

## Resistivity due to Domain Wall Scattering

Peter M. Levy and Shufeng Zhang

*Physics Department, New York University, 4 Washington Place, New York, New York 10003*

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Domain walls in ferromagnetic metals are known to be a source of resistance since the early experiments on iron whiskers. Recently it has been possible to identify this contribution from data on cobalt and nickel films which display stripe domains in which the current is driven normal to the domain walls. With the same Hamiltonian as used to explain giant magnetoresistance in structures with collinear magnetic alignments we have determined the spin flip, as well as nonflip, scattering present in domain walls. We calculate the resistivity in zero field, i.e., in the presence of striped domains, and at saturation to show the amount of magnetoresistance that is attributable to domain wall scattering. [S0031-9007(97)04820-5]

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Since the early experiments on iron whiskers [1], it was recognized that walls between domains in ferromagnets are a source of electrical resistance in addition to that present in the domains. By applying magnetic fields to saturate magnetization, and thereby erase domains in an otherwise multidomain ferromagnet, the resistance of iron was found to drop significantly. Cabrera and Falicov [2] considered two mechanisms by which the walls produce additional scattering: paramagnetic effects from the reflection of incoming electron waves from the ferromagnetically ordered domains as they enter the twisted spin structure of a wall, and diamagnetic effects “due to the zigzagging character of the electron orbits when going between up and down regions of the magnetization.” In metals with few impurities, such as iron whiskers, the relaxation times are sufficiently long, and Cabrera and Falicov concluded that these diamagnetic effects can account for the observed negative magnetoresistance (MR) [3]. Indeed, both Cabrera and Falicov, and Berger [4], found that the reflection for an electron at the Fermi surface from a 180° wall which is 10 nm thick is negligible; unless the walls are so abrupt to be of monolayer thickness, electron scattering from reflections do not contribute to the electrical resistance.

While the resistivity of iron whiskers at low temperatures (about 4.2 K) is small, of the order of 0.01  $\mu\Omega$  cm, most of the ferromagnetic layers that are used in magnetoresistive elements, e.g., spin valves, have a considerably higher resistivity due to inherent defects such as grain boundaries and roughness at the boundaries of these thin layers. Recently Gregg *et al.* [5] obtained the first direct observation of ferromagnetic domain wall scattering by passing a current that is nominally perpendicular to a striped domain structure in thin films of cobalt (1000 Å). The resistivity of their films was about 10  $\mu\Omega$  cm, so that the diamagnetic effects that are putatively responsible for the negative MR in pure iron whisker cannot be responsible. Also, as the thickness of the walls is estimated to be 15 nm, reflections of impinging electrons with the Fermi wavelength cannot account for the additional resis-

tivity due to domain walls which was estimated to be about 0.52  $\mu\Omega$  cm. Gregg *et al.* [5] propose that scattering of conduction electrons by domain walls is due to a combination of (1) how well the precessional behavior of the carrier spins allows it to track the changing local exchange field direction as it traverses the wall, and (2) the same type of spin dependent scattering due to impurities that gives rise, *inter alia*, to giant magnetoresistance. The ability of an electron spin to track the reorientation of the magnetization in a domain wall is a necessary ingredient for understanding the electron states produced by these walls, however, this mistracking is not a *source* of scattering; and by itself it does not produce resistance. In this Letter we use the same Hamiltonian used to understand the giant MR (GMR) of magnetic multilayers, and show that when the spin dependent scattering due to defects present in the film is evaluated in the wave functions appropriate to the spin structure in a domain wall we can reproduce the additional resistivity observed by Gregg *et al.*

The Hamiltonian used to describe GMR consists of two parts. The spin dependent electronic structure is described by

$$H_0 = -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + J\sigma \cdot \hat{M}(\mathbf{r}), \quad (1)$$

where  $J$  denotes the exchange splitting,  $V(\mathbf{r})$  is the nonmagnetic periodic potential, and the unit vector  $\hat{M}(\mathbf{r})$  points in the direction of the local magnetization. The scattering of electrons is given by

$$V_{\text{scatt}} = \sum_i [v + j\sigma \cdot \hat{M}(\mathbf{r})]\delta(\mathbf{r} - \mathbf{r}_i), \quad (2)$$

where  $\mathbf{r}_i$  is the position of the impurities and  $j$  represents the spin dependence of the scattering. Its origin can be either the band structure, as given by Eq. (1), or the intrinsic spin dependence of the defect-impurity scattering potential. In homogeneous systems, where the magnetization is collinear,  $\hat{M}(\mathbf{r}) = \hat{M}$ , and it is natural to choose this direction for the axis of quantization of spin  $\sigma$ . Alternately, if one prefers another axis, the

Hamiltonian Eq. (1) can be diagonalized by rotating the spin operator  $\sigma$  to be parallel to  $\hat{M}$ ,

$$\Psi(\mathbf{r}) = R_\theta \begin{pmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{pmatrix}, \quad (3)$$

where  $R_\theta \equiv \exp(-i \frac{\theta}{2} \hat{n} \cdot \sigma)$  and  $\hat{n}$  represents the axis about which the magnetization rotates, so that  $\sigma(\theta) \cdot \hat{M} = \sigma_z$  and the rotated Hamiltonian diagonal in spin space is

$$H_\theta \equiv R_\theta^{-1} H_0 R_\theta = -\frac{\hbar^2}{2m} \nabla^2 + V + J \sigma_z. \quad (4)$$

The eigenstates of this Hamiltonian are referred to as the spin dependent band structures of ferromagnetic metals.

When the magnetization is noncollinear, as in a domain wall, its direction varies as a function of distance and the angle of rotation in Eq. (3) is a function of position. As position and momentum are noncommuting variables the rotation operator for spin in a domain wall does not commute with the kinetic energy operator, therefore the spin Hamiltonian, Eq. (1), for a domain wall is not diagonalized by the rotation as in Eq. (4). Rather, we find

$$R_\theta^{-1} \frac{\hbar^2 \nabla^2}{2m} R_\theta = \frac{\hbar^2 \nabla^2}{2m} + V_{\text{pert}}, \quad (5)$$

where

$$\begin{aligned} V_{\text{pert}} &= R_\theta^{-1} [P^2/2m, R_\theta] \\ &= \frac{\hbar^2}{2m} (\sigma \cdot \hat{n}) (\nabla \theta) \cdot p - \frac{i \hbar^2}{4m} (\sigma \cdot \hat{n}) \nabla^2 \theta \\ &\quad + \frac{\hbar^2}{8m} |\nabla \theta|^2. \end{aligned} \quad (6)$$

The additional term generated by the rotation represents corrections to the wave functions due to the twisting of magnetization in domain walls. This term is the stationary representation of the mistracking referred to by Gregg in Ref. [5]. The Hamiltonian for the wall, Eqs. (4) and (5), does not have pure spin eigenstates; therefore the impurity potential, Eq. (2), scatters electrons from one eigenstate to another and thereby mixes the two channels of current that would be independent were it not for this additional term. The application of a field that is large enough to saturate the magnetization erases domains and the walls separating them. It produces a homogeneous sample whose eigenstates [see Eq. (4)] are pure spin states. The impurity potential, Eq. (2), does not scatter between states of different spin so that the spin current channels are independent of one another. As the resistivity of one channel in a ferromagnetic metal is usually lower than the other, the currents in the channels are unequal, and a short circuit exists at saturation. This is

partially removed when domains are present because the scattering in domain walls mixes the currents. This is the origin of the additional resistance due to domain walls.

To estimate the size of this perturbation we consider a  $180^\circ$  wall with the magnetization continuously rotating over a distance  $d$ , i.e.,  $\theta(x) = \pi x/d$  for  $0 < x < d$  and  $\sigma \cdot \hat{n}$  equals  $\sigma_x$  ( $\sigma_y$ ) for a Bloch (Néel) wall. For these walls the second term in Eq. (6) is zero, and the third term represents a constant shift in the potential which will not be relevant to the spin dependent scattering by domain walls. We believe this simplified wall profile captures the essential physics. Other profiles, e.g.,  $\theta(x) = 2 \arctan(x/d)$ , make  $\nabla_x \theta$  position dependent; they do not produce new physics.

Up to the first order in  $V_{\text{pert}}$ , the eigenstates of  $H_0 + V_{\text{pert}}$  are

$$\Psi_\uparrow(\mathbf{k}, \mathbf{r}) = \alpha^{-2}(k_x) \left[ R_\theta \begin{pmatrix} e^{i\mathbf{k}_\uparrow \cdot \mathbf{r}} \\ 0 \end{pmatrix} - \frac{ik_x}{k_F} \xi R_\theta \begin{pmatrix} 0 \\ e^{i\mathbf{k}_\uparrow \cdot \mathbf{r}} \end{pmatrix} \right] \quad (7)$$

and

$$\Psi_\downarrow(\mathbf{k}, \mathbf{r}) = \alpha^{-2}(k_x) \left[ R_\theta \begin{pmatrix} 0 \\ e^{i\mathbf{k}_\downarrow \cdot \mathbf{r}} \end{pmatrix} + \frac{ik_x}{k_F} \xi R_\theta \begin{pmatrix} e^{i\mathbf{k}_\downarrow \cdot \mathbf{r}} \\ 0 \end{pmatrix} \right], \quad (8)$$

where the eigenstate energy is  $\epsilon_{\mathbf{k}\sigma} = \frac{\hbar^2 \mathbf{k}_\sigma^2}{2m} + \sigma J$  ( $\sigma = \pm$  or  $\uparrow\downarrow$ ),  $\xi \equiv \pi \hbar^2 k_F / 4mdJ$ , and the coefficient  $\alpha^2(k_x) = 1 + (\xi k_x / k_F)^2$ . In an adiabatic approximation, in which we retain only the first terms in Eqs. (7) and (8), the spin channels would also be decoupled even in the presence of the domain walls. It is the second terms on the right-hand side of Eqs. (7) and (8) which go beyond such an adiabatic approximation. As we will presently see, the correction term is quite small for the walls we consider, of the order of 0.03 for a  $180^\circ$  wall with a wall thickness of 150 Å, and it is not necessary to consider higher order terms of the perturbation Eq. (6).

To calculate the resistivity of a domain wall we evaluate the spin dependent electron scattering potential, Eq. (2), in states of  $H_0 + V_{\text{pert}}$ , Eqs. (7) and (8), i.e., calculate the matrix elements

$$V_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma'} \equiv \int \Psi_\sigma^+(\mathbf{k}, \mathbf{r}) V_{\text{scatt}} \Psi_{\sigma'}(\mathbf{k}', \mathbf{r}) d^3r. \quad (9)$$

As the walls are thick compared to the Fermi wavelength, we neglect scattering due to reflections of electrons as they go from the collinearly aligned domain into the twisted wall between domains [2,4]. Adopting the Boltzmann transport approach, the nonequilibrium distribution function for each eigenstate of  $H_0 + V_{\text{pert}}$  satisfies the following:

$$-e\mathbf{v}^\sigma \cdot \mathbf{E} \delta(\epsilon_F - \epsilon_{\mathbf{k}\sigma}) = \frac{1}{8\pi^3} \int W_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma'} [f^\sigma(\mathbf{k}) - f^\sigma(\mathbf{k}')] d^3\mathbf{k}' + \frac{1}{8\pi^3} \int W_{\mathbf{k}\mathbf{k}'}^{\sigma-\sigma} [f^\sigma(\mathbf{k}) - f^{-\sigma}(\mathbf{k}')] d^3\mathbf{k}', \quad (10)$$

where the scattering rates  $W$  are given by

$$W_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma'} = \frac{2\pi}{\hbar} |V_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma'}|^2 \delta(\epsilon_{\mathbf{k}\sigma} - \epsilon_{\mathbf{k}'\sigma'}), \quad (11)$$

and the matrix elements of the scattering potential are

$$|V_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma}|^2 = c_i \alpha^2(k_x) \alpha^2(k'_x) \times \left[ (v + \sigma j) + \frac{k_x k'_x}{k_F^2} \xi^2 (v - \sigma j) \right]^2 \quad (12)$$

and

$$|V_{\mathbf{k}\mathbf{k}'}^{\uparrow\downarrow}|^2 = c_i \alpha^2(k_x) \alpha^2(k'_x) [(v + j)k'_x - (v - j)k_x]^2 \times \xi^2 / k_F^2, \quad (13)$$

where  $c_i$  is the impurity concentration. Here the index  $\sigma$  does *not* represent pure spin states; rather it denotes the eigenstates of  $H_0 + V_{\text{pert}}$  in spin space, i.e., the spinors [see Eqs. (7) and (8)].

For current parallel to the domain walls (CIW), reminiscent of the current in the plane of the layer (CIP) geometry for multilayers, there are no “scattering in” terms for the following reason. The distribution function  $f(\mathbf{k})$  can be written as  $f(\mathbf{k}) = f_0(\mathbf{k}) + \mathbf{k} \cdot \mathbf{E}g(\mathbf{k})$  where  $f_0(\mathbf{k})$  is the equilibrium distribution function and  $g(\mathbf{k})$  is an even function of  $\mathbf{k} \cdot \mathbf{E}$ . Since the scattering rates Eqs. (12) and (13) depend on the component of momentum parallel to  $\nabla_x \theta$ , the integration over  $\mathbf{k}'$  for the scattering in terms vanish identically. Thus we obtain a simple solution of the distribution function, [from Eq. (10)],

$$f^\sigma(\mathbf{k}) = f_0(\mathbf{k}) - e v_y^\sigma E \delta(\epsilon_F - \epsilon_{\mathbf{k}\sigma}) \tau^\sigma(\mathbf{k}), \quad (14)$$

where the relaxation time  $\tau^\sigma$  is given by

$$[\tau^\sigma(\mathbf{k})]^{-1} = (1/2\pi)^3 \int d^3k' (W_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma} + W_{\mathbf{k}\mathbf{k}'}^{\uparrow\downarrow}) \quad (15)$$

and the conductivity is  $\sigma_{\text{CIW}} = \sum_\sigma \int e v_y^\sigma f^\sigma(k) d^3k$ . By using Eqs. (11)–(15) and carrying out the integrations over momenta we find, up to second order in  $\xi$  [note that one also needs to expand  $\alpha^2(k_x)$  and  $\alpha^2(k'_x)$  to second order in  $\xi$ ], the CIW resistivity  $\rho_{\text{CIW}} = 1/\sigma_{\text{CIW}}$  of a domain wall is

$$\rho_{\text{CIW}} = \rho_0 \left[ 1 + \frac{\xi^2}{5} \frac{(\rho_0^\uparrow - \rho_0^\downarrow)^2}{\rho_0^\uparrow \rho_0^\downarrow} \right], \quad (16)$$

where  $\rho_0^\delta$  is the resistivity for spin  $s$  of the ferromagnet,  $\rho_0^{-1} = 1/\rho_0^\uparrow + 1/\rho_0^\downarrow$  is the conductivity of the ferromagnet without domain walls, and we have used for simplicity the same Fermi wave vector for spin up and spin down. The first term in Eq. (16) comes from two independent current channels and the second term represents resistance due to the wall, which is inversely proportional to the squares of the wall thickness.

The extra resistivity due to domain walls, i.e., second term in Eq. (16), is dependent on the spin dependence of the resistivity. If the two spin channel resistivities are the same, i.e.,  $\rho_0^\uparrow = \rho_0^\downarrow$ , domain walls do not contribute

additional resistance. This is quite understandable: The role of domain walls is to “mix” two current channels, and thereby partially remove the “short circuit” effect in a perfectly ferromagnetic aligned domain. Without spin dependence of the resistivity to start with, mixing has no effect on the resistivity. The spin orbit coupling in the domains themselves has an analogous effect on the resistivity [6]. Although the spin-orbit coupling energy is very small compared to exchange and Coulomb energies in electronic structure calculations, its effect on the resistivity is significant because the scattering, Eq. (2), mixes the two current channels [6].

To estimate the MR due to walls we choose commonly accepted values of  $k_F = 1 \text{ \AA}^{-1}$ ,  $J = 0.5 \text{ eV}$ , and  $\rho_0^\uparrow/\rho_0^\downarrow = 5-20$  for typical ferromagnetic materials of Co, Fe and Ni. With these parameters, we find the magnetoresistance ratio  $R$ , which is defined as

$$R_{\text{CIW}} \equiv \frac{\rho_{\text{CIW}} - \rho_0}{\rho_0} = \frac{\xi^2}{5} \frac{(\rho_0^\uparrow - \rho_0^\downarrow)^2}{\rho_0^\uparrow \rho_0^\downarrow}, \quad (17)$$

ranges from 0.3% to 1.8% for a wall 150  $\text{\AA}$  thick, which is the estimated thickness for the cobalt films used in Ref. [5].

We now turn to the calculation for currents perpendicular to the domain walls (CPW); this is reminiscent of the current perpendicular to the plane (CPP) of the layer in magnetic multilayers. In this geometry, the scattering in terms in the Boltzmann equation, Eq. (10), do not vanish, and it is necessary to introduce an approximation to solve the integral equation. We take the distribution function in the “scattering in terms” in the form  $f^\sigma(\mathbf{k}) = f_0(\mathbf{k}) + \mathbf{k}'_x \bar{g}^\sigma$  ( $\bar{f}^\sigma$  denotes the angular average over the momentum variable), so that the scattering in terms become

$$-\frac{V}{8\pi^3} \int W_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma} f^\sigma(\mathbf{k}') d^3\mathbf{k}' - \frac{V}{8\pi^3} \int W_{\mathbf{k}\mathbf{k}'}^{\sigma-\sigma} f^{-\sigma}(\mathbf{k}') d^3\mathbf{k}' = \frac{f^{-\sigma}(\mathbf{k}) - f^\sigma(\mathbf{k})}{\tau_0}, \quad (18)$$

where the “spin mixing” relaxation time is defined as

$$1/\tau_0 = \frac{2mc_i}{3\pi\hbar^2} (v^2 - j^2) \xi^2. \quad (19)$$

By placing this into the Boltzmann equation, Eq. (10), and by some algebraic manipulations, we find that the resistivity for CPW is

$$\rho_{\text{CPW}} = \rho_0 \left[ 1 + \frac{\xi^2}{5} \frac{(\rho_0^\uparrow - \rho_0^\downarrow)^2}{\rho_0^\uparrow \rho_0^\downarrow} \left( 3 + \frac{10\sqrt{\rho_0^\uparrow \rho_0^\downarrow}}{\rho_0^\uparrow + \rho_0^\downarrow} \right) \right]. \quad (20)$$

By comparing with the resistivity of CIW, we find that the ratio of CPW and CIW magnetoresistance due to domain wall scattering is

$$R_{\text{CPW}}/R_{\text{CIW}} = 3 + \frac{10\sqrt{\rho_0^\uparrow\rho_0^\downarrow}}{\rho_0^\uparrow + \rho_0^\downarrow}. \quad (21)$$

To compare our results with experimental data for cobalt, we choose the same parameters as before, i.e.,  $k_F = 1 \text{ \AA}^{-1}$ ,  $J = 0.5 \text{ eV}$  and  $\rho_0^\uparrow/\rho_0^\downarrow$  in the range of 5–20; this range of values hold is for a variety of impurities and at room temperature as well as for low temperatures, because for cobalt the contributions from phonon and magnon scattering produces spin dependent scattering as the electron density of states at the Fermi level depends on the spin direction [7]. We find that the CPW magnetoresistance is between 2% and 11%, which is consistent with the 5% found by Gregg [5] for cobalt at room temperature. For nickel, the values for  $\rho_0^\uparrow/\rho_0^\downarrow$  at low temperatures can be as large as for cobalt; however at room temperature they are smaller because the temperature dependent spin scattering is weaker in nickel [8]. In iron the temperature dependent scattering seems to be independent of spin [8], so that, even though there is some spin dependent scattering due to impurities at low temperatures of the order of  $\rho_0^\uparrow/\rho_0^\downarrow = 1/11$  to 3, at room temperature this ratio may be not far from 1. In this case, contributions to the resistivity from scattering in domain walls in iron will be considerably smaller at room temperature than at low temperatures [4.2 K].

In summary, we have taken into account the admixture of spin states due to the noncollinearity of the magnetization in domain walls; we find that impurities scatter electrons between eigenstates and thereby mix heretofore independent channels of current. We calculated the resistivity for currents parallel and perpendicular to the walls and find we are able to reproduce the additional resistance due to domain walls found in recent experiments on cobalt films. The inability of an electron spin to track the reorientation of magnetization in a domain wall, epitomized by the ratio  $\xi$  introduced in Ref. [5], shows up in our Eqs. (7) and (8) as admixing states with opposite spins. It is not a

source of scattering or resistance; rather the impurity scattering, Eq. (2), produces the resistance.

*Note added*—Since completion of this work, Tatara and Fukuyama [9] have published a study in which they focus on quantum transport in magnetic wires, where it is found that the effect of domain walls is to *reduce* resistivity [10]. In particular, they stress that a magnetic field removes domain walls that break the weak localization that is otherwise present when the wire is uniformly magnetized. In our study we are interested in explaining the observed *increase* of resistivity in thin magnetic films due to domain walls that comes from the spin dependence of the scattering from impurities; this effect was not considered in Ref. [9].

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