Domain-wall resistance in metal nanocontacts

Julian Velev and William H. Butler
Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA
and Center for Materials for Information Technology, University of Alabama, Tuscaloosa, Alabama 35487, USA
(Received 9 June 2003; revised manuscript received 11 December 2003; published 23 March 2004)

We present a study of ballistic conductance through Ni, Co, and Fe nanocontacts within a semiempirical tight-binding model. In our model, both spin channels are treated simultaneously, which allows us to simulate a domain wall pinned in the nanocontact. We observe that the interplay of the contact and the domain wall resistance can produce very large giant magnetoresistance ratios. However, at least within our model, very large giant magnatoresistance appears to be limited to geometries in which the nanocontacts are very narrow and have very small aspect ratios.

DOI: 10.1103/PhysRevB.69.094425 PACS number(s): 75.47.Jn, 72.10.−d, 72.25.−b

I. INTRODUCTION

The decade and a half following the discovery of giant magnetoresistance (GMR) in Fe-Cr multilayers,[1,2] has witnessed a continuing growth of interest in spin-dependent electron transport.[3–7] During this period several novel GMR geometries were proposed, including spin valves, multilayered nanowires, and recently nanocontacts. García *et al.*[8] reported MR in Ni and Co nanocontacts of 300%, which they later extended to 700% and 1000%, respectively.[9] The same group reported MR in Fe nanocontacts to be an order of magnitude smaller.[10] In the experiments, two different geometries were used. In the first geometry,[8] two sharpened wires were brought into contact. A magnetic field was applied along the common axis of the two wires by two separate coils. The field applied to one of the wires was kept constant while the field applied to the other could be oriented parallel or antiparallel to the first. Increased resistance was observed when the field applied to the two wires was in opposite directions, presumably trapping a domain wall at the nanocontact region. The second geometry[9] consisted of a sharpened wire touching the surface of another wire perpendicular to it. Increased resistance was observed when a magnetic field was applied along the axis of the first wire causing the magnetization of the two wires to be perpendicular to each other due to shape anisotropy. In that case a domain wall was also presumed to be formed in the nanocontact region. These experiments have become a matter of debate because of the possibility that the conductance changes might be due to effects related to magnetostriction.

On the theoretical side, Bruno[11] showed that the anisotropy of the contact can pin the domain wall in the contact, and thus, shorten the length of the domain wall by two orders of magnitude as compared to bulk. This is important because it has been shown that electrons traveling through a wide domain wall in which neighboring atomic moments are nearly parallel experience very weak scattering. However, electrons passing through a narrow, abrupt wall cannot adjust to the sharp change of magnetization, and experience increased reflection. It is, however, very difficult to obtain analytical results for realistic nanocontacts because of the difficulty of taking into account the crucial aspects of the electronic structure in the vicinity of the nanocontact.

Calculations of the domain-wall resistance taking into account the band structure of the material have just begun to appear. The resistance of abrupt domain walls in Ni, Co, and Fe was studied in both model and realistic calculations.[12] It was shown that model calculations are deficient because they poorly approximate the band structure near the Fermi energy, in particular, the large number of bands at the Fermi energy. More recently, the domain-wall resistance in Co was studied in an *ab initio* linear muffin-tin orbital study[13] both in the ballistic and diffuse regimes. In all studies diffuse (thick) domain walls were found to increase the conductance and decrease MR compared to sharp abrupt walls. However, the geometries studied so far have been infinite and uniform in the plane perpendicular to the current and therefore have not been consistent with the small domain-wall width. In addition, this type of calculation misses the effects of the contact resistance between the leads and the constriction which is, in fact, the leading source of resistance in atomic size constrictions.[14]

In this paper we report on a study of the conductance through domain walls pinned in a constriction accounting simultaneously for the constriction and the noncollinear spin. We calculate (i) the transmission through planar domain walls in bulk Ni, Co, and Fe; (ii) the transmission through Ni, Co, and Fe nanocontacts for several aspect ratios of the nanocontacts; and (iii) the transmission through structures in which the constriction is made of nonmagnetic material, systems such as Co-Cu-Co and Fe-Cr-Fe. This latter geometry is chosen because the nonmagnetic material would be expected to break the exchange interaction allowing an abrupt change in magnetization which should maximize the domain-wall plus constriction effect.

II. MODEL

Our calculations are based on a semiempirical tight-binding (TB) model fitted to *ab initio* band structures. We utilize a supercell formulation that allows us to study contacts with arbitrary length and cross-section size. We treat both spins simultaneously which allows us to study the cases in which the spin is not collinear with the magnetization.

Some important aspects of this problem are not accounted for in our model. We do not attempt to calculate the magnetic

structure of the junction from first principles. Although such calculations would be very interesting and useful, they would also be fraught with uncertainties, because the experimental systems are very difficult to characterize at the atomic scale. We believe that it is also important to understand the effects of the aspects of the problem which we do model, i.e., the effects of the noncollinearity of the moments, the thickness of the domain wall, the width of the nanocontact, and the effects of nonmagnetic atoms in the contact.

For a sample sandwiched between two leads at zero temperature, the ballistic conductance in each spin channel is given by the total transmission probability through the sample,[16]

$$\Gamma = \frac{e^2}{h} \sum_{\mathbf{k}_\parallel, i, \mathbf{k}'_\parallel, j} T_{\mathbf{k}_\parallel, i; \mathbf{k}'_\parallel, j}(E_F), \tag{1}$$

where $(\mathbf{k}_\parallel, i)$ labels an incident Bloch state with transverse wave vector $\mathbf{k}_\parallel$ in one lead and $(\mathbf{k}'_\parallel, j)$ labels a transmitted Bloch state in the other. The additional integer quantum numbers i and j are are needed because each of the leads may have several Bloch states for a given value of transverse momentum. The total transmission probability, summed over all incident and transmitted states, can be written in a basis of planar orbitals using the Caroli formula[17] as

$$\Gamma = \frac{e^2}{h} \mathrm{Tr}[\tilde{\Sigma}_L G^R_{LR} \tilde{\Sigma}_R G^A_{RL}], \tag{2}$$

where $G^{R/A}_{LR}$ is the retarded/advanced Green's function (GF) matrix element between the first-principal layer of the left and right leads and $\tilde{\Sigma} = i(\Sigma^R - \Sigma^A)$ is the imaginary part of the self-energy of one of the semi-infinite leads evaluated at its end. In the calculation of the conductance, all Green's functions and self-energies are evaluated at the Fermi energy.

The method we use to calculate the conductance, when the spin is not collinear with the magnetization, is the same as that used in a study of the angular dependence of the conductance in spin valves.[15] The Hamiltonian matrix is transformed locally as follows:

$$H(\theta, \phi) = U(\theta, \phi) H U^\dagger(\theta, \phi), \tag{3}$$

where H is the is a block diagonal 2×2 matrix when the spin-quantization axis is aligned with the magnetization (off-diagonal elements are zero if there are no spin-flip terms in the Hamiltonian). The Hamiltonian matrix elements for majority and minority electrons are different in magnetic materials. The spin rotation matrix $U(\theta, \phi)$ is the well known

$$U(\theta, \phi) = \begin{pmatrix} \cos\frac{\theta}{2} e^{i\phi/2} & \sin\frac{\theta}{2} e^{-i\phi/2} \\ -\sin\frac{\theta}{2} e^{i\phi/2} & \cos\frac{\theta}{2} e^{-i\phi/2} \end{pmatrix}. \tag{4}$$

The method we use to calculate the conductance through a constriction was originally developed to study the conductance of nanowires.[14] We model the constriction using a supercell surrounded by enough empty sites that the constriction is isolated. Then the supercell is repeated periodically in the plane. The obtained superlattice has a square lattice with lattice constant $L = Na$, where a is the bulk lattice constant and N is an integer, which indicates the size of the supercell. We use a semiempirical TB Hamiltonian constructed by fitting to *ab initio* band structures.[18] The orthogonal two-center integral approximation was used. The matrix elements between different species are obtained by averaging the corresponding matrix elements of the compound species. The TB parameters were fitted to bulk band structures. This represents a limitation because the potentials of the atoms in the constriction may differ from the bulk potentials. This is especially true for atoms close to the surface which become increasingly important as the constriction becomes narrower. The constriction is surrounded by empty sites.

The transmission probability is first obtained in the supercell basis $|\mathbf{k}_{||}, i, \alpha, R_z\rangle$ where $\mathbf{k}_{||} = (k_x, k_y)$ $(|k_x|, |k_y| < \pi/L)$ denotes a two-dimensional (2D) wave vector within the superlattice Brillouin zone (BZ), α labels the symmetry type for the sp^3d^5 orbitals, R_z labels the layer, and i labels the atom coordinates in the supercell. Consequently, the conductance is transformed to the basis of the reciprocal lattice vectors of the superlattice $|\mathbf{k}_{||} + \mathbf{g}_n, \alpha, R_z\rangle$ where $\mathbf{g}_n = (2\pi/L) \times (n_1, n_2)$ denotes the reciprocal lattice vectors of the superlattice that fall in the first bulk Brillouin zone $(0 \leqslant n_1, n_2 \leqslant N)$. Finally, after integration over the supercell BZ we obtain the conductance in the form

$$\Gamma = \sum_{n,n'} [\Gamma_\uparrow(\mathbf{g}_n, \mathbf{g}_{n'}) + \Gamma_\downarrow(\mathbf{g}_n, \mathbf{g}_{n'})]. \tag{5}$$

Here the labels α have been summed over. Due to translational symmetry, the bulk layer orbitals associated with different wave vectors $\mathbf{g}_n$ are decoupled in the leads, but coupled in the constriction region.

III. RESULTS AND DISCUSSION

We have studied three ferromagnetic $3d$ transition metals Ni, Co, and Fe. The first two, fcc Ni and fcc Co, were the first to be reported to show large contact MR.[8] The last, bcc Fe, was reported to have much smaller contact MR, which was attributed to the fact that Fe is a weak ferromagnet, i.e., its majority d band is not filled.[10] In all three cases, we work with the (001) lattice orientation.

As a first step, we studied the conductance through domain walls in bulk Ni, Co, and Fe. The width of the wall was artificially limited to w monolayers (ML). In Fig. 1, the conductance (a) and MR (b) are shown as a function of the domain-wall width. The angle of magnetization in consecutive layers changes with the step $180°/(w-1)$. The straight lines in Fig. 1(a) are the conductances of bulk Ni, Co, and Fe, respectively. The conductance in the presence of a domain wall of width w increases with w. In the case of a domain wall, we define MR as the ratio,

$$\mathrm{MR} = \frac{\Gamma_{||} - \Gamma_{\mathrm{wall}}}{\Gamma_{\mathrm{wall}}}, \tag{6}$$

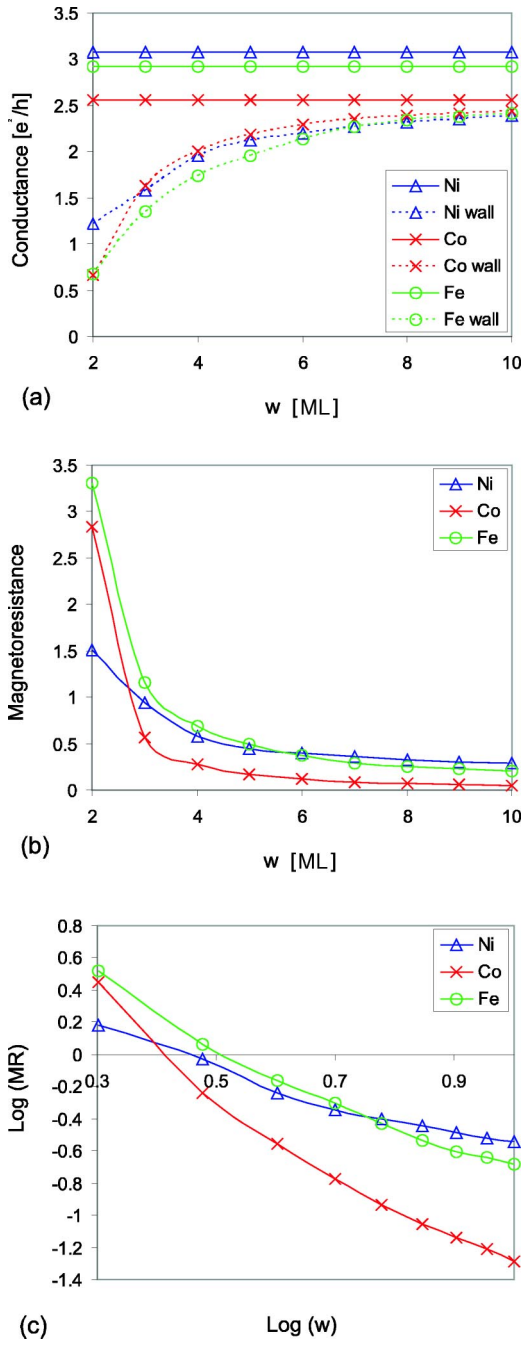

FIG. 1. Bulk and domain-wall conductance (a), MR (b), and MR scaling (c) in bulk Ni, Co, and Fe as a function of the domain-wall width w. The conductance is expressed in units of e^2/h (i.e., $0.386\times10^{-4}\ \Omega^{-1}$) per two-dimensional unit cell.

where $\Gamma_\parallel$ is the the conductance for parallel alignment of the moments in the two leads, i.e., no domain wall is present.

The resultant MR of a bulk domain wall, Fig. 1(b), is largest for $w=2$ ML, where the magnetization in the second layer is at 180° with respect to the magnetization of the first one. As expected, the domain-wall resistance drops very rapidly as the domain-wall width increases. In the case of $w=2$ ML, the observed MR ratios can be calculated using the collinear approach. In the absence of a domain wall, the conductances [Fig. 1(a)] are simply proportional to the number of propagating states per two-dimensional cell. All states are transmitted with unit probability. In the presence of the abrupt domain wall, an upper limit to the conductance (and a lower limit to the MR) can be obtained by assuming that all states that are not blocked by the requirement of $\mathbf{k}_\parallel$ conservation, are transmitted with unit probability. This approach would lead to MR's of 1.04, 1.17, and 0.87 for Ni, Co, and Fe, respectively. The actual MR's are much higher, 2.8, 1.5, and 3.3, indicating that the transmission probability is substantially less than unity, especially for Fe. The low transmission probabilities have been related to the different nature of the wave functions for majority and minority.[10] This is not surprising for Co and Ni for which the Fermi level falls above the d bands for majority and near the top of the d bands for minority. For Fe, although the Fermi level falls in the d bands for both majority and minority, the minority Fermi surface falls near the bcc pseudogap where the states have significant free-electron character and are qualitatively different from the d states of the majority.

The rate of decrease of MR with w is shown in Fig. 1(c). It is found to be of the form d^{-x}, where $x=1.04$, 2.37, and 1.68 for Ni, Co, and Fe, respectively. This scaling is different from the free-electron prediction ($x=2$) which indicates that it is sensitive to the details of the electronic structure. The value and scaling of MR are in quantitative agreement with other band-structure calculations.[13]

The bulk geometry is unrealistic for two reasons: first, the domain-wall widths in bulk materials are much larger than the length of the constriction we would like to consider; second, the mismatch between the bands in the semi-infinite lead and the levels in the constriction, rather than the domain-wall resistance, is the dominant source of resistance in this geometry. The calculation of the conductance and MR of a domain wall in bulk is, nevertheless, instructive because it constitutes a limiting case which the nanocontact conductance and MR must approach when the aspect ratio of the nanocontact approaches zero. The aspect ratio of the nanocontact we define to be w/N, where w is the domain-wall width and N is the lateral size of the constriction.

Therefore, we proceeded to study finite-size constrictions with the domain wall pinned in the constriction. We model the constriction by a wire of length d ML in the direction of the current and a cross section of $N\times N$ unit cells perpendicular to the current. The wire is placed between semi-infinite leads of the same material. When the size of the constriction is negligible compared to the size of the leads, the domain-wall width is predicted[11] to be material independent and determined from the length of the constriction $w=8d/\pi^2$, therefore, we consider the domain-wall width to be equal to the constriction length. We vary the length d from 2 ML for which the first layer is at 0° and the second at 180° to some d_{max} for which the magnetization of consecutive layers changes by $180°/(d-1)$. We vary the supercell size N from 1 representing a zigzag chain of atoms to some N_{max}. The atomic chain ($N=1$) is somewhat unrealistic because we take the atoms to reside on the bcc lattice sites. All spins on the same layer have the same orientation. As the domain-

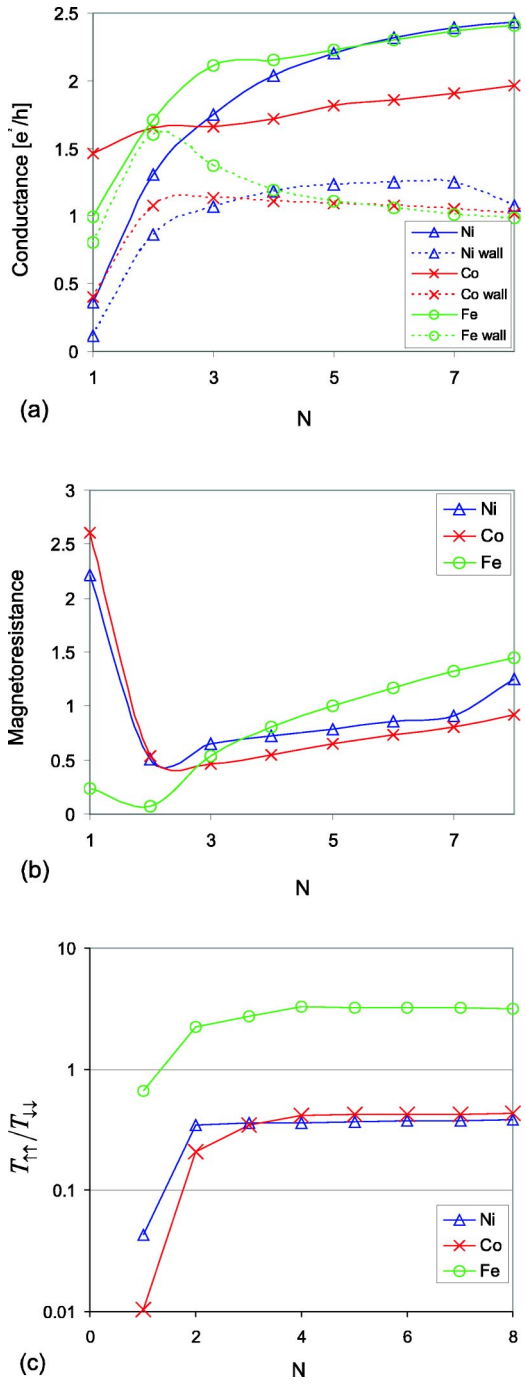

FIG. 2. Nanocontact and domain-wall transmission per unit cell (a) magnetoresistance (b), and ratio of majority to minority conductance (c) in Ni, Co, and Fe nanowires of 2 ML length with semi-infinite leads of the same material.

wall aspect ratio $w/N \to 0$, the result should approach the value of the conductance and MR of the domain wall of width w in bulk.

In Fig. 2(a), the conductance of a nanocontact of length $d=2$ ML in Ni, Co, and Fe is shown as a function of the lateral size of the constriction N. In contrast to the bulk case studied earlier, the conductance of the constriction when all magnetizations are parallel steadily increases with N beginning from a small fraction of the bulk value. This is due to the finite size of the constriction for which there are only a few transverse modes (channels) which match poorly with the bands in the semi-infinite leads. As N is increased, the density of states (DoS) in the constriction resembles more and more the bulk DoS and more channels become open for conductance.

The domain wall acts only on the fraction of the carriers that are permitted through the constriction. At small constriction widths ($N=1,2$), the domain-wall magnetoresistance is very large for the strong ferromagnets Ni and Co and very small for Fe, which is shown in Fig. 2(b). This is due to the fact that the transmission, when the magnetizations are antiparallel to each other, is very low for the cases of Ni and Co and fairly large for the case of Fe.

The constriction appears to transmit some states more readily than others. Figure 2(c) shows the ratio of majority to minority conductance (for no domain wall) for Fe, Co, and Ni. For Co and Ni, the minority conductance is significantly higher than the majority for large constriction widths. This can be understood simply from the fact that there are more Bloch states in the minority channel at the Fermi energy. However, as the constriction becomes smaller, the ratio of minority to majority conductance becomes extremely large, approaching a factor of 100 for Co and 25 for Ni. For Fe, the majority conductance exceeds the minority except for the smallest constrictions which again favor minority transmission. It is tempting to explain the relative enhancement of minority transmission for narrow constrictions in terms of d electrons being transmitted more easily than s electrons. The effect, however, is not as simple as smaller bandwidth equals enhanced transmission. A calculation of the transmission probability through a narrow constriction in a single band tight-binding model as a function of bandwidth yielded a transmission probability independent of bandwidth. The effect may result from a combination of bandwidth and hybridization between bands. Regardless of the origin, the enhanced transmission of minority compared to majority appears to correlate with the very large MR observed for Co and Ni for the narrowest constrictions.

As the constriction gets larger, the MR of Fe becomes comparable to the MR of Ni and Co because the ratio of the total number of propagating states in the minority and majority channels is comparable for all three elements. The opening of new channels for conduction increases the conductance of the constriction towards the bulk value in the absence of a domain wall but the conductance in the presence of the domain wall decreases slightly due to the band mismatch between the majority and minority bands. As a result, the MR increases steadily towards the MR of a 2 ML domain wall in bulk. However, the width at which the constriction is indistinguishable from bulk is significantly greater than the range we are considering.

As the length of the constriction increases and the domain wall becomes thicker, its resistance decreases rapidly so that the conductance of the constriction with and without a wall become closer and closer. In Fig. 3(a), the conductances of a 7 ML constriction of Ni, Co, and Fe are shown as a function of N. There is now very little difference in the conduction through the constriction with and without a domain wall

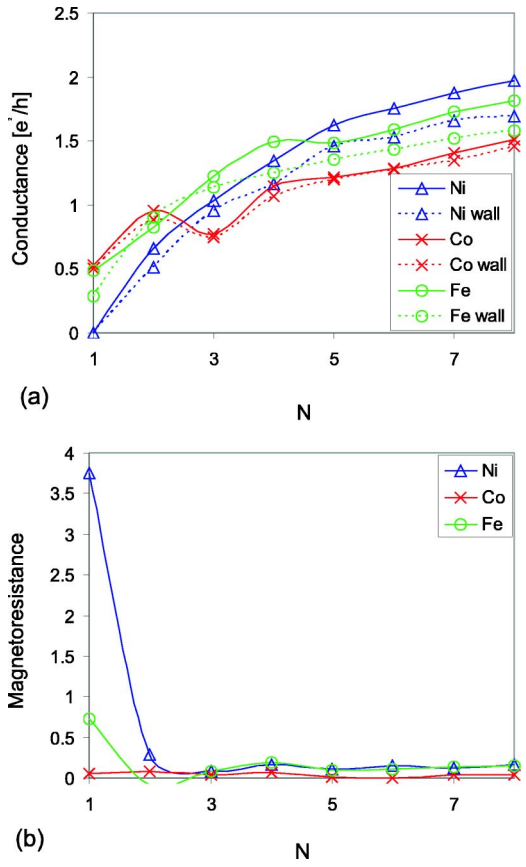

FIG. 3. Nanocontact and domain-wall transmission per unit cell (a) and MR (b) in a Ni, Co, and Fe nanowire of 7 ML length with semi-infinite leads of the same material.

pinned inside. In Fig. 3(b), the corresponding MR is shown. The MR is relatively small for the entire range from atomic width constrictions to bulk except in the case of an atomic width Ni constriction. This could be due to a very poor match between the levels on a single Ni atom and the bands of the semi-infinite Ni leads. In addition, the levels that match are of *d* type, so, they are poorly matched within the domain wall. This enables Ni to show consistently MR of order of 350% at atomic sizes.

In Fig. 4, we show the MR obtained in various constrictions of aspect ratio 1:1 ($w=N$). The MR of all three materials becomes very small for larger *N*. Relatively large MR is obtainable in atomic-size constrictions if the aspect ratio is kept constant. For the same *N*, large MR is obtainable when the aspect ratio gets smaller, i.e., for shorter domain walls.

The shortest possible domain wall is 2 ML thick which is difficult to make if we use the same magnetic material throughout because the constriction has to consist only of a few atoms. However, if we replace the material in the constriction by a nonmagnetic material then effectively the domain wall will always be abrupt regardless of the length of the constriction. In Fig. 5(b), the MR of a Cu wire between Ni and Co semi-infinite leads, as well as a Cr wire between Fe semi-infinite leads is shown. The length of the constriction is 3 ML. At atomic sizes, appreciable MR is only obtainable for the Co-Cu-Co case. However, for larger constrictions both the Co-Cu-Co and the Fe-Cr-Fe systems show

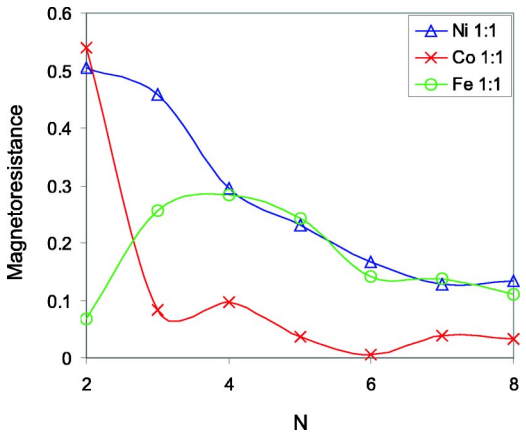

FIG. 4. MR of a Ni, Co, and Fe nanocontact of aspect ratio 1:1 as a function of the size of the constriction (either *N* or *d*).

significant MR. The band matching between the Ni leads and the Cu wire is equally poor for both spin channels at all *N* resulting in very small MR for the entire range of wire sizes. The conductance of the three different systems is shown in Fig. 5(a) for the cases in which the magnetization in the leads are parallel and antiparallel to each other. At atomic sizes, there is a very small difference between the two spin channels in all systems. However, the conductance of the

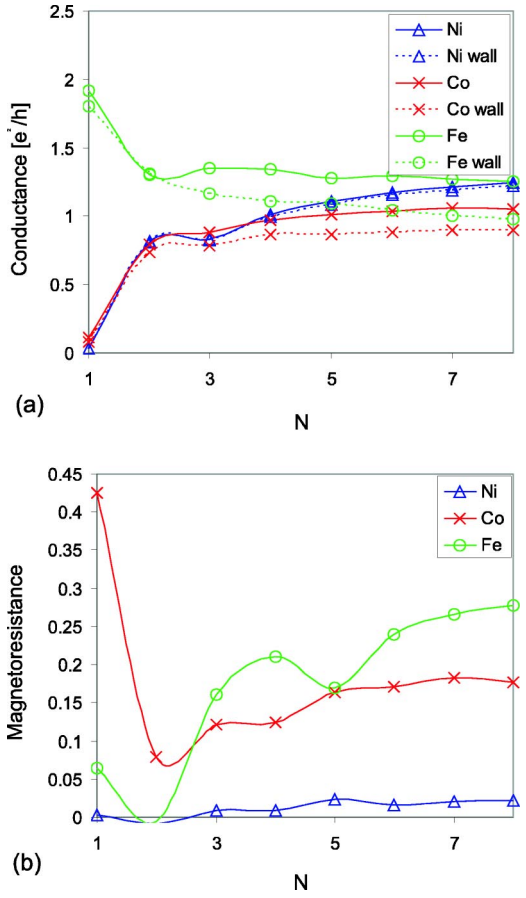

FIG. 5. Parallel and antiparallel conductance per unit cell (a) and MR (b) of a Ni-Cu-Ni, Co-Cu-Co, and Fe-Cr-Fe nanocontact as a function of the size of the constriction.

Co-Cu-Co case is very low, enabling a large MR ratio. The conductance of the Fe-Cr-Fe system is fairly large resulting in a small MR ratio. At larger sizes, there are enough states in the wire to make the band mismatch between the two leads noticeable. Thus, the MR actually increases with the lateral size of the constriction *N*, in contrast to all-magnetic constrictions. This is a result of the fact that the nonmagnetic material allows a sharp domain wall for all sizes. A similar picture is obtained for larger lengths of the nonmagnetic wire. These larger constrictions may be easier to manufacture in practice and their MR actually increases with the size, in contrast to all-magnetic constrictions, which display useful MR ratios only at atomic sizes.

Although, for very narrow constrictions the TB approximation may not be completely adequate it is illustrative of the mechanism of the constrained domain-wall resistance. For a better understanding of this mechanism a more rigorous method of treating the electronic structure in the constriction is needed.

IV. CONCLUSION

We have developed a method to study the resistance of a domain wall pinned by a constriction. We found that the interplay between contact resistance and domain-wall resistance can produce very large MR ratios. The effect is largely due to the fact that narrow constrictions make possible much narrower domain walls than the domain walls common in bulk, thus, the domain wall can have a significant resistance. The weak ferromagnet Fe has an order of magnitude smaller MR at atomic sizes but above this range its MR is comparable with Ni and Co. A particular feature of Ni is that a chain of Ni atoms has consistently large MR regardless of the width of the domain wall, probably due to the poor level matching between the Ni atom and the Ni solid. In general, the very large MR effect is limited to atomic size constrictions.

ACKNOWLEDGMENTS

This research was supported in part by the Oak Ridge Institute for Science and Education and the Oak Ridge National Laboratory. Work at the University of Alabama was supported in part by National Science Foundation MRSEC Grant No. NSF-DMR 0213985 and by DARPA through Office of Naval Research Grant No. N00014-02-1-0590.

[1] M.N. Baibich, J.M. Broto, A. Fert, F. Nguyen Van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. **61**, 2472 (1988).
[2] G. Binasch, P. Grunberg, F. Saurenbach, and W. Zinn, Phys. Rev. B **39**, 4828 (1989).
[3] P.M. Levy, Solid State Phys. **47**, 367 (1994).
[4] M. Gijs and G. Bauer, Adv. Phys. **46**, 285 (1997).
[5] E.Y. Tsymbal and D.G. Pettifor, Solid State Phys. **56**, 113 (2001).
[6] J. Bras and W.P. Pratt, J. Magn. Magn. Mater. **200**, 274 (1999).
[7] *Magnetic Multilayers and Giant Magnetoresistance: Fundamentals and Industrial Applications*, edited by U. Hartmann (Springer, New York, 2000).
[8] N. García, M. Muñoz, and Y.-W. Zhao, Phys. Rev. Lett. **82**, 2923 (1999).
[9] N. García, M. Munízz, G.G. Qian, H. Rohrer, I.G. Saveliev, and Y.-W. Zhao, Appl. Phys. Lett. **79**, 4550 (2001).
[10] N. García, M. Muñoz, and Y.-W. Zhao, Appl. Phys. Lett. **76**, 2586 (2000).
[11] P. Bruno, Phys. Rev. Lett. **83**, 2425 (1999).
[12] J. van Hoof, K. Schep, A. Brataas, G. Bauer, and P. Kelly, Phys. Rev. B **59**, 138 (1999).
[13] J. Kudrnovský, V. Drchal, C. Blaas, P. Weinberger, I. Turek, and P. Bruno, Phys. Rev. B **62**, 15 084 (2000); J. Kudrnovský, V. Drchal, I. Turek, P. Středa and P. Bruno, Surf. Sci. **482-485**, 1107 (2001).
[14] J. Velev and Y.C. Chang, Phys. Rev. B **67**, 144425 (2003); J. Magn. Magn. Mater. **250**, 219 (2002).
[15] J. Velev and Y.C. Chang, Phys. Rev. B **64**, 104404 (2001).
[16] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).
[17] C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J. Phys. C **4**, 916 (1971).
[18] D. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).