Domain Wall Scattering Explains 300% Ballistic Magnetoconductance of Nanocontacts

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We present theory and experiments in good agreement for ballistic magnetoresistance in nanoscopic-size contacts in 3*d* metals (Ni and Co). It is found that values of the ballistic magnetoconductance of ~300% at room temperature can be explained by scattering by the domain wall which is trapped in the constriction region. These values are obtained for very small contacts and they decrease very fast as the contact size increases. The theory also explains this behavior.

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Because of many possibilities of application to devices, a large magnetoresistance effect has been searched for during the past several decades. In particular, a breakthrough came with the discovery of the giant magnetoresistance (GMR) in magnetic multilayers [1,2] and also in heterogeneous AgCo and CuCo granular alloys [3,4]. There have also been studies of magnetoresistance (MR) in very thin Ni wires of 30 nm diameter with values of MR of 8% (much smaller than those of GMR) at 1–10 K and 2 kOe applied field [5]. Work describing the interaction mechanism of domain wall with current has been developed [6]. Very recently there have been measurements of ballistic magnetoresistance (BMR) in nanometer-size Ni contacts reporting values of up to 300% BMR at room temperature (RT) and 100 Oe applied field [7]. It has also been observed that the value of the BMR decreases very fast as the size of the contact increases to a few hundred atoms; see Fig. 1.

Earlier work by Cabrera and Falicov [8] showed that the effect is negligibly small in bulk materials where the domain wall width (DWW) is much larger than the Fermi wavelength (λ_F). Analogous results were obtained by Tatara and Fukuyama [9]. The reason for that is that if the DWW is much larger than λ_F the electron spin can then accommodate itself adiabatically from one side of the domain wall to the other, or in other words the reflection of the electron at the wall is negligible, resulting in a very small MR. However, this is no longer true if the contact size becomes nanometer scale, showing quantized conductance in units of $2e^2/h$ [10], where e and h are the electron charge and the Planck constant, respectively. The DWW may then be very thin, of the order of the contact size, and the BMR should be very large even at RT because, in this case, adiabaticity does not hold. This has indeed been indicated in the calculation in the limit of a vanishing domain wall width [8,11].

In this paper a theoretical study of the BMR, based on a linear response theory and experimental results for Ni and Co contacts of nanoscale at RT and under 120 Oe applied field, is presented.

In order to proceed, the resistivity is calculated based on the exchange interaction (J) between the local spin S and the electron spin. Considering a narrow wire,

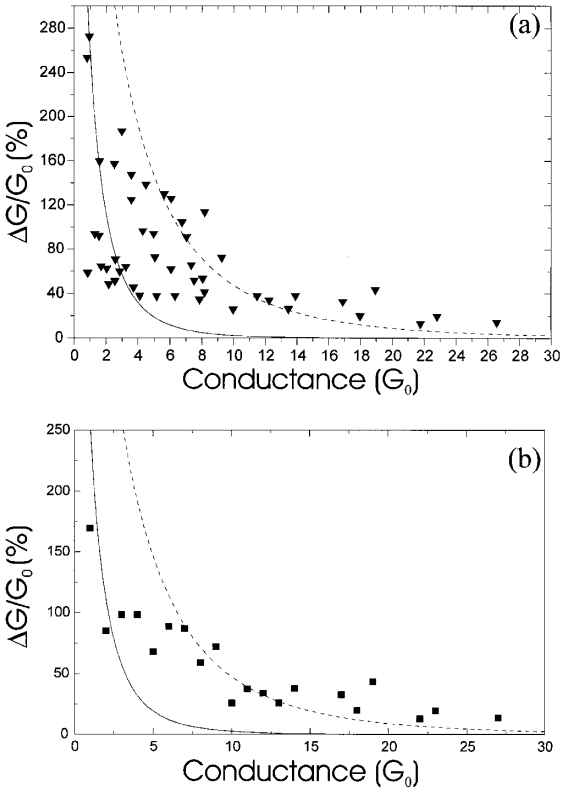

FIG. 1. (a) Experimental values of ballistic magnetoconductance as a function of the nanocontact conductance for Ni (triangles). The conductance is expressed in units of $G_0 = (e^2/h)N$. The solid and dashed lines are the calculations with the theory developed here for the parameter values $\beta = 13$ and 40, respectively. Notice that for large G the magnetoconductance is practically constant, in agreement with theory (see text). (b) The same as in (a) but for the average experimental data.

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the system is treated as one dimensional. The Hamiltonian is

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} - J \int dx\, \mathbf{S}(x)\,(c^\dagger \boldsymbol{\sigma} c)\,, \qquad (1)$$

where $\epsilon_k \equiv \hbar^2 k^2/2m - \epsilon_F$ (ϵ_F being the Fermi energy). The spin index is denoted by $\sigma = \pm$ and $\boldsymbol{\sigma}$ is the Pauli matrix (spin indices are suppressed in the second term). Here, the local spin $\mathbf{S}$ has the spatial dependence of a domain wall. In terms of a polar coordinate ($S_Z \equiv S\cos\theta$) the wall is represented in the bulk case as $\cos\theta = \tanh(x/\lambda)$, λ being the thickness of the wall. Correctly speaking this expression is rigorous in the bulk case, where the wall is determined by the exchange and uniaxial anisotropy energy. Here we use this expression to describe the wall in nanocontact. What is essential is that λ, being determined by the geometry of the contact, is of the size of the contact, as will be discussed later. To calculate the resistivity based on this Hamiltonian, it is convenient to carry out a local gauge transformation in the electron spin space so that the Z axis is chosen to be along the local direction of spin $\vec{S}$ [9]. The transformation is written as

$$a_\sigma = \sigma \cos\frac{\theta}{2}\, c_\sigma - i \sin\frac{\theta}{2}\, c_{-\sigma}\,, \qquad (2)$$

where the electron in the new frame is denoted by a_σ. The Hamiltonian is modified to be

$$H = \sum_{k\sigma} \epsilon_{k\sigma} a^\dagger_{k\sigma} a_{k\sigma} + H_{\rm int}\,, \qquad (3)$$

where

$$\epsilon_{k\sigma} \equiv \epsilon_k - \sigma\Delta \qquad (4)$$

is the energy of the uniformly polarized electron with the exchange splitting $\Delta \equiv J|\mathbf{S}|$. The term $H_{\rm int}$ describes the interaction between the electron and the wall [12]

$$H_{\rm int} \equiv \frac{\hbar^2}{2m}\frac{1}{L}\sum_{kq}\Big[-\Big(k + \frac{q}{2}\Big)A_q a^\dagger_{k+q}\sigma_x a_k + \frac{1}{4L}\sum_p A_p A_{-p+q} a^\dagger_{k+q} a_k\Big], \qquad (5)$$

where

$$A_q \equiv \int dx\, e^{-iqx}\nabla\theta = \pi\,\frac{1}{\cosh(\pi q\lambda/2)}\,, \qquad (6)$$

is a domain-wall form factor which plays the role of a classical gauge field. Because of the gauge transformation, the electronic current is also modified to be

$$J = \frac{e\hbar}{m}\sum_k\Big(k a^\dagger_k a_k - \frac{1}{2}\frac{1}{L}\sum_q A_q a^\dagger_{k+q}\sigma_x a_k\Big). \qquad (7)$$

The resistivity calculation is based on the linear response theory. In the ballistic case we consider, it is convenient to use the Mori formula, which relates the resistivity to the correlation of random forces in the case of weak scattering as [13]

$$\rho_w = \Big(\frac{e^2 n}{m}\Big)^{-2} \lim_{\omega\to 0}\frac{1}{\hbar\omega}\,{\rm Im}[\chi_{\dot J\dot J}(\hbar\omega) - \chi_{\dot J\dot J}(0)]. \qquad (8)$$

Here $\chi_{\dot J\dot J}(i\omega_\ell) \equiv -(\hbar/V)\langle \dot J(i\omega_\ell)\dot J(-i\omega_\ell)\rangle$, where $\dot J \equiv dJ/dt = \frac{i}{\hbar}[H, J]$, n is the electron density, $V = L$ is the system volume. This function $\chi_{\dot J\dot J}(i\omega_\ell)$ is defined in the imaginary time, with $\omega_\ell \equiv 2\pi\ell/\beta$ being a bosonic Matsubara frequency [$\beta \equiv 1/(k_B T)$]. The function $\chi_{\dot J\dot J}(\hbar\omega)$ which appears in Eq. (8) is an analytical continuation of the correlation function for imaginary time, i.e., $\chi_{\dot J\dot J}(\hbar\omega) \equiv \chi_{\dot J\dot J}(i\omega_\ell \to \hbar\omega + i0)$, where $i0$ denotes an infinitesimally small positive imaginary part. The nonconservation of the current (i.e., finite $\dot J$) arises from the scattering by the wall, which is calculated from Eqs. (5) and (7) as

$$\dot J = -i\Big(\frac{e}{m}\Big)\Delta\,\frac{1}{L}\sum_{kq\sigma}\sigma A_q a^\dagger_{k+q,-\sigma} a_{k,\sigma}\,. \qquad (9)$$

The imaginary-time correlation function is then calculated as

$$\chi_{\dot J\dot J}(i\omega_\ell) = -\frac{\hbar}{L^3}\Big(\frac{e\Delta}{m}\Big)^2 \times \sum_{kq\sigma}|A_q|^2\,\frac{1}{\beta}\sum_n G_{k+q,n+\ell,-\sigma} G_{kn\sigma}\,, \qquad (10)$$

where $G_{kn\sigma} \equiv [i\omega_n - \epsilon_{k\sigma}]^{-1}$ is the electron Green function, with $\omega_n \equiv (2n-1)\pi/\beta$ being a fermionic Matsubara frequency. After summing over ω_n, the imaginary part of the analytical continuation is calculated in the limit of $\omega \to 0$ as

$${\rm Im}\chi_{\dot J\dot J}(\hbar\omega + i0)|_{\omega\to 0} = \pi\hbar\omega\,\frac{\hbar}{L^3}\Big(\frac{e\Delta}{m}\Big)^2\sum_{kq\sigma}|A_q|^2\delta(\epsilon_{k,\sigma})\delta(\epsilon_{k+q,-\sigma} - \epsilon_{k,\sigma})\,, \qquad (11)$$

which leads to the resistivity

$$\rho_w = \pi\hbar\Big(\frac{\Delta}{en}\Big)^2\frac{1}{L^3}\sum_{kq\sigma}|A_q|^2\delta(\epsilon_{k+q,-\sigma} - \epsilon_{k,\sigma})\delta(\epsilon_{k,\sigma}) = \frac{\pi}{\hbar^3 L}\Big(\frac{m\Delta}{en}\Big)^2\frac{1}{k_{F\uparrow}k_{F\downarrow}}\Big[\frac{1}{\cosh^2\pi(k_{F\uparrow} + k_{F\downarrow})\lambda/2} + \frac{1}{\cosh^2\pi(k_{F\uparrow} - k_{F\downarrow})\lambda/2}\Big]. \qquad (12)$$

The resistance due to the wall, which is given by $R_W \equiv L\rho_W/N$ (N being the number of the channels in the cross sectional area) is therefore obtained as

$$R_W = \frac{h}{e^2}\frac{1}{N}\frac{\pi^2}{4}\frac{\zeta^2}{1-\zeta^2}F(\zeta,\lambda), \tag{13}$$

where the function $F(\zeta,\lambda)$ is

$$F(\zeta,\lambda) \equiv \frac{1}{2}\left[\frac{1}{\cosh^2\pi k_F\lambda} + \frac{1}{\cosh^2\pi k_F\zeta\lambda}\right], \tag{14}$$

and $\zeta \equiv (k_{F\uparrow} - k_{F\downarrow})/(k_{F\uparrow} + k_{F\downarrow})$, $k_F \equiv (k_{F\uparrow} + k_{F\downarrow})/2$. We can show that this result (13) is also derived by use of the Landauer formula [14], which assumes the linear response and locality of conductance and has been known to describe the transport in (nonmagnetic) nanocontacts quite well.

In the absence of the wall the conductance is determined by the number of channels through the contact, N, as $G_0 = (e^2/h)N$. Since the two resistance $G_0^{-1}$and R_W are from different origins, the total resistance in the presence of the wall is written as $R \equiv G_0^{-1} + R_W$. Thus the magnetoconductance, defined as the relative change of conductance when a domain wall is introduced, i.e., $\Delta G/G \equiv (G_0 - G)/G$, $(G \equiv R^{-1})$, is obtained as

$$\frac{\Delta G}{G} = \frac{\pi^2}{4}\frac{\zeta^2}{1-\zeta^2}F(\zeta,\lambda). \tag{15}$$

Because of the function F, the magnetoconductance decays very rapidly for $k_{F\sigma}\lambda \gtrsim 1$, which indicates that the electron can adiabatically follow the magnetization change inside the wall. It should be noted that in the limit of a single band spin, i.e., $\zeta \to 1$, the magnetoconductance goes to infinity, corresponding to total reflection.

Calculation so far is applicable to both s and d electrons. The feature of the band is taken into account in parameters ζ, k_F (and β below). We assume that, in the case of ballistic nanocontact, the d band carries the most current, due to a much larger density of states at the Fermi level as compared with the s band. In fact, the ratio of the density of states of d and s electrons, obtained from the band structure calculations [15], is given by $\beta \equiv D_{\rm tot}/D_s = 13$ and 11 for Ni and Co, respectively. The splitting ζ is related to the density of states of the d band as $\zeta = (D_\uparrow - D_\downarrow)/(D_\uparrow + D_\downarrow)$. The number of channels N is written by use of Sharvin's formula [16] as $N = \beta(k_F a)^2/4$, where a is the radius of the contact and the parameter β takes into account the large density of states of the d band. It should be noticed that $N = 1$ may correspond to a section of 1–3 atoms.

In nanocontacts the width of the wall is smaller than that of the bulk system. This fact leads to the enhancement of MR in nanocontacts. The profile of the wall is determined by the geometry of the constriction and the wall width becomes comparable to the length d of the narrowest part of the constriction, where the cross section of the contact varies rapidly, $2\lambda \sim d$. Therefore it would be natural to assume $2a \sim d$ in the contact. From these considerations the essential parameter in ΔG, λ, is related to N as

$$k_F\lambda \simeq k_F a \simeq \sqrt{\frac{4N}{\beta}}. \tag{16}$$

Thus the magnetoconductance (15) as a function of N (or G) is large at small N if ζ is close to 1 but decreases rapidly for $N \gtrsim \beta/4$. So far we have not described the mechanism that makes the domain wall shift, but probably mechanisms such as those due to point singularities [17] may account for the reversal of magnetization in our experiments.

The BMR experiments have been performed recently for Ni [7] at room temperature and at a maximum applied field of 120 Oe, showing MR values of up to 300% and also showing that the MR drops very fast with increasing conductance (or cross section) of the nanocontact (see Ref. [7] for experimental details). Using the same technique, we have also measured Co nanocontacts. The results are presented in Figs. 1 and 2.

Using the previous theory, we have calculated the BMR values for the values $\zeta = 0.87$ and 0.83 corresponding

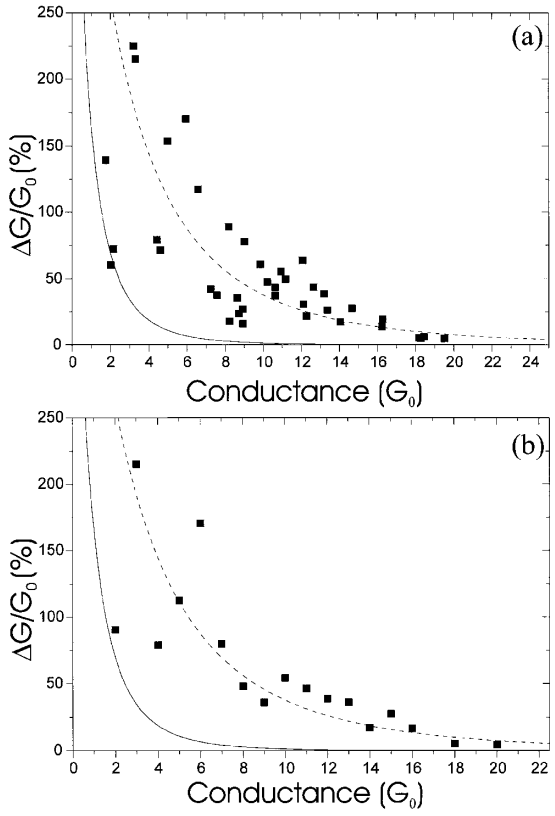

FIG. 2. The same as in Fig. 1 but for Co and the values $\beta = 11$ and 40, respectively.

to Ni and Co, respectively, as obtained from band structure calculations [15]. The results of the calculations are plotted in Figs. 1 and 2 as continuous lines for $\beta = 13$ and 11, respectively, in comparison with the experimental data, and we also find a decrease of calculated BMR with an increasing conductance of the nanocontact. Figures 1(a) and 2(a) are for all of the raw data, while Figs. 1(b) and 2(b) are for the average values of the data with the same conductance. Discontinuous lines show calculations for a value of $\beta = 40$ for both metals, and now the calculations fall better on the data. The deviation of the value of β obtained from band structure calculations and with that which fits the data can be easily justified, because the density of states and the spin configuration at the nanocontact do not necessarily have to be the same as those of the bulk materials [18].

Let us check the validity of the assumption of the weak scattering. For $\zeta = 0.87$, the function F is $F \sim 0.1$ even for $N = 1$ and thus the relevant expansion parameter is $\zeta^2/(1 - \zeta^2)F \sim 0.3$, which is small enough. Thus our calculation would be applicable to a whole range of G observed in the experiment. Note that the assumption of weak scattering can be valid even when the magnetoconductance is 300%. The weak scattering justifies the perturbative calculation of R_W up to the second order in A_q, and even in this case the magnetoresistance, governed by the ratio of R_W to G_0^{-1}, can be large.

We have estimated the resistance in nanowire based on one-dimensional calculation and have taken into account the number of channels N as a multiplying factor [Eq. (13)]. This treatment is valid in the small N region which we are most interested in.

In our analysis, ΔG decreases exponentially for large λ, leading to $\Delta G \propto e^{-4\pi\zeta\sqrt{N/\beta}}$ for large N. This asymptotic behavior, however, is an artifact of the use of $\cos\theta = \tanh(x/\lambda)$. If we approximate the wall as uniform, i.e., $\nabla\theta = \pi/2\lambda$ for $-\lambda < x < \lambda$, the function $[\cosh\pi k_F\lambda]^{-1}$ in the function F [Eq. (14)] is replaced by $[\sin k_F\lambda/k_F\lambda]^2$ and thus $\Delta G \propto 1/N$ for large N. Therefore, the asymptotic behavior is dependent on the shape of the contact. This means that BMR is practically constant for large G, in agreement with the data. On the other hand, the ΔG feature, which peaked at about $N \sim 0$ and decayed rapidly for $N \gtrsim \beta/4$, is general.

Also the scatter of BMR data may be due to different contacts with different spin densities at the Fermi level. We have assumed only one nanocontact but when the conductance increases there may be several nanocontacts produced in different regions of the macroscopic wires. Each of these regions may have different domain configurations.

Before concluding, we acknowledge that Mathon [19] presented BMR calculations as a function of the DWW, using tight binding models, and found similar results: large values of the BMR (200%) for Ni and Co for atomic size DWW, and these values drop very fast as the DWW increases.

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