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Magnetoresistance in domain walls: effect of randomness

J. Kudrnovský [a,*], V. Drchal [a], I. Turek [b], P. Středa [c], P. Bruno [d]

[a] *Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-182 21 Praha 8, Czech Republic*
[b] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic*
[c] *Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, CZ-162 00 Praha 6, Czech Republic*
[d] *Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*

Abstract

The Landauer–Büttiker approach formulated in the framework of the spin-polarized surface Green function technique and the tight-binding linear muffin-tin orbital method is used to study the magnetotransport in the presence of the domain walls (DW) from first principles. Our approach allows to treat both the ballistic and the diffusive regime of the DW transport on equal footing. The effect of disorder is included in terms of lateral supercells confined to individual atomic layers within a DW. In this paper we apply the method to fcc(0 0 1)-based DW of elemental ferromagnets. © 2001 Published by Elsevier Science B.V.

Keywords: Density functional calculations; Green's function methods; Conductivity; Metal–metal magnetic heterostructures

1. Introduction

Transport in layered materials has been subject of intensive theoretical investigations, in particular in view of the discovery of the giant magnetoresistance (GMR) in metallic multilayers [1,2]. In ferromagnets, the domain walls (DW) are a source of magnetoresistance which recently attracted experimental and theoretical interest (see Ref. [3] and references therein). The DW magnetoresistance (DWMR) is rather small in conventional ferromagnets with DW thicknesses of order of hundredths of atomic layers, but it can be quite large in ferromagnetic ballistic nanocontacts (see Ref. [4] and references therein), where the mean free path is much larger than the DW width. Both the model and realistic calculations [5] agree on that the presence of the DW reduces the ballistic magnetoresistance of the sample. The combined effect of impurity and DW scattering on the magnetoresistance of the sample still needs to be clarified. Some authors [3,6,7] conclude that the presence of the DW in the sample with impurities reduces its conductance while others discuss a possibility of the enhancement of the sample conductance due to the presence of DWs there [8,9]. It should be noted that both reduction [10,11] and enhancement [12,13] of magnetoresistance due to DWs were found also in the experiment. All theoretical studies were, however, done using oversimplified (mostly free-electron like) models. It was clearly demonstrated recently [5] that realistic ab initio calculations can give very different results as compared to model calculations, but until now such calculations were limited to the ballistic

* Corresponding author. Tel.: +420-2-6605-2905; fax: +420-2-8689-0527.
E-mail address: kudrnov@fzu.cz (J. Kudrnovský).

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DWMR only [5]. Realistic calculations for systems with the combined impurity and DW scattering are thus quite interesting.

In this paper we will formulate such an approach within the first principles tight-binding linear muffin-tin orbital (TB-LMTO) method [14] and by employing the Landauer–Büttiker approach to the transport in the framework of the surface Green function formalism. The substitutional randomness in the system will be described in terms of lateral two-dimensional supercells within each disordered sample layer.

2. Formalism

Suppose the magnetic system consists of a semi-infinite left ($\mathscr{L}$) and a semi-infinite right ($\mathscr{R}$) magnetic lead sandwiching a sample of varying thickness (1–N monolayers) (monolayer, ML). Vectors of magnetization in the left and right lead are aligned antiparallel to each other in the case of the DW and parallel to each other for the reference ferromagnetic (F) case. Within a DW the magnetic moments of individual atoms in the layer p are collinear and rotated by an angle θ_p with respect to the reference ferromagnetic system. The angle θ_p changes across the DW from $\theta_p = 0$ to $\theta_p = \pi$, usually a linear profile of θ_p as a function of the layer p is assumed. In principle each atomic layer can be viewed in terms of $n \times n$ supercells ($n \times n$ two-dimensional complex lattice). In order to describe disorder (substitutional binary alloys) it is then necessary to average over different sizes n of supercells and for each n over different occupations of the sites within the supercell with the two constituents involved. It should be noted that the present supercell approach allows to consider also non-collinear alignments of atomic moments within a given layer. We neglect possible layer and lattice relaxations in the system: all our calculations refer to a fcc Co parent lattice.

The resulting expression for the DW conductance C_{DW} is given by (see Ref. [15] for details)

$$C_{\mathrm{DW}} = \frac{e^2}{h}\frac{1}{N_\parallel}\sum_{\mathbf{k}_\parallel} \mathrm{Tr}\{B_{\mathscr{L}}(\mathbf{k}_\parallel, E_{\mathrm{F}})\, g_{1,N}(\mathbf{k}_\parallel, E_{\mathrm{F}}^{+}) \times B_{\mathscr{R}}(\mathbf{k}_\parallel, E_{\mathrm{F}})\, g_{N,1}(\mathbf{k}_\parallel, E_{\mathrm{F}}^{-})\}. \quad (1)$$

Here $N_\parallel$ is the number of $\mathbf{k}_\parallel$-points in the surface Brillouin zone (SBZ), E_{F} is the Fermi energy, $E_{\mathrm{F}}^{\pm} = E_{\mathrm{F}} \pm \mathrm{i}\delta$, and Tr denotes the trace over the angular momentum index $L = (\ell m)$ and over the spin index. It should be noted that due to non-collinear alignments of magnetizations in the DW the spin index is no longer a good quantum number. The quantities $B_{\mathscr{L}}$ and $B_{\mathscr{R}}$ are expressed as

$$B_{\mathscr{L}}(\mathbf{k}_\parallel, E) = \mathrm{i}(\Gamma_{\mathscr{L}}(\mathbf{k}_\parallel, E_+) - \Gamma_{\mathscr{L}}(\mathbf{k}_\parallel, E_-)),$$
$$B_{\mathscr{R}}(\mathbf{k}_\parallel, E) = \mathrm{i}(\Gamma_{\mathscr{R}}(\mathbf{k}_\parallel, E_+) - \Gamma_{\mathscr{R}}(\mathbf{k}_\parallel, E_-)), \quad (2)$$

where $\Gamma_{\mathscr{L}/\mathscr{R}}$ denote the so-called embedding potentials of the left and right lead, respectively, and $g_{1,N}$ and $g_{N,1}$ are off-diagonal blocks of the TB-LMTO Green function of the system evaluated between the terminal layers $p = 1$ and $p = N$ of the DW. It should be noted that the DW Green functions have to be transformed from the reference coordinate system to the local coordinate system in a given layer by the unitary rotation corresponding to the spin 1/2. The TB-LMTO Green function is defined in terms of site-diagonal quantities, the so-called potential functions, which describe the scattering properties of individual atoms, and site-off diagonal quantities, the so-called structure constants, which characterize the lattice structure and are independent of the properties of individual atoms [16]. Only the potential functions need to be transformed as the structure constants are spin independent. All relevant quantities are treated as 2×2-supermatrices in the spin subspace.

The input potentials needed for the evaluation of the layered DW Green function were determined self-consistently for the ferromagnetic alignment using the local spin-density approximation and the TB-LMTO method as described in detail in Ref. [16]. We have then used the frozen-potential approach, i.e., the potentials in the transformed coordinate system (angle θ_p for a given layer p) are the same as those for the reference, ferromagnetic system. This approximation is justified by the so-called magnetic force theorem [17,18]. The potentials of individual atoms A and B of a binary substitutional alloy $\mathrm{A}_{100-x}\mathrm{B}_x$ as simulated by $n \times n$-supercells are approximated by

the potentials of A and B atoms calculated within the coherent potential approximation (CPA). For their evaluation in the present context we refer to Ref. [16]. In this way we neglect very small fluctuations due to a varying local environment of atoms A and B within a supercell.

Finally, we will define the DWMR as $R_{DW}/R_F - 1 = C_F/C_{DW} - 1$, where the subscripts DW, and F refer, respectively, to the DW and reference ferromagnetic alignment (no DW). The resistance $R = 1/C$ where C is the conductance given by Eq. (1).

3. Results and discussion

We performed calculations for both the ballistic and diffusive DW transport assuming an fcc(0 0 1) layer stack and a linear profile for θ_p as a function of the DW thickness. The following model of the DW was considered:

Co(001) semi-infinite left lead	random sample layers	random DW layers with layer-wise rotation angles θ_p	random sample layers	Co(001) semi-infinite. right lead

(3)

In the case of ballistic transport the leads and the sample layers are formed by the same ferromagnetic atoms (Co or Ni) and the thickness of the DW is up to 100 ML. The disordered sample containing a single DW is restricted to a narrow region of 10 ML thick sandwiched by two ferromagnetic Co leads. The sample randomness is modeled by 5×5-supercells simulating a substitutional alloy $Co_{84}X_{16}$ (21 Co atoms and four impurity atoms X in each supercell, X = Cu, Ni, Cr). Configurational average extends over a few configurations only as the current fluctuations for metallic systems were found to be small for 5×5-supercells [15]. The $\mathbf{k}_\parallel$-integration extends over 10 000 points in the full fcc(0 0 1)-SBZ (400 points in the corresponding SBZ of the supercell) and $|\mathrm{Im}\, E_F^{\pm}| = 10^{-7}$ Ry.

3.1. Ballistic domain-wall transport

The dependence of the DWMR and corresponding conductances for an ideal fcc(0 0 1)-Co DW on the DW thickness is plotted in Fig. 1. The zero DW thickness corresponds to an abrupt F/AF interface, where AF denotes antiferromagnetic alignment, and it is included for a completeness. Large values of the DWMR for DW thicknesses on an atomic scale, which are found in nanocontacts [4], can be seen while their values for thicknesses corresponding to classical DWs (hundredths of MLs) are negligibly small (see also Fig. 2). Calculations also unambiguously illustrate that the presence of the DW in the system decreases its ballistic conductance. These results are in a good agreement with similar realistic calculations of the DWMR [5] performed, however, for the case of infinite spin spiral rather than for a single DW like in the present case. A more detailed study of the dependence of the DWMR on the DW thickness $d \in (1,100)$ MLs is plotted in Fig. 2 with the aim to estimate its functional dependence. We compare

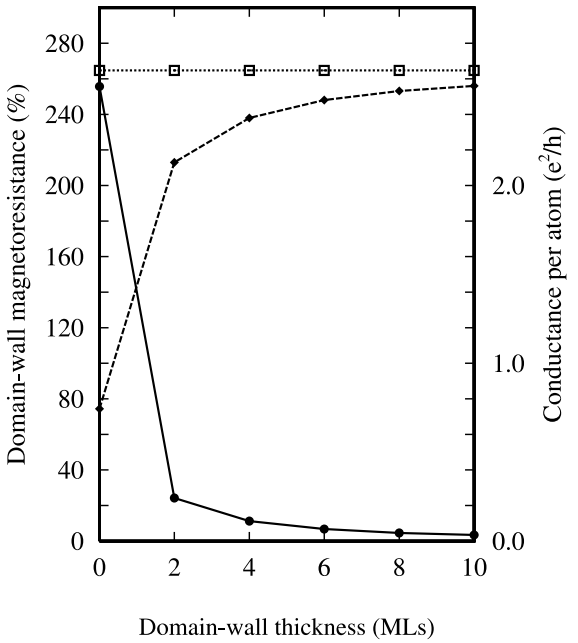

Fig. 1. The ballistic DW transport in fcc(0 0 1)-Co as a function of the DW thickness: DWMR ratio (–●–) and DW conductance per atom (-◆-) together with the reference sample conductance without the DW (-□-). Note the different labelings of vertical axes. Symbols are calculated values and lines serve as a guide for eye.

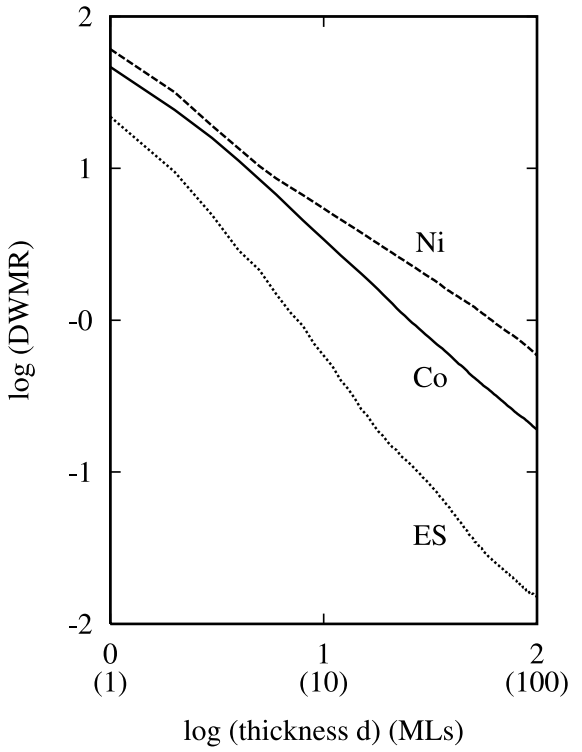

Fig. 2. The ballistic DWMR ratio as a function of the DW thickness of 100 layers calculated for fcc(0 0 1)-based DWs: Co (—), Ni (- - -), and the free-electron model (···). Note logarithmic scales on x- and y-axes.

here cases of fcc(0 0 1) Co- and Ni-based DWs, and their free-electron counterpart simulated here by the empty sphere (ES) model, i.e., the flat-potential model studied by using the same codes as for Co and Ni metals. The so-called potential parameters [14,16] describing the flat potentials were chosen such that the ES bands are close to corresponding sp bands of Co up states including the relative position of the Fermi energy with respect to the band bottom. The exchange splitting of the up- and down-ES bands was chosen as that of the d bands in an fcc Co ferromagnet. We have assumed a linear profile for the angle θ inside the DW. The calculated d^{-2}-dependence for the ES model is in a good agreement with the analytical result of Ref. [5] for a spin spiral. On the other hand, Co- and Ni-DWs behave quite differently, namely, we obtain approximately the d^{-1}-dependence for fcc-(0 0 1)-Ni DWs and the $d^{-1.3}$-dependence for fcc(0 0 1)-Co DWs. This qualitative difference between realistic and model calculations can be explained [5] by the occurrence of many nearly degenerate states close to the Fermi energy. We have also tested other angle profiles in the DW, in particular the angle dependence corresponding to the classical Bloch wall ($\theta(x) \propto \arcsin(\tanh(x/d))$) was also studied with similar results as compared to the linear profile. Scattering of electrons at layers with differently oriented magnetic moments is an origin of the DWMR. It should be mentioned that one can also expect corresponding changes in layer-resolved densities of states, in particular at the Fermi energy. Such a study, however, is beyond the scope of the present paper.

3.2. Diffusive domain-wall transport

We have studied the transport through a DW containing non-magnetic impurities ($Co_{84}Cu_{16}$, spin-independent scattering), as well as magnetic impurities with their moments aligned parallel ($Co_{84}Ni_{16}$) or antiparallel ($Co_{84}Cr_{16}$) to the host Co atoms. The linear dependence of magnetization angle θ_p on the DW thickness was assumed. The results were compared to the reference case of the (ferromagnetic) sample without the DW but containing impurities. The thickness of disordered region was kept fixed (10 ML) but the thickness of the DW introduced inside this disordered region was varied from 10 to 0 ML (abrupt DW) in steps of 2 ML (see Eq. (3)). It should be noted that this is the only way in which the results for a reference disordered region without the DW and the case with the DW can be meaningfully compared. Results are summarized in Fig. 3a–c. The following conclusions can be drawn: (i) The presence of the DW in each case lowers the DW conductance for the present model, in agreement with conclusions of Refs. [3,6,7]. (ii) The DW conductance increases with the DW thickness, and its slope is roughly indirectly proportional to the strength of the disorder in the system. In particular, the largest slope is found for ballistic sample (see Fig. 1). The measure of the disorder strength in the present study is simply the value of the reference conduc-

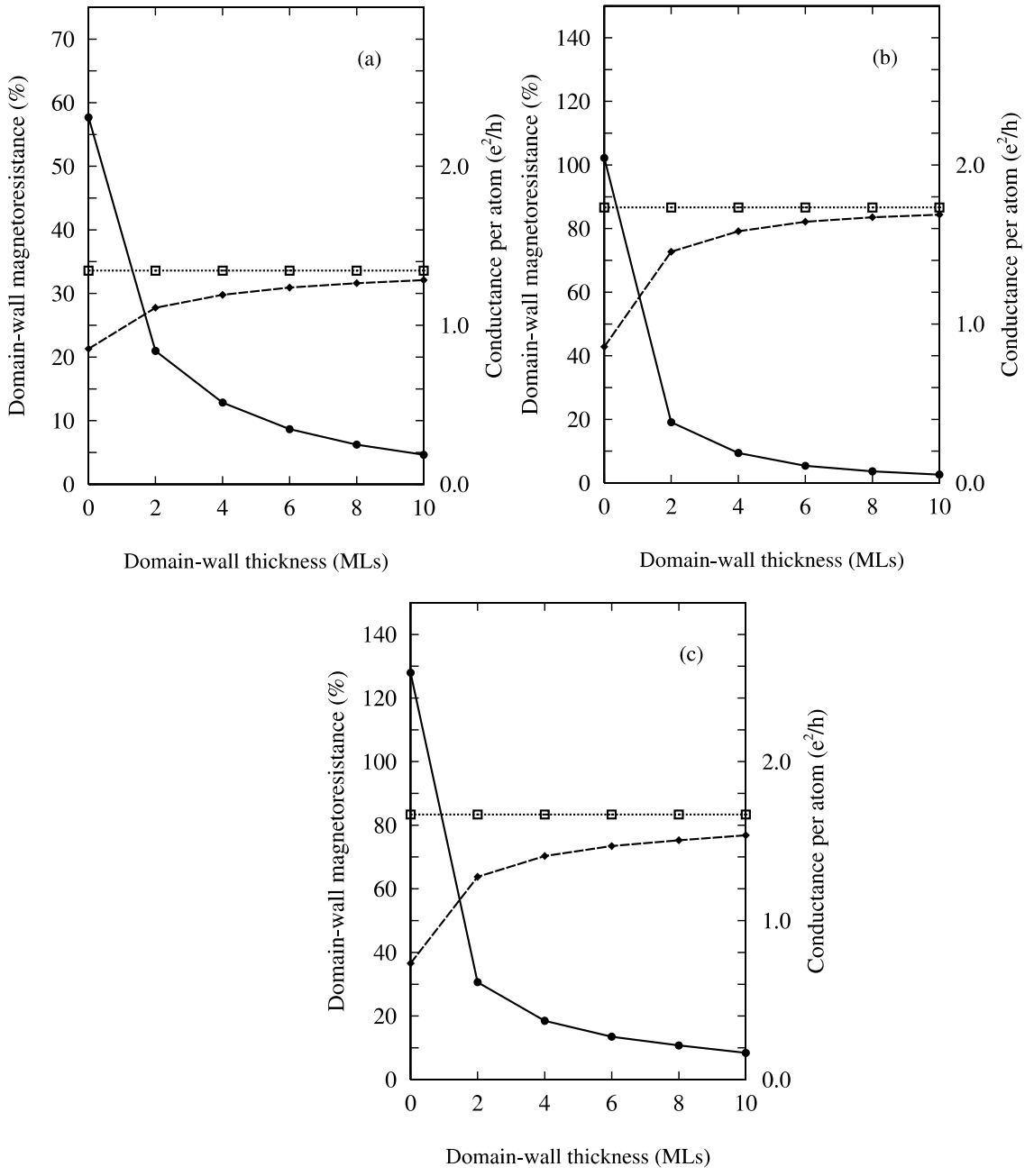

Fig. 3. (a) The diffusive DW transport in fcc(0 0 1)-$Co_{84}Cu_{16}$ as a function of the DW thickness: DWMR ratio (–●–) and DW conductance per atom (-◆-) together with the reference sample conductance without the DW (-□-). Note the different labelings of vertical axes. Symbols are calculated values and lines serve as a guide for eye; (b) the same for fcc(0 0 1)-$Co_{84}Ni_{16}$; (c) the same for fcc(0 0 1)-$Co_{84}Cr_{16}$.

tance across the disordered ferromagnetic sample without the DW which, in turn, is related to the imaginary part of the CPA coherent potential function evaluated at the Fermi energy E_F. It is

zero for an ideal Co, approximately the same for CoNi or CoCr alloys, and the largest for CoCu alloys. The effect of the additional DW scattering thus becomes weaker the stronger the disorder in the systems is. (iii) The DWMR of disordered samples is quickly reduced with increasing DW thickness. Larger differences among various disordered samples can be seen only for very short DWs. This indicates that also in disordered samples the key mechanism for a reduction of the DWMR with the DW thickness is a quick decrease of the rotation angle $\theta(d)$ between layers in DWs as its thickness d increases.

In conclusion, it thus seems that intrinsic mechanisms, i.e., the spin dependence of the scattering at impurities as well as the realistic multiband electronic structure cannot explain an increase of the sample conductance due to the presence of DW observed in some recent experiments.

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