alpha\beta}(a+b,z') \tag{6}$$

in the first approximation, i.e., on the assumption of sufficiently small scattering at the interfaces (with coordinates a and $a+b$ along the z axis). Upon rotation of the quantization axis, the matrix $\Sigma_{\rm int}^{\alpha\beta}$ is transformed according to the same law (3), (4) as the volume scattering matrix. In Eq. (6) $G_0^{\alpha\beta}(z,z')$ is the zeroth-approximation Green's function (2). If by analogy with (5) we introduce a parameter having the dimensions of length, $\lambda^{\uparrow(\downarrow)}=\hbar^2 k_F/m{\rm Im}\Sigma_{\rm int}^{\uparrow(\downarrow)}$, which characterizes the effective mean free path corresponding to spin-dependent scattering at the interfaces, then by assumption this length is much shorter than the lattice constant a_0.

To calculate the two-point conductivity, we use the Kubo equation in the form given in Ref. 14, which appears as follows in the mixed $k-z$ representation:

$$\sigma^{\alpha\beta\eta\nu}(z,z')=-\frac{e^2\hbar^3}{4m^2\pi}\sum_{\mathbf{k}}\left[G^{\beta\eta+}(z,z')-G^{\beta\eta-}(z,z')\right]\times\nabla^{\leftrightarrow}{}_z\nabla^{\leftrightarrow}{}_{z'}\left[G^{\nu\alpha+}(z',z)-G^{\nu\alpha-}(z',z)\right], \tag{7}$$

where $G^{\alpha\beta\pm}(z,z')$ denotes the advanced and retarded Green's functions (6), the spin indices $\alpha,\beta,\eta,\nu=\uparrow,\downarrow$, $\nabla^{\leftrightarrow}{}_z=\frac{1}{2}\nabla^{\rightarrow}{}_z-\nabla^{\leftarrow}{}_z)$ is the antisymmetric operator of differentiation with respect to the coordinate z, and e is the electron charge. Now the current density at a point z has the form of a second-rank spinor and is given by the expression

$$J^{\alpha\beta}(z)=\int\sigma^{\alpha\beta\eta\nu}(z,z')E^{\eta\nu}(z')dz', \tag{8}$$

where $E^{\eta\nu}(z')$ is the effective electric field, which is also a second-rank spinor. It has been shown[14] that the introduction of this quantity is equivalent to the calculation of a vertex correction to the expression for the conductivity (7).

From the energy conservation law we obtain equations for determining the fields $E^{\eta\nu}(z')$:

$$\frac{\partial}{\partial z}J^{\alpha\beta}(z)=0. \tag{9}$$

Equations (8) and (9) are solved self-consistently on the basis of the assumption that the effective fields $E^{\eta\nu}(z')$ do not depend on the coordinate within each layer, but jump at the interfaces as a result of the surface scattering of electrons:

$$E^{\eta\nu}(z)=E_i^{\eta\nu}+C_1^{\eta\nu}\delta(z-a)+C_2^{\eta\nu}\delta(z-a-b), \qquad (10)$$

where $C_1^{\eta\nu}$ and $C_2^{\eta\nu}$ are the voltage drops across the interfaces due to spin-dependent scattering as distinct from volume scattering, $E_i^{\eta\nu}$ denotes quantities that are independent of the coordinate z and differ for different layers ($i=a,b,c$). These quantities are chosen in such a way as to satisfy the conditions of continuity of the expressions for the currents in different layers $J_a^{\alpha\beta}(z)$, $J_b^{\alpha\beta}(z)$, and $J_c^{\alpha\beta}(z)$:

$$J_a^{\alpha\beta}(z)\big|_{z=a}=J_b^{\alpha\beta}(z)\big|_{z=a},$$

$$J_b^{\alpha\beta}(z)\big|_{z=a+b}=J_c^{\alpha\beta}(z)\big|_{z=a+b}, \qquad (11)$$

and the constants $C_1^{\eta\nu}$ and $C_2^{\eta\nu}$ are chosen so that all coordinate-dependent terms in these expressions will vanish. This choice can be made even though such terms are much greater than the evaluated constants.

To obtain the complete system, Eq. (9) must be augmented with expressions for the total voltage drop

$$aE_a^{\alpha\alpha}+bE_b^{\alpha\alpha}+cE_c^{\alpha\alpha}+C_1^{\alpha\alpha}+C_2^{\alpha\alpha}=U,$$

$$aE_a^{\alpha\beta}+bE_b^{\alpha\beta}+cE_c^{\alpha\beta}+C_1^{\alpha\beta}+C_2^{\alpha\beta}=0 \quad \text{for} \quad \alpha\neq\beta. \qquad (12)$$

We have thus written a system of equations for the quantities $E_i^{\alpha\beta}$, $C_1^{\alpha\beta}$, and $C_2^{\alpha\beta}$, each of which is a second-rank spinor. We can solve this system to obtain the total resistance of the sandwich: $R=U/(J^{\uparrow\uparrow}+J^{\downarrow\downarrow})$.

The final equation for the resistance of the sandwich ($a/b/c$) has the form

$$R=\frac{6\pi^2\hbar}{e^2k_F^2}A^{-1}\left\{\left[(a+c)^2+(a+c)(l^{\uparrow}+l^{\downarrow})\left(\frac{b}{l}+2\Sigma_0\right)\right.\right.$$
$$+l^{\uparrow}l^{\downarrow}\left(\frac{b}{l}+2\Sigma_0\right)^2+(1-\cos\gamma)ac\frac{(l^{\uparrow}-l^{\downarrow})^2}{2l^{\uparrow}l^{\downarrow}}$$
$$\left.+(1+\cos\gamma)((a+c)(l^{\uparrow}-l^{\downarrow})\Sigma_1-2l^{\uparrow}l^{\downarrow}\Sigma_1^2)\right]$$
$$\times\left[a+c+\frac{2\xi l^{\uparrow}l^{\downarrow}}{l^{\uparrow}+l^{\downarrow}}\left(\frac{b}{l}+2\Sigma_0\right)\right]+\sin^2\gamma(1-\xi)$$
$$\times\left[ac\frac{(l^{\uparrow}+l^{\downarrow})^2(1-\xi)}{4l^{\uparrow}l^{\downarrow}\xi}\left(a+c+\frac{2l^{\uparrow}l^{\downarrow}}{l^{\uparrow}+l^{\downarrow}}\left(\frac{b}{l}+2\Sigma_0\right)\right)\right.$$
$$\left.\left.+\frac{ac(a+c)(l^{\uparrow}-l^{\downarrow})^2}{4l^{\uparrow}l^{\downarrow}}+(a+c)l^{\uparrow}l^{\downarrow}\Sigma_1^2-ac(l^{\uparrow}-l^{\downarrow})\Sigma_1\right]\right\}, \qquad (13)$$

where $1/\xi=1+[(k^{\uparrow}-k^{\downarrow})l^{\uparrow}l^{\downarrow}/(l^{\uparrow}+l^{\downarrow})]^2$, l is the mean free path of conduction electrons in the nonmagnetic interlayer, and the following notation has been introduced:

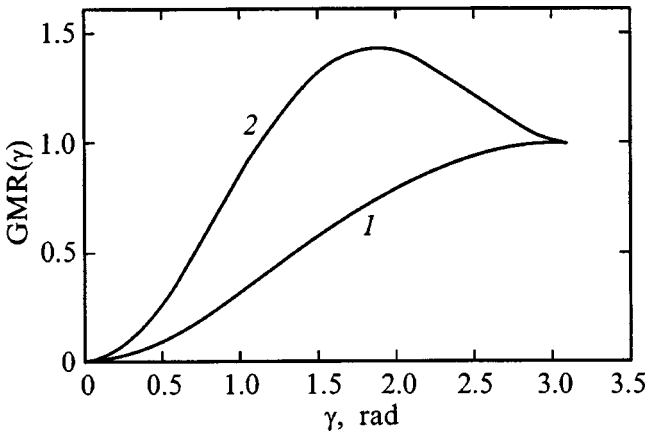

FIG. 1. Dependence of the normalized magnetoresistance on the angle between the directions of the magnetizations of ferromagnetic layers with thicknesses $a=c=23$, $b=11$, $l^{\uparrow}=60$, $l^{\downarrow}=20$, $l=180$; (*1*) $\lambda^{\uparrow}\to\infty$, $\lambda^{\downarrow}\to\infty$; (*2*) $\lambda^{\uparrow}=200$, $\lambda^{\downarrow}=10$.

$$A=(l^{\uparrow}+l^{\downarrow})\left[\left(a+c+\frac{2\xi l^{\uparrow}l^{\downarrow}(b/l+2\Sigma_0)}{l^{\uparrow}+l^{\downarrow}}\right)\right.$$
$$\left.\times\left(a+c+\frac{2l^{\uparrow}l^{\downarrow}(b/l+2\Sigma_0)}{l^{\uparrow}+l^{\downarrow}}\right)+ac\sin^2\gamma\frac{(1-\xi)^2}{\xi}\right],$$

$$\Sigma_0=\frac{ma_0}{\hbar^2k_F}\mathrm{Im}(\Sigma_{\mathrm{int}}^{\uparrow}+\Sigma_{\mathrm{int}}^{\downarrow}),$$

$$\Sigma_1=\frac{ma_0}{\hbar^2k_F}\mathrm{Im}(\Sigma_{\mathrm{int}}^{\uparrow}-\Sigma_{\mathrm{int}}^{\downarrow}). \qquad (14)$$

2. DISCUSSION OF THE RESULTS

We have derived an analytical equation (13) for the resistance of a magnetic sandwich in the case of noncollinear magnetization of the magnetic layers, taking into account spin-dependent scattering that differs in the bulk and at the interfaces of the layers. This property enables us to investigate the role of interfacial scattering in the gigantic magnetoresistance of such multilayer magnetic structures.

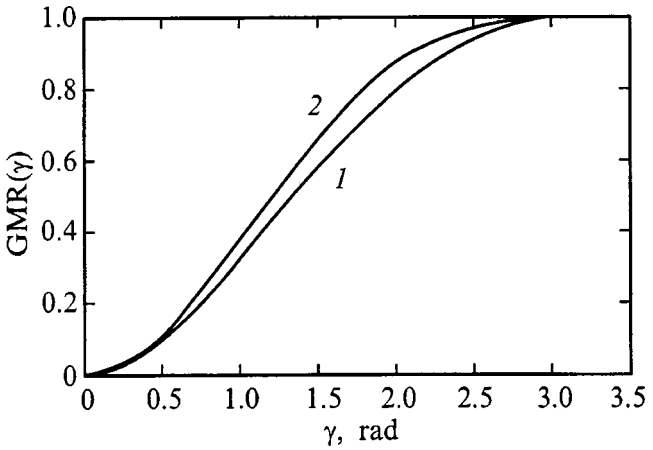

FIG. 2. The same as Fig. 1 for $a=c=39$, $b=11$, $l^{\uparrow}=60$, $l^{\downarrow}=20$, $l=180$; (*1*) $\lambda^{\uparrow}\to\infty$, $\lambda^{\downarrow}\to\infty$; (*2*) $\lambda^{\uparrow}=200$ $\lambda^{\downarrow}=10$.

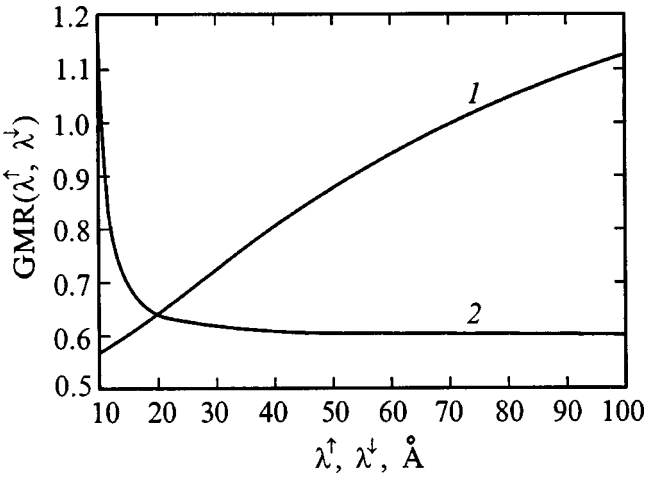

FIG. 3. Dependence of the normalized magnetoresistance on the mean free paths corresponding to scattering at the interfaces: (*1*) $\lambda^{\uparrow}=100$, $\lambda^{\downarrow}=10-100$; (*2*) $\lambda^{\uparrow}=10$, $\lambda^{\downarrow}=10-100$. The angle between the directions of the magnetizations of the ferromagnetic layers is $\gamma=\pi/2$. The parameters are $a=c=23$, $b=11$, $l^{\uparrow}=60$, $l^{\downarrow}=20$, $l=180$. All lengths are given in angstroms.

In the limit without surface scattering, i.e., assuming infinite effective-mean-free paths corresponding to spin-dependent scattering at the interfaces, $\lambda^{\uparrow(\downarrow)}\to\infty$, we find that Eq. (13) coincides with the equation for the angular dependence of the magnetoresistance in Ref. 9. But if the magnetization of the layers is assumed to be strictly collinear ($\gamma=0,\pi$), there is no interference between coherent electron waves with different directions of the spin projection: The term that contains the difference $k^{\uparrow}-k^{\downarrow}$ and is proportional to $\sin^2\gamma$ vanishes. The expression for the magnetoresistance then coincides with the one given in Ref. 13. The results can therefore be regarded as a generalization of the previously published calculations.

To plot graphs, we use the normalized form of the magnetoresistance

$$\mathrm{GMR}=\frac{R(\gamma)-R(\gamma=0)}{R(\gamma=\pi)-R(\gamma=0)} \tag{15}$$

with realistic values of the electron scattering parameters and the Fermi wave vector $k_F^{\uparrow(\downarrow)}$. In particular, we assume that $(k_F^{\uparrow}-k_F^{\downarrow})/(k_F^{\uparrow}+k_F^{\downarrow})=0.1$, as in the experiments reported in Ref. 9. Allowance for interfacial as well as volume scattering introduces a contribution to the angular dependence of the magnetoresistance of the multilayer structure. Specifically, surface scattering can have the effect that the resistance is observed to be a maximum for other than an antiparallel configuration of the magnetizations of adjacent ferromagnetic layers (Fig. 1). This unexpected result could not happen as a consequence of previous calculations and is most likely typical of the CPP geometry only, because the CIP resistance depends linearly on $\cos\gamma$, owing to the absence of interference between electronic states. Naturally, when the thickness of the magnetic layers is increased, the influence of scattering at the interfaces diminishes, volume scattering begins to play an ever-increasing role, and this effect no longer occurs (Fig. 2). The change in the surface scattering parameters for electrons with spins $\uparrow$ and $\downarrow$, the ratio of which can differ from the ratio of the mean free paths of the electrons in the bulk, $(\lambda^{\uparrow}-\lambda^{\downarrow})/(\lambda^{\uparrow}+\lambda^{\downarrow})\neq(l^{\uparrow}-l^{\downarrow})/(l^{\uparrow}+l^{\downarrow})$, also influences the value of the magnetoresistance (Fig. 3).

*)E-mail: pugach@magn.phys.msu.su

[1] M. N. Baibich, J. M. Broto, A. Fert, F. Nguyen Van Dau, and F. Petroff, Phys. Rev. Lett. **61**, 2472 (1988).
[2] R. E. Camley and J. Barnas, Phys. Rev. Lett. **63**, 664 (1989).
[3] P. M. Levy, S. Zhang, and A. Fert, Phys. Rev. Lett. **65**, 1643 (1990).
[4] X.-G. Zhang and W. H. Butler, Phys. Rev. B **51**, 10 085 (1995).
[5] A. Barthelemy, J. Childress, V. Cros, O. Durant, O. Duvail, P. Etienne, A. Fert, J. M. George, R. Loloee, R. Morel, D. N. Mosca, L. G. Pereira, F. Petroff, A. Schuhl, P. A. Schroeder, and L. Steren, Phys. Low-Dimens. Struct. **3**, 17 (1994).
[6] R. Q. Hood and L. M. Falicov, Phys. Rev. B **46**, 8682 (1992).
[7] J. Mathon, M. Villert, and H. Itoh, Phys. Rev. B **52**, R6983 (1995).
[8] A. Vedyaev, B. Dieny, N. Ryzhanova, J. B. Genin, and C. Cowache, Europhys. Lett. **25**, 465 (1994).
[9] A. Vedyayev, N. Ryzhanova, B. Dieny, P. Dauguet, P. Gandit, and J. Chaussy, Phys. Rev. B **55**, 1 (1997).
[10] K. M. Schep, P. J. Kelly, and G. E. W. Bauer, Phys. Rev. Lett. **74**, 586 (1995).
[11] P. Zahn, I. Mertig, M. Richter, and H. Eschrig, Phys. Rev. Lett. **75**, 2996 (1995).
[12] W. H. Butler, X.-G. Zhang, D. M. C. Nicholson, and J. M. MacLaren, Phys. Rev. B **52**, 13 399 (1995).
[13] A. Vedyaev, M. Chshiev, N. Ryzhanova, B. Dieny, C. Cowache, and F. Brouers, J. Magn. Magn. Mater. **172**, 53 (1997).
[14] H. E. Camblong, P. M. Levy, and S. Zhang, Phys. Rev. B **51**, 16 052 (1995).

Translated by James S. Wood