

## Ballistic electron transport through magnetic domain walls

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(Received 2 October 1998)

Electron transport limited by the rotating exchange potential of domain walls is calculated in the ballistic limit for the itinerant ferromagnets Fe, Co, and Ni. When realistic band structures are used, the domain-wall magnetoresistance is enhanced by orders of magnitude compared to the results for previously studied two-band models. Increasing the pitch of a domain wall by confinement in a nanostructured point contact is predicted to give rise to a strongly enhanced magnetoresistance. [S0163-1829(99)02302-4]

The application potential of magnetoresistive effects has rekindled interest in the study of electrical transport in metallic (Stoner) ferromagnets such as Fe, Co, and Ni. One complicating factor that is still an open problem is the influence on the transport properties of the magnetic domain structure. Domain walls (DW's) result from minimizing the sum of the magnetostatic, magnetic anisotropy, and exchange energies and they can be driven out of a material by applying a magnetic field. This modifies the transport properties but the magnitude and even the sign of the magnetoresistance (MR) [ $(R_{\text{sat}} - R_0)/R_0 = [G_0 - G_{\text{sat}}]/G_{\text{sat}}$  (where  $R_0 = 1/G_0$  and  $R_{\text{sat}} = 1/G_{\text{sat}}$  are the zero-field and saturation-field resistances, respectively)] remain a matter of controversy.

Early experimental studies on very pure iron samples showed a large MR of up to 90% at low temperatures<sup>1</sup> that was attributed to percolation through numerous domains.<sup>2</sup> Using a free-electron model, Cabrera and Falicov<sup>3</sup> interpreted transport through a single DW as a tunneling process and the corresponding MR was found to be exponentially small. More recently, Tataru and Fukuyama<sup>4</sup> calculated the DW conductivity in the clean limit where the mean free path  $l$  resulting from defect scattering is much larger than the wall width  $\lambda_{DW}$ . For a free-electron model in a semiclassical approximation they found an MR that scales like  $-n_{DW}/(\lambda_{DW}\bar{k}_F^2)$ , where  $n_{DW}$  is the domain-wall density and  $E_F \equiv \hbar^2\bar{k}_F^2/2m$  is the Fermi energy. This MR is also very small for DW widths and Fermi energies of transition metals. In room-temperature measurements of transport through Ni and Co films exhibiting stripe domain structures, Gregg *et al.*<sup>5</sup> measured significant negative MR's, much larger than predicted by any of the above theoretical work (but in a regime where  $l \leq \lambda_{DW}$ ). Levy and Zhang<sup>6</sup> subsequently pointed out that spin-dependent impurity scattering

can strongly enhance the (negative) DW MR. Breaking of the weak localization quantum correction by the exchange field leads to a positive MR at low temperature<sup>4</sup>. Otani *et al.*<sup>7</sup> and Ruediger and co-workers<sup>8</sup> measured a positive DW MR in thin magnetic wires, but up to high temperatures.

In the spirit of previous work on the giant magnetoresistance of magnetic multilayers<sup>9</sup> we study DW scattering in the ballistic limit, i.e., in the limit where the defect scattering mean free path  $l$  is sufficiently larger than the system size.<sup>10</sup> These results are appropriate for clean point contacts with diameters  $d$  sufficiently smaller than  $l$ . We disregard lateral quantization, assuming  $d \gg \lambda_F$ , with  $\lambda_F$  the Fermi wavelength. For perpendicular transport in multilayers, the ballistic MR is of the same order of magnitude as the MR in diffuse systems.<sup>9,11</sup> When  $l \gg \lambda_{DW}$ , our calculated transport coefficients can be used as boundary conditions in the semiclassical Boltzmann equations.<sup>12</sup>

The conductance  $G$  is given by Landauer's formula as

$$G = \frac{e^2}{h} \sum_{\mathbf{k}_{\parallel}} \sum_{\nu\mu} |t_{\nu\mu}(\mathbf{k}_{\parallel})|^2, \quad (1)$$

where  $\mathbf{k}_{\parallel}$  is the conserved Bloch vector parallel to the DW. The transmission amplitude of an incoming state  $\mathbf{k}_{\parallel}\mu$  to an outgoing state  $\mathbf{k}_{\parallel}\nu$  through the DW sandwiched by the two bounding domains of the ferromagnet is denoted by  $t_{\nu\mu}(\mathbf{k}_{\parallel})$ ,  $\mathbf{k}_{\parallel}\mu$ , and  $\mathbf{k}_{\parallel}\nu$  labeling flux-normalized states at the Fermi energy to the left and right of the DW, respectively, including the spin labels.

A constant modulus for the local magnetization vector is assumed; its direction may be represented by a single rotation angle  $\theta$  since we disregard the spin-orbit interaction.  $\theta$  varies along the  $z$  direction but is constant in the  $x, y$  directions. The exchange field of the DW can be diagonalized by

a local gauge transformation at the cost of an additional spin-rotation energy. Instead of treating this term by perturbation theory<sup>4,6</sup> we employ here the WKB approximation, which has the important advantage of being valid also for vanishing exchange splittings.

In order to understand the basic physics, let us first consider a simple two-band model in which the plane-wave states with parallel wave vector  $\mathbf{k}_{\parallel}$  and energy  $E_{\uparrow,\downarrow} = \hbar^2 k^2/2m \pm \Delta$  are modified by the domain wall. In the WKB method the spinor wave functions are multiplied by  $z$ -dependent phase factors  $\exp\{i\int^z dz' \sqrt{2mE_{\pm}[q(z')]/\hbar^2 - k_{\parallel}^2}\}$ . The eigenenergies of the local Hamiltonian in which the gradient  $q(z) = \partial\theta/\partial z$  is taken to be constant are those of a ‘‘spin spiral’’.<sup>13</sup>

$$E_{\pm}(q) = \frac{\hbar^2}{2m} [k^2 + q^2/4 \pm \sqrt{k_z^2 q^2 + p^4}], \quad (2)$$

with  $\Delta = \hbar^2 p^2/2m$  and  $k_z$  determined by  $E_{\pm}(q) = E_F$ . The WKB factor is imaginary for states propagating through the whole DW and exponentially damped otherwise. In our adiabatic approximation we disregard all tunneling states, which is allowed in the limit  $\lambda_{DW} k_F \gg 1$ . The eigenstates are not pure spin states: the DW/spin spiral system acts like a spin-orbit scatterer to mix the two spin directions. The DW conductance is thus limited by the local band structure with the smallest number of modes at the Fermi energy that is at the center of the DW, where  $q$  is maximal,  $q_{\max} = \pi/\lambda_{DW}$ . For perpendicular transport<sup>14</sup>

$$G(q) = \frac{e^2}{h} \frac{A}{2\pi} \begin{cases} \bar{k}_F^2 - q^2/4 & \text{for } q^2 \leq 2p^2 \\ \bar{k}_F^2 - p^2 + p^4/q^2 & \text{for } q^2 > 2p^2. \end{cases} \quad (3)$$

This equation holds when  $\bar{k}_F^2 > q^2/4 + p^2$ , i.e., when both spin bands are occupied. Note that transport parallel to the spin spiral is much less affected by the DW:  $G_{\parallel}(q) = G(0) + O(q^4)$ .

In bulk transition metals in which  $q^2 \ll p^2$ , the DW MR becomes  $[G(q_{\max}) - G(0)]/G(0) = (\pi/2\lambda_{DW}\bar{k}_F)^2$  for DW's independent of the exchange splitting. Using Eq. (3), the Fermi wave vectors for one conduction electron per atom, and the experimental width of the DW, we obtain the numbers in Table I for Ni, Co, and Fe. The effect appears to be very small and likely to be swamped by other magnetoresistive effects such as the anisotropic or ordinary MR. The reason is clearly the smallness of the kinetic spin rotation energy as compared to the exchange splitting, i.e.,  $q^2 \ll p^2$ . The DW only slightly deforms the Fermi spheres, resulting in a tiny magnetoconductance. In transition metals, however, many bands at the Fermi energy are much closer than the exchange splitting. When spin-up and spin-down states close to the Fermi energy are (nearly) degenerate, a DW that gives rise to a repulsive interaction between them may push the bands away from the Fermi energy and reduce the conductance. Realistic band structures must be used in order to evaluate the importance of these splittings. To this end we carried out first-principles calculations of defect-free DW's in Ni(fcc), Co(fcc), and Fe(bcc) within the local spin-density approximation (LSDA) to density-functional theory (DFT).

TABLE I. Parameters for Fe, Ni, and Co, calculated saturation (single-domain) conductances, and magnetoresistances (MR) as defined in the text. DW thicknesses are taken from Ref. 24.

Property	Fe	Ni	Co
Crystal structure	bcc	fcc	fcc
Layer direction	(100)	(100)	(111)
$G_{sat}[10^{15} \Omega^{-1} \text{m}^{-2}]$	1.531	1.923	1.529
DW thickness $\lambda_{DW}$			
(in nm)	40	100	15
(in monolayers)	276	570	72
Spiral angle/monolayer	0.65°	0.32°	2.5°
DW-MR			
two-band model	-0.0008%	-0.0001%	-0.008%
Adiabatic model	-0.13%	-0.11%	-0.33%
Linear model	-0.39%	-0.16%	-0.46%
Abrupt DW	-71%	-58%	-67%

The open character of the leads can be captured by the embedding Green's function technique<sup>16-18</sup> based on the linearized augmented plane-wave (LAPW) method and the muffin-tin-shape approximation for the crystal potential. The transport coefficients and the conductance of samples with arbitrary stacking of atomic monolayers with noncollinear spins can be calculated with this method. The technical details of the method are given in Refs. 17 and 18.

In the adiabatic limit the DW may be represented by a spin spiral, which can be computed using conventional band-structure techniques by the generalized Bloch theorem based on a combined translation and spin-rotation operator.<sup>15</sup> For narrow DW's a ‘‘linear’’ model is more accurate, in which we calculate the transmission (numerically) exactly for a magnetization that is rotated by a constant rate  $q_{\max}$  in a *finite* region of width  $\lambda_{DW}$  between single domain leads.<sup>18</sup>

The results are summarized in Table I for the two models just considered for (i) experimental bulk DW widths and (ii) for DW's of monolayer width, both for a total spin rotation  $\pi$ . Note the large difference between the first-principles calculations and the two-band model. Figure 1 displays the width-dependent DW conductance as a function of the magnetization rotation angle per monolayer for Fe and Ni, respectively. We observe a *linear dependence*,  $\text{MR} \sim -q_{\max}$ , in clear contradiction of the two-band model [Eq. (3)].

We can understand these features using perturbation theory. The spin spiral can be represented by an interaction Hamiltonian that contains two operators  $H_{\text{int}}^{(1)} \sim q$  and  $H_{\text{int}}^{(2)} \sim q^2$ , respectively.<sup>4</sup> The energy-band structure of the bulk ferromagnet and thus the conductance is modified by this interaction. In nondegenerate perturbation theory the first-order term corresponding to  $H_{\text{int}}^{(1)}$  vanishes. The second-order term due to  $H_{\text{int}}^{(1)}$  and first-order term due to  $H_{\text{int}}^{(2)}$  both contribute to the order of  $q^2$ , which explains the leading term in Eq. (3). However, in the presence of degeneracies simple perturbation theory breaks down. Instead, the Hamiltonian must be diagonalized first in the subspace of (nearly) degenerate states. The splitting of the degenerate states is directly

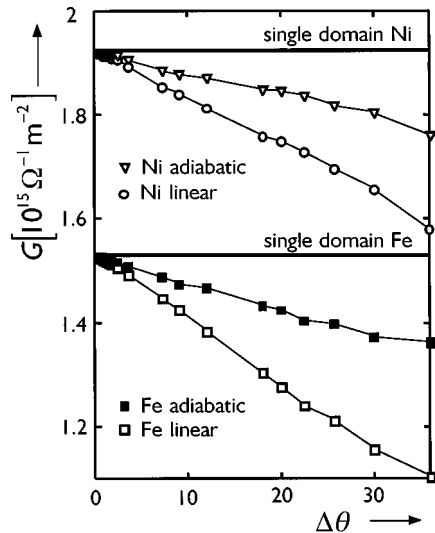


FIG. 1. Conductance of domain walls in Ni and Fe as a function of the magnetization rotation angle per monolayer,  $\Delta\theta = \pi a / \lambda_{DW}$ , where  $a$  is the monolayer width and  $\lambda_{DW}$  the width of the domain wall. Results are given for the adiabatic approximation (spin spiral) and the linear approximation (see text). The bulk ballistic conductances are indicated by the horizontal lines.

proportional to the matrix elements of the interaction Hamiltonian, thus in leading order proportional to  $q$ . As the energy splittings increase, conducting channels are removed from the Fermi surface and the conductance is reduced proportionally. The linear dependence observed in Fig. 2 can thus be explained by the occurrence of many (nearly) spin-degenerate states close to the Fermi energy. Naturally, the MR is also much larger for closely spaced states that are not strictly degenerate. This explains the large difference between the results for the two-band model and the full-band structures in Table I.

We observe that the relative effect of the DW is still rather small, smaller than the experiments by Gregg *et al.*<sup>5</sup> and smaller than the theoretical results by Levy and Zhang for very spin-asymmetric bulk defect scattering.<sup>6</sup> Bloch DW's in thin films can be significantly narrower than in bulk material,<sup>19</sup> which means that the bulk DW magnetoresistance

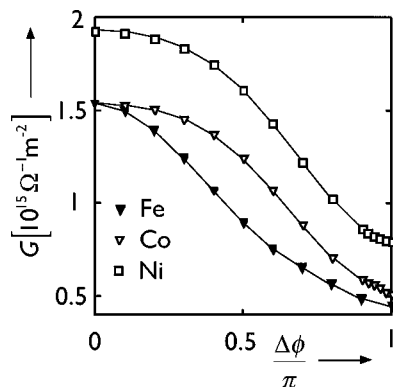


FIG. 2. Conductances of abrupt domain walls in Ni, Fe, and Co as a function of the angle  $\Delta\phi$  between the magnetization vectors of the bounding domains.

should be larger in thin films than the bulk values in Table I, but still smaller than in Refs. 5 and 6. The present calculations show unambiguously that the DW's *increase* the resistance. The experimentally observed DW-induced decrease of the resistance<sup>7,8</sup> can therefore not be an intrinsic effect, but must be an as yet unidentified defect-related, size-related, or other extrinsic phenomenon. Previous results obtained by perturbation theory and a two-band model<sup>4,6</sup> should be reconsidered in the light of the present findings. Unfortunately, implementing degenerate perturbation theory for diffuse systems<sup>4</sup> with realistic band structures appears to be quite cumbersome.<sup>20</sup> In the recent work of Levy and Zhang<sup>6</sup> the DW scattering is calculated on the basis of a two-band model. In spite of the small forward spin-flip scattering in this model they can explain a significant MR due to a strongly spin-dependent bulk-defect scattering. The band structure crowding at the Fermi surface enhances not only the backward scattering that causes the ballistic MR discussed here, but also the forward scattering. The bulk defects might therefore be less important than initially apparent.

The DW scattering increases with  $q = \partial\theta / \partial z$ , which can be achieved by reducing the DW width or by increasing the winding number for a given width. Both operations become possible by trapping a DW in a nanostructured ferromagnetic point contact. Ballistic point contacts have been fabricated successfully in simple metals,<sup>21,22</sup> but not yet in ferromagnetic materials.<sup>23</sup> When the magnetization on one side of the contact is pinned by shape anisotropy or exchange biasing, the magnetization vector on the other side can be rotated independently by rotating the sample in an external magnetic field. The maximal effect is expected for an abrupt domain wall, for which we predict a huge MR (see Table I), much larger than what has been achieved with tunnel junctions of the same materials. The material dependence on the angle between the two magnetizations (Fig. 2) betrays again the importance of the details of the band structure. In a similar fashion an  $n\pi$  DW could be created by repeated rotation in the magnetic field. The conductance is then predicted to decrease linearly with the number of turns as in Fig. 1, up to some value at which phase slips occur, or the spiraling magnetization spills out of the constriction. We stress that this somewhat naive picture needs to be supported by micromagnetic calculations.<sup>23</sup>

In conclusion, we presented and analyzed model and first-principles calculations of electron transport through magnetic domain walls. The large number of bands close to the Fermi surface causes a strong enhancement of the DW MR as compared to two-band calculations. Evidence that degeneracies at the Fermi surface of Fe, Co, and Ni can give rise to relatively large effects is found. DW's always decrease the ballistic conductance, causing a negative MR. The ballistic DW magnetoresistance is found to be somewhat smaller than measured recently in thin films, which can be partly due to the reduction of domain-wall widths in thin films as compared to bulk ferromagnets. Trapping a domain wall in nanostructured constrictions is predicted to give rise to a strongly enhanced magnetoresistance.

We acknowledge helpful discussions with Jaap Caro, Ramon van Gorkom, Junichiro Inoue, Andrew Kent, and Gen

Tatara. This work is supported by the ‘‘Stichting voor Fundamenteel Onderzoek der Materie’’ (FOM), and the ‘‘Nederlandse Organisatie voor Wetenschappelijk Onderzoek’’ (NWO). We acknowledge benefits from the TMR Research

Network on ‘‘Interface Magnetism’’ under Contract No. FMRX-CT96-0089 (DG12-MIHT). G.E.W.B. would like to thank Seigo Tarucha and his group members for their hospitality at the NTT Basic Research Laboratories.

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