Numerical study of magnetoresistance for currents perpendicular to planes in spring ferromagnets

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Magnetoresistance (MR) for currents perpendicular to planes is calculated within the ballistic limit for spring ferromagnets in which an artificial domain wall is formed by the external magnetic fields. We consider two contributions to the MR: one is caused by a twisting of the magnetization and the other is due to a mismatch of the electronic structure between the two ferromagnets comprising the spring ferromagnets. We show that the resulting MR may show a nonmonotonic dependence on the width of the domain walls and can be either positive or negative according to the magnitude of these two contributions. We further show that oscillatory behavior appears in the MR when the soft ferromagnet is sandwiched between hard ferromagnets.

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The past decade has seen growing interest in magnetoresistive phenomena such as giant magnetoresistance (GMR) and tunnel magnetoresistance in artificial magnetic multilayers.[1–3] The effect of GMR is caused by a spin-dependent scattering, which makes the total resistivity larger in the anti-parallel (AP) than that in the parallel (P) alignment of the magnetization of magnetic layers. The magnetoresistance (MR) effect is also observed in nonartificial materials, that is, the resistance due to domain walls (DW) in ferromagnets is reduced when the external magnetic field (h) eliminates the DW. When the ferromagnets are submicron size wires, the DW magnetoresistance (DWR) is similar to the GMR in the geometry of the current perpendicular to planes (CPP) because the current runs mainly perpendicular to the DW. Because the width of the DW is of the order of several 10 nm, the DWR from each DW is usually small, at most a few percent.[4] However, it has been pointed out theoretically that the DWR can be as large as the GMR when the width of the DW is reduced to a length of an atomic scale.[5,6] Concerning the DWR in ferromagnetic wires, negative MR (decrease in resistivity with increasing h) has been reported.[7,8] Change in the Lorentz motion, elimination of weak localization, and change in the carrier number by vanishing DW have so far been proposed as the origin of the negative MR.[8–10]

In order to further understand the phenomenon of DWR, control of the DW is strongly required, which is, however, rather difficult to perform experimentally. This difficulty may be removed by using spring ferromagnets (SFM) which consist of two types of ferromagnets: one a soft ferromagnet and the other a hard ferromagnet. When we apply an external magnetic field h, the soft ferromagnet rotates its magnetization towards the external field and thereby a twisted state of the magnetization, similar to DW, is realized at the interfaces between two ferromagnets. Because the twisted region shrinks with increasing h, the resistance is expected to increase with increasing h.

Measurements of MR in SFM have been performed for both CPP and current in plane geometries by several groups.[11–14] Wegrowe *et al.*[12] have indicated that CPP-MR in SFM is the superposition of the two effects of GMR and DWR. The former effect is naturally superimposed on the effect of DWR because the spin dependent scattering in the ferromagnets varies with the alignments of the magnetization of SFM. In reality, another effect of MR (contact MR), which is caused by a mismatch of the electronic states at the interface between two ferromagnets, should be added to CPP-GMR of SFM. The contact MR is nothing but the DWR of SFM with zero DW thickness. These three effects of GMR, DWR, and contact MR may be either additive or subtractive depending on the initial alignment of the magnetization of two ferromagnets. In addition, the contact MR can be either positive or negative according to the difference between the electronic states of two ferromagnets. Because of these features of MR, the dependence of MR in SFM on DW thickness can be nonmonotonic, and the sign of the MR can be changed by varying the DW thickness.

The purpose of this paper is to calculate the contact MR and DWR in A/B-type SFM for a wide range of parameter values by using a simple model and to show that the MR can actually be nonmonotonic and may change its sign with decreasing DW thickness. The conductance and MR of SFM are calculated using the Kubo-Landauer formula in the ballistic limit for finite size systems. A contribution to the MR from diffusive conductance will be taken into account in a method proposed by Schep *et al.*[15] We will show that the qualitative features of the calculated MR may be unchanged by the diffusive conductance. The effects of GMR caused by the spin-dependent scattering will be discussed later. We also present results for $A/B/A$-type SFM, in which an oscillatory MR may be realized due to the quantum confinement effect in the ballistic regime.

We use a single band tight-binding model, the Hamiltonian of which is given as

$$H=-t\sum_{i,j,\sigma} c^{\dagger}_{i\sigma}c_{j\sigma}+\sum_{i,\sigma} v_{i\sigma}c^{\dagger}_{i\sigma}c_{i\sigma}, \quad (1)$$

where t is a nearest-neighbor site hopping and $v_{i\sigma}$ is the spin-dependent potential of site i. The energy band in the paramagnetic state extends from $-6.0t$ to $6.0t$ for the simple cubic lattice. We, hereafter, take t as the unit of energy. For an A/B-type spring ferromagnet, $v_{i\sigma}=v_{A\sigma}$ and $v_{B\sigma}$ for A and B ferromagnets, respectively. We take

$$v_{A\sigma}=v_A-s\Delta_A/2, \tag{2}$$

$$v_{B\sigma}=v_B-s\Delta_B/2, \tag{3}$$

with $s=+(-)$ for $\sigma=\uparrow(\downarrow)$ spin. In the following, we take $v_A=0$, $v_B-v_A\equiv\delta v$. We have not performed self-consistent determination of the magnetization near the interface but have assumed an abrupt change of the magnetizations of A and B ferromagnets at the interface. It is also assumed that the magnetization of each atomic planes rotates uniformly within the DW. The spin indices are defined for systems without the external field.

The conductance Γ is calculated by using the Kubo-Landauer formula in the mixed representation of $(k_\parallel,\ell)$ where ℓ stands for the layer index.[16,17] The number of k points are 200×200 unless specified. The MR ratio is defined as

$$\text{MR ratio}=2\times\frac{\Gamma(h=0)-\Gamma(h\neq0)}{\Gamma(h=0)+\Gamma(h\neq0)}. \tag{4}$$

In an A/B-type SFM without a twisted region of magnetization (no DW), the contact resistance $(1/\Gamma_{C\sigma})$ may be given as[15,18]

$$\frac{1}{\Gamma_{C\sigma}}=\frac{1}{\Gamma_\sigma}-\frac{1}{2}\left(\frac{1}{N_{A\sigma}}+\frac{1}{N_{B\sigma}}\right), \tag{5}$$

when the electron transport is diffusive, but spin conserving. Here, Γ_σ is the calculated conductance and $N_{A\sigma}$ and $N_{B\sigma}$ are the numbers of channels with spin σ in the ferromagnetic leads A and B, respectively. The correction due to the diffusive transport is given by adding the diffusive resistance $(1/\Gamma_d)$ to $1/\Gamma_{C\sigma}$ in such a way that

$$\frac{1}{\tilde{\Gamma}_\sigma}=\frac{1}{\Gamma_{C\sigma}}+\frac{1}{\Gamma_d}, \tag{6}$$

where Γ_d is given in a unit of $[e^2/h]$. Now the conductance in the definition of the MR ratio is given by $\Gamma=\Sigma_\sigma\tilde{\Gamma}_\sigma$ with or without magnetic field h. In this work we will treat the diffusive conductance as a variable parameter because it may be strongly sample dependent in real systems.

When there is a DW in B magnet, which is the situation we are dealing with, there occurs spin mixing in B magnet due to the twisting of the magnetization in the DW region, which makes the definition of the spin-dependent channel number difficult. Here we assume that the effective number of channels in B magnet can be given as

$$\tilde{N}_{B\uparrow}=N_{B\uparrow}\cos^2(\theta/2)+N_{B\downarrow}\sin^2(\theta/2), \tag{7}$$

$$\tilde{N}_{B\downarrow}=N_{B\uparrow}\sin^2(\theta/2)+N_{B\downarrow}\cos^2(\theta/2), \tag{8}$$

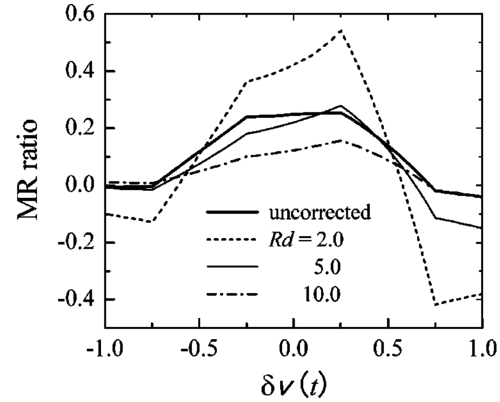

FIG. 1. Calculated results of the contact MR as a function of the potential difference of A and B magnets for $\Delta_A=1.0$ and $\Delta_B=0.5$. Thick solid curve is the MR ratio without correction due to diffusive conductance. Broken, thin-solid, and chained curves are corrected MR with diffusive resistance R_d.

where θ is the angle of the magnetization direction between the nearest-neighbor layers within the DW. Although no rigorous proof has yet been given for the above expressions, they give correct results for $\theta=0$ and π. The contact resistance $\Gamma_{C\sigma}$ is given by replacing $N_{B\sigma}$ in Eq. (5) with $\tilde{N}_{B\sigma}$. In this case $\Gamma_{C\sigma}$ should be interpreted as a contact resistance including the DW contribution. The validity of the approximation will be discussed in relation to the numerical results.

In the following, we consider two cases for the MR in an A/B-type SFM having a hard magnet A and a soft one B: (1) The magnetizations of A and B magnets are parallel for $h=0$, and become antiparallel for $h\neq0$; and (2) The magnetizations of A and B magnets are antiparallel when $h=0$ which are changed to be parallel by $h\neq0$.

For both cases, the DWR is positive, that is, the resistance increases with increasing h, while the contact MR may be either positive or negative according to the degree of mismatch of the electronic states at the interface. We also calculate the MR for an $A/B/A$-type SFM, in which two DW regions appear by twisting the magnetization of the B magnet.

We first study the contact MR (MR with zero DW thickness) of the A/B-type SFM. The contact MR can be either positive or negative depending on the degree of mismatch of the electronic states between A and B magnets. Figure 1 shows the calculated results of the contact MR as functions of δv with $v_A=0$, $\Delta_A=1.0$, and $\Delta_B=0.5$. The Fermi level is taken as $\epsilon_F=-4.0$ throughout this paper. The uncorrected MR ratio is shown by a thick solid curve. When δv is small, the MR ratio is positive but it tends to change sign for larger values of $|\delta v|$. The results can be easily interpreted in the following way. Let us start with the result for $\delta v=0.75$. In this case the matching of the down-spin state of A magnet with the up-spin state of B magnet is perfect. Therefore $\Gamma_\uparrow+\Gamma_\downarrow$ at $h\neq0$ (AP alignment) is much larger than that at $h=0$ (P alignment) and the MR ratio is negative. As δv is decreased to 0.25, the matching between the down-spin state of A magnet and the down-spin state of B magnet becomes perfect, and therefore $\Gamma_\uparrow+\Gamma_\downarrow$ at $h=0$ is much larger than

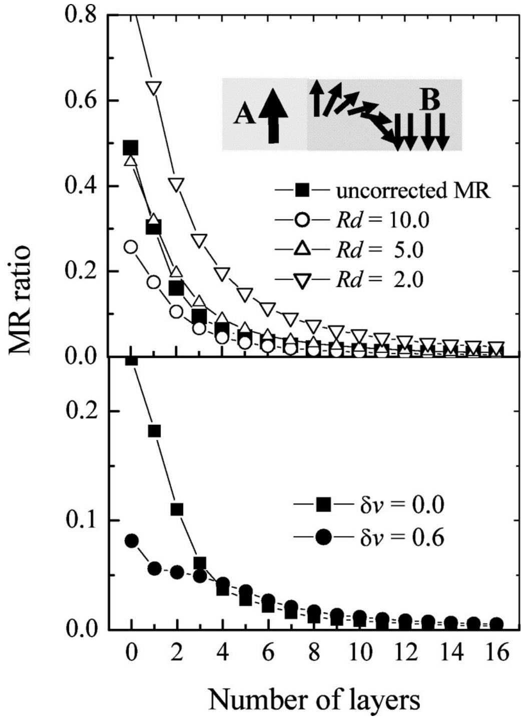

FIG. 2. Calculated results of the MR ratio as functions of domain wall thickness (number of atomic layers) for (a) $\Delta_A = \Delta_B = 1.0$ with $\delta v = 0$ and (b) $\Delta_A = 1.0, \Delta_B = 0.5$ with $\delta v = 0.0$ and 0.6. Solid and open symbols are uncorrected and corrected MR due to diffusive resistance R_d, respectively. The inset of (a) is a schematic figure of the AP magnetization alignment.

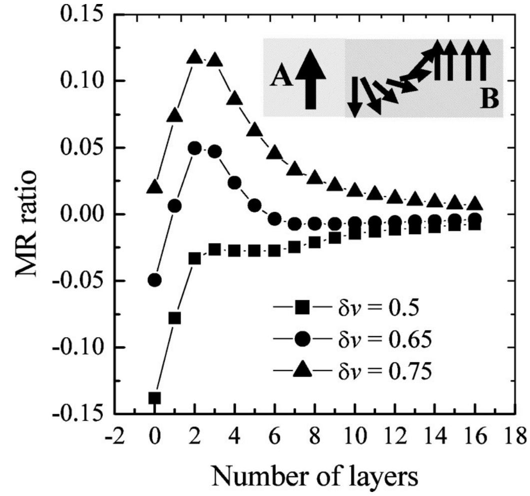

FIG. 3. Calculated results of uncorrected MR ratio as function of DW thickness (number of atomic layers) for $\Delta_A = 1.0, \Delta_B = -0.5$ with several values of δv.

$\Gamma_\uparrow + \Gamma_\downarrow$ at $h \neq 0$ and the MR ratio is positive. A similar situation occurs for $\delta v = -0.25$ and -0.75. It should be noted that the MR ratio calculated using the conductance given by Eq. (5) should be ± 2.0 at $\delta v = \pm 0.75$ and ± 0.25 because of the perfect matching in the electronic states at $h = 0$ or $h \neq 0$.

The MR ratios corrected by taking into account the diffusive resistance are shown by broken, thin-solid, and chained curves for $R_d (= 1/\Gamma_d) = 2.0$, 5.0, and 10.0, respectively. Here the values of $1/R_d$ have been taken to be the same order of magnitude as those of $\Gamma_\sigma, \sim 10^{-1}[e^2/h]$ per channel. For a smaller value of R_d, the singular feature of MR ratios at $\delta v = \pm 0.75$ and ± 0.25 can be seen clearly. The corrected MR shows a dependence on δv similar to that of the uncorrected MR ratios as long as $R_d \sim 1/(\Gamma_\uparrow + \Gamma_\downarrow) \sim 5.0$.

Figures 2(a) and 2(b) show the calculated results of MR ratio as functions of DW thickness (number of layers) for case (1), where the magnetizations of A and B magnets align P for $h = 0$ and change AP for $h \neq 0$. The inset of Fig. 2(a) shows schematically the magnetic configuration in AP alignment. Parameter values are taken to be $\delta v = 0$ with $\Delta_A = \Delta_B = 1.0$ for Fig. 2(a), and $\delta v = 0$ and 0.6 with $\Delta_A = 1.0$ and $\Delta_B = 0.5$ for Fig. 2(b). The curves shown by solid squares and circles are the uncorrected MR ratios. These MR ratios are positive and increase with decreasing DW thickness because the resistance caused by the electronic state mismatch at the interface, and by the twisting of the magnetization increases with an increasing magnetic field. The MR ratio given by circles in Fig. 2(b) is not significantly large at zero DW thickness because the contact MR is small, but shows a shoulder at the thin DW region. The latter result indicates that the contribution to the MR from the twisting of the magnetization becomes large for the thin DW region as will be discussed later.

The corrected MR ratios by taking into account the diffusive resistance are shown by open circles, triangles, and squares with several values of $R_d (= 1/\Gamma_d)$. The corrected MR ratio in Fig. 2(a) shows a similar magnitude and dependence on the DW thickness as compared with the uncorrected MR ratios when Γ_d has values similar to Γ_σ. The dependence of the MR ratio on the DW thickness is about $1/(\text{DW thickness})^2$, which agrees qualitatively with the theoretical predictions.[5,9,10] The corrected MR ratios decrease naturally with the increase in the diffusive resistance because we have not included any spin dependence in the diffusive resistance.

Now we present the calculated results of the MR ratio for case (2) shown in Fig. 3. Here the magnetizations of A and B magnets are AP at $h = 0$ and P at $h \neq 0$. The configuration of the magnetization in P alignment is shown in the inset of Fig. 3. The parameter values are taken as $\delta v = 0.5, 0.65$, and 0.75 with $\Delta_A = 1.0, \Delta_B = -0.5$. Because the sign of Δ_B is negative, the sign of the contact MR ratios is opposite to that of the MR ratios shown in Fig. 1. Therefore, the contact MR (zero DW thickness) is negative or quite small for these parameter sets.

As can be seen in Fig. 3, the MR ratio may change its sign with DW thickness. When $h = 0$, the magnetizations of A and B magnets are AP. By applying the magnetic field h, a DW appears near the interface of A and B magnets. The DWR is small for thicker DW. The contact MR is also small because the magnetization of the B atomic layer at the interface remains AP to that of A magnet due to a strong coupling between A and B magnetizations at the interface. With increasing h, the DW shrinks and its positive contribution to MR increases. Therefore, the MR ratio becomes positive as shown by solid circles and triangles. At a sufficiently high magnetic field, the magnetization of *A* and *B* magnets may be parallel and DW thickness becomes zero. Because the MR ratios at zero DW thickness are negative or small, the MR ratios tend to decrease with decreasing DW thickness. Thus, the MR ratio shows a nonmonotonic dependence on the DW thickness and even changes its sign according to the parameter values. When the negative MR at zero DW thickness is too large in magnitude, the MR ratio remains negative irrespective of the DW thickness. The change in sign of the MR ratio may occur when the negative contribution from the contact MR and positive one from DW are comparable to each other.

The dependence of the MR ratio on the DW thickness may not be altered by inclusion of the diffusive conductance as long as $1/R_d$ is the same order of magnitude of $\Gamma_\uparrow+\Gamma_\downarrow$. The corrected MR ratios for $\delta v=0.65$ with $R_d=10.0$ are almost the same as the results indicated by circles in Fig. 3 (not shown).

The effect of spin-dependent scattering may give rise to complexity in the dependence of the MR ratio on DW thickness. Different spin asymmetry of the scattering of *A* and *B* magnets can cause the dependence more complex. Let us assume for the sake of simplicity that the GMR caused by the spin-dependent scattering is positive; that is, the conductance in P alignment is always larger than that in AP alignment. Under this assumption, the GMR is positive (negative) in case (1) [case (2)]. Therefore, in case 1, the GMR, DWR, and the contact MR are additive, and give rise to positive MR. In contrast, in case 2, the GMR, DWR, and contact MR can be subtractive, and cause a complex dependence of MR as a function of DW thickness. A nonuniform rotation of magnetization in DW observed in experiments may give rise to a modification of the present results; however, the qualitative features will be unchanged. The sign change in MR predicted in the present study may be observable by applying a suitable magnetic field or adopting magnets of appropriate thickness in the spring ferromagnets. Such a result has been recently reported by Nagura *et al*.[13] for Gd/Co multilayers.

Finally, we study the MR of *A*/*B*/*A*-type spring ferromagnets. We assume that magnet *B* is a soft magnet and two DW's are produced within *B* magnet by the external field. The width of the *B* layer is taken to be 70 atomic layers. Solid circles and open squares in Fig. 4 show the calculated results of the uncorrected MR ratio as a function of DW thickness for $\Delta_A=1.0$ with $\Delta_B=0.2$ (solid circles) and -0.2 (open squares), respectively. We find an oscillatory behavior in the MR as functions of DW thickness. This is due to the quantum confinement of electrons within the *B* magnet caused by the mismatch of the electronic states between *A* and *B* magnets. The period of the oscillation, which is much longer than the Fermi wave length, is a result of a beat of two different wave lengths of the up- and down-spin states in *B* magnet. In the present choice of the Fermi energy and Δ_B, the Fermi wave numbers of the up- and down-spin states of *B* magnet are about $0.5\pi\pm0.05$, which give the period of the beat $\Delta L=2\pi/(k_{F\downarrow}-k_{F\uparrow})\sim20\pi$ in units of the lattice constant. Because the results in Fig. 4 are shown as a function of the thickness of one DW within *B* layer, half of the oscillation period should be $20\pi/4\sim16$ atomic layers, which is in good agreement with the results shown in Fig. 4. The short period oscillation caused by the Fermi wavelength itself is not observed in the figure because the period is an order of the lattice constant. The long period oscillation might be observable in sufficiently clean samples.

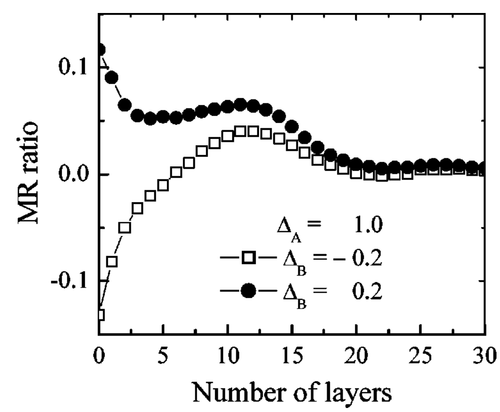

FIG. 4. Calculated results of the MR ratio as functions of DW thickness (number of atomic layers) for *A*/*B*/*A*-type spring ferromagnets with $\delta v=0$.

We have shown that the assumption to the effective channel numbers, Eqs. (7) and (8) would not alter the qualitative feature of the thickness dependence of the DWR. The assumption, however, has not yet proved to be valid. In order to check the validity, one should first generalize the results obtained by Schep *et al.*[15] to a contact of two ferromagnets. Because this is a generalization of their method used to explain the angular dependence of CPP-GMR observed,[18–20] the resultant expression of the interface resistance should be consistent with the observation. However, the present geometry of the interface with DW-like structure might violate the necessary conditions for their theory.[18,19] The DW region may give rise to quantum size effects because the magnetization rotates layer by layer in the region, and the elastic mean free path might be longer than the DW thickness. Derivation of proper expression for the interface resistance for the present geometry may thus be a problem in future.

In conclusion, we have performed a numerical study of the CPP-MR in spring ferromagnets within the ballistic limit. We have demonstrated that the MR ratio depends nonmonotonically on DW thickness in spring ferromagnets and that even a change in sign of the MR ratio may be possible. The results are attributed to competitive contributions from the DWR and contact MR caused by spin mixing within the DW and the electronic state mismatch at the interface, respectively. Although we have calculated the ballistic conductance, the qualitative features may be unchanged after taking into account the diffusive resistance of the order of $1/(\Gamma_\uparrow+\Gamma_\downarrow)$. We have also predicted an oscillation of MR for *A*/*B*/*A*-type spring ferromagnets, which might be observed in clean samples. For quantitative comparison between theory and experiment, however, realistic models might be required, which will be a subject of research in the near future.

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[1] M.N. Baibich, J.M. Broto, A. Fert, F. Nguyen Van Dau, F. Petroff, P. Etienna, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. **61**, 2472 (1988).
[2] T. Miyazaki and N. Tezuka, J. Magn. Magn. Mater. **139**, L231 (1955).
[3] J.S. Moodera, L.R. Kinder, T.M. Wong, and R. Meservey, Phys. Rev. Lett. **74**, 3273 (1995).
[4] J.F. Gregg, W. Allen, K. Ounadjela, M. Viret, M. Hehn, S.M. Thompson, and J.M.D. Coey, Phys. Rev. Lett. **77**, 1580 (1996).
[5] P.M. Levy and S. Zhang, Phys. Rev. Lett. **79**, 5110 (1997).
[6] J.B.A.N. van Hoof, K.M. Schep, P.J. Kelly, and G.E.W. Bauer, J. Magn. Magn. Mater. **177**, 188 (1998); J.B.A.N. van Hoof, K.M. Schep, A. Brataas, G.E.W. Bauer, and P.J. Kelly, Phys. Rev. B **59**, 138 (1999).
[7] K. Hong and N. Giordano, Phys. Rev. B **51**, 9855 (1995).
[8] U. Ruediger, J. Yu, S. Zhang, A.D. Kent, and S.S.P. Parkin, Phys. Rev. Lett. **80**, 5639 (1998).
[9] G. Tatara and H. Fukuyama, Phys. Rev. Lett. **78**, 3773 (1997).
[10] R.P. van Gorkom, A. Brataas, and G.E.W. Bauer, Phys. Rev. Lett. **83**, 4401 (1999).
[11] S.N. Gordeev, J.-M.L. Beaujour, G.J. Bowden, B.D. Rainford, P.A.J. de Groot, R.C.C. Ward, M.R. Wells, and A.G.M. Jansen, Phys. Rev. Lett. **87**, 186808 (2001).
[12] J.-E. Wegrowe, A. Comment, Y. Jaccard, J.-Ph. Ansermet, N.M. Dempsey, and J.-P. Nozieres, Phys. Rev. B **61**, 12 216 (2000).
[13] H. Nagura, K. Takanashi, S. Mitani, K. Saitoh, and T. Shima, J. Magn. Magn. Mater. **240**, 183 (2002).
[14] J.L. Prieto, M.G. Blamire, and J.E. Evetts, Phys. Rev. Lett. **90**, 027201 (2003).
[15] K.M. Schep, J.B.A.N. van Hoof, P.J. Kelly, G.E.W. Bauer, and J.E. Inglesfield, Phys. Rev. B **56**, 10 805 (1997).
[16] H. Itoh, T. Kumazaki, J. Inoue, and S. Maekawa, Jpn. J. Appl. Phys. **37**, 5554 (1998).
[17] H. Itoh, A. Shibata, T. Kumazaki, J. Inoue, and S. Maekawa, J. Phys. Soc. Jpn. **68**, 1632 (1999).
[18] G.E.W. Bauer, K.M. Schep, K. Xia, and P.J. Kelly, J. Phys. D **35**, 2410 (2002).
[19] G.E.W. Bauer, Y. Tserkovnyak, D. Huertas-Hernando, and A. Brataas, Phys. Rev. B **67**, 094421 (2003).
[20] J. Bass and W.P. Pratt, Jr., J. Magn. Magn. Mater. **200**, 274 (1999).