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Ab initio theory of perpendicular transport in layered magnetic systems

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Abstract

The spin-polarized electron conductance perpendicular to layers of a random magnetic multilayer is evaluated from first principles. We employ the Landauer formulation in the framework of the tight-binding linear muffin-tin orbital approach and the surface Green-function technique. The disorder in the bulk and at interfaces is included in terms of lateral supercells confined to individual atomic layers. The application is made to interleave and separate multilayers with a different order of magnetic and non-magnetic layers with generally non-collinear alignments of layer magnetizations.

Keywords: Magnetoresistance – theory; Ferromagnetic multilayers; Disorder – alloys; Electronic structure

Transport in layered materials is subject of intensive theoretical investigations, in particular in view of the discovery of the giant magnetoresistance (GMR) in metallic multilayers. From the theoretical point of view the current perpendicular to plane geometry (CPP) differs from the more common current in plane (CIP) geometry [1,2] in several aspects: the high symmetry of the CPP geometry makes its theory easier which is particularly convenient for an ab initio study in this paper, it is better suited for testing of theoretical models, and it gives larger value of the GMR as compared to the CIP geometry.

In this contribution, as motivated by a recent paper [3], we wish to present the ab initio study of the effect of order of magnetic and non-magnetic layers on the CPP–GMR of interleaved and separated multilayers. In particular, the emphasis is put on the effect of non-collinear alignments of layer magnetizations omitted in a previous study [3]. In addition, we consider two possible type of *disorder* in a system, namely an alloying in the spacer and the interdiffusion at interfaces between magnetic and non-magnetic layers. Recently two related ab initio studies of the CPP–GMR analyzing the effect of disorder in the system either in magnetic and/or non-magnetic layers and at interfaces between them have appeared [4,5]. The electronic structure of a multilayer is described in the framework of the tight-binding linear muffin-tin orbital (TB-LMTO) approach while realistic boundary conditions at the sample-lead interfaces (semi-infinite leads) were included via the surface Green-function technique. The substitutional disorder in the sample is included in terms of lateral $n \times n$-supercells confined to individual atomic layers while the sample leads are assumed to be ideal. We assume that orientations of moments in magnetic layers may be in general non-collinear. In the spirit of Landauer

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formulation the conductance is determined by the corresponding transmission coefficient.

The resulting expression for the conductance $\mathscr{C}$ is given by (see Ref. [4] for details)

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

Here $N_\parallel$ is the number of $\mathbf{k}_\parallel$-points in the surface Brillouin zone (SBZ), E_F is the Fermi energy, $E_\mathrm{F}^\pm = E_\mathrm{F} \pm \mathrm{i}\delta$, Tr denotes the trace over the angular momentum index $L = (\ell m)$ and over the spin index, and θ is the angle between magnetizations in magnetic layers. It should be noted that due to non-collinear alignments of magnetizations the spin index is no longer a good quantum number. All quantities are therefore treated as 2×2-supermatrices in the spin subspace. Properties of semi-infinite leads are fully described by the quantities $B_{\mathscr{L}}$ and $B_{\mathscr{R}}$ which can be expressed in terms of lead surface Green functions (see Ref. [4] for more details), while $g_{1,N}$ and $g_{N,1}$ are layer off-diagonal blocks of the TB-LMTO Green function of the whole system evaluated between the terminal sample layers $p = 1$ and $p = N$. Finally, we will define the magnetoresistance ratio as $\mathrm{MR} = \mathscr{R}(\theta)/\mathscr{R}(0) - 1 = \mathscr{C}(0)/\mathscr{C}(\theta) - 1$, where $\mathscr{R}(\theta) = 1/\mathscr{C}(\theta)$, and $\mathscr{C}(\theta)$ is given by Eq. (1).

The potentials of individual atoms of a binary substitutional alloy $A_{100-x}B_x$ as simulated by $n \times n$-supercells are approximated by the potentials of A and B atoms calculated within the coherent potential approximation (CPA), i.e., we neglect very small fluctuations due to a varying local environment of atoms A and B within a supercell. In addition, we used the same potentials for the reference ferromagnetic system and for the system with non-collinear alignment of magnetic moments which is justified by the magnetic force theorem [7,8]. For more details see Refs. [4,6].

We have performed calculations for two types of FCC(0 0 1)-multilayers sandwiched by ideal Cu(0 0 1) leads which differ from each other only in the ordering of magnetic and non-magnetic layers, namely the the interleaved (IL) and separated (SP) multilayers. The IL geometry is described by the structure formula $[\mathrm{M}(m_1)/\mathrm{S}(s)/\mathrm{M}(m_2)/\mathrm{S}(s)]_4$ while the SP geometry can be described as $[\mathrm{M}(m_1)/\mathrm{S}(s)]_4\,[\mathrm{M}(m_2)/\mathrm{S}(s)]_4$, where $m_1 = 10$ Co monolayers (MLs) and $m_2 = 5$ Co ML for both IL and SL samples. We have considered two models of randomness: (i) Co/Cu multilayers with $Cu_{50}Co_{50}$ *interface interdiffusion* at adjoining two interface layers, and (ii) $Co/Cu_{84}Ni_{16}$ multilayers with *random spacer* slabs and flat interfaces. The spacer thickness is 5 Cu ML in the former case and 5/15 CuNi ML in the latter case so that the total sample thicknesses are 95 and 165 ML, respectively. Sample interfaces with leads are assumed to be ideal and we neglect possible lattice and layer relaxations (parent FCC(0 0 1) Cu layers). The sample randomness is modeled by 5×5-supercells simulating a substitutional alloy $Cu_{84}Ni_{16}$ (21 Cu atoms and 4 Ni atoms) in each supercell, or a substitutional alloy $Cu_{50}Co_{50}$ (25 Cu and 25 Co atoms in two adjoining interface layers). Configurational average extends over 5 configurations in each case and current fluctuations for present systems were found to be only 1–2% (see also Ref. [4]).

Magnetic moments in narrower magnetic layers (5 Co MLs) are rotated with respect to thicker layers by an angle $\theta = 0^\circ$, $45^\circ, 90^\circ$, 135°, and 180° (only $\theta = 0^\circ$, 90°, 180° for a larger sample). Reference parallel (P) and antiparallel (AP) alignments correspond to $\theta = 0$ and $\theta = 180$, respectively. The $\mathbf{k}_\parallel$-integration extends over 1600 points in the full FCC(0 0 1)-SBZ (64 points in the SBZ of the 5×5-supercell) and $|\mathrm{Im}\, E_\mathrm{F}^\pm| = 10^{-7}$ Ry. It should be noted that a similar system was studied in the framework of the empirical multiband tight-binding model employing the Anderson level disorder in both Co and Cu layers of the same thicknesses (10 ML) for two-repetitions (sample thickness of 70 ML [3]). The parameters of level disorder were fitted to reproduce approximately bulk resistances of pure Cu and Co samples. The most important difference of our study as compared to Ref. [3] is the non-collinear alignment of magnetic moments which simulates the influence of external magnetic field on magnetic layers with different coercitivities.

We have first evaluated the conductance of an FCC(0 0 1) trilayer 5 Co|n $Cu_{84}Ni_{16}$|5 Co ($n = 1-600$ ML) sandwiched by ideal semi-infinite Cu leads. The bulk resistivity of the alloy spacer was estimated from the slope of the linear dependence of the resistance as a function of the spacer thickness while the interface resistance was estimated from the offsets of the parallel (P) and antiparallel (AP) resistances. We have found the resistivity of FCC-$Cu_{84}Ni_{16}$ alloy 11.8 μΩ cm as compared to the experimental value [9] of 15.3 μΩ cm. Recent theoretical calculations based on the KKR-CPA method including vertex corrections give of 13.32 μΩ cm [10] for FCC-$Cu_{80}Ni_{20}$. It should be noted that present supercell calculations include effect of vertex corrections properly. The interface resistivity is characterized by dimensionless quantity $\gamma = (AR^\downarrow - AR^\uparrow)/(AR^\downarrow + AR^\uparrow)$ and by $AR^* = (AR^\downarrow + AR^\uparrow)/4$, where R^σ ($\sigma = \uparrow, \downarrow$) denotes interface resistance and A is the area of interface. Typical experimental results for Cu/Co multilayers [2] are $\gamma = 0.71$–0.77 and $AR^* = 0.38-0.51\,\mathrm{f\Omega\,m^2}$. Present results $\gamma = 0.76$ and $AR^* = 0.56\,\mathrm{f\Omega\,m^2}$ compare well with the experiment. Theoretical results [5] for parallel and antiparallel interface resistances for ballistic Co/Cu system [11] are 0.35 and $1.90\,\mathrm{f\Omega\,m^2}$, respectively, 0.33 and $1.79\,\mathrm{f\Omega\,m^2}$ for Co/Cu/Co system with interface disorder [5] to be compared to $0.27/2.00\,\mathrm{f\Omega\,m^2}$ in the

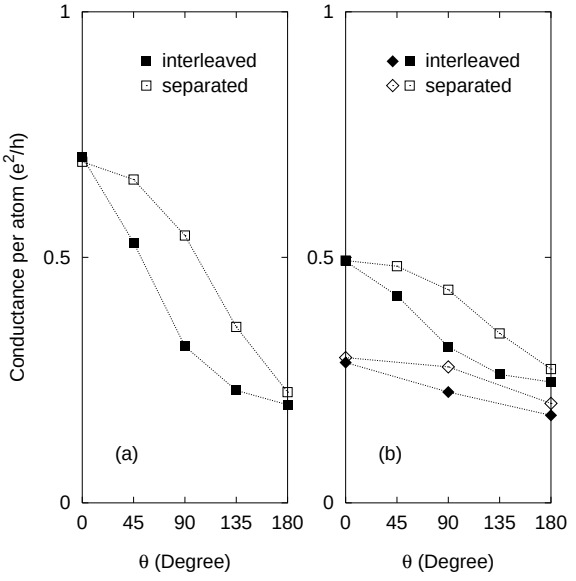

Fig. 1. The conductance of interleaved (full symbols) and of separated (empty symbols) multilayeres: (a) interdiffusion at sample interfaces, and (b) alloying in spacer layers (squares: 5 ML spacer slabs, diamonds: 15 ML spacer slabs). The lines serve as a guide for eye.

present $Co/Cu_{84}Ni_{16}/Co$ system. The interface resistance thus seems to be determined primarily by differences in the electronic structure of magnetic and spacer layers at sample interfaces while the influence of various kinds of disorder is less important. The present approach thus gives a reasonable agreement with existing experimental and theoretical data for both the bulk and interface resistivites.

The results for IL and SP multilayers are presented in Fig. 1 and the following conclusions can be drawn: (i) The differences between IL and SP geometries are quite small for collinear alignments (P and AP), for P in particular; (ii) The rotated samples show a pronounced dependence on the layer order in a qualitative agreement with the experiment [3]. There is, however, no simple relation between the angle θ and the value of the applied external field in the experiment [3]. The results also indicate that above differences become smaller with increasing thicknesses of disordered spacer slabs (see Fig. 1b). On the contrary, the differences between the IL and SP samples increase with number of repetitions, as it can be concluded by comparing results for 2 and 4 repetitions, again in an agreement with [3]; (iii) The conductance of the SP sample is larger as compared to the IL sample in a qualitative agreement with experiment [3]: electrons passing through the IL sample suffer additional spin scatterings at interfaces with thicker and narrower magnetic slabs with rotated magnetizations as compared to the SP sample with magnetizations rotated only at the interface which separates thicker and narrower slabs; (iv) The parallel alignment for interdiffusion case (Fig. 1a) has larger conductance as the number of disordered layers is smaller as compared to the case of random spacer sample.

In conclusion, we have found only small differences between the IL and SP geometries for P and AP alignments but non-negligible deviations for samples with rotated magnetizations. These differences become larger with increasing number of repetitions but the opposite tendency is observed for increasing number of disordered layers. Further studies are thus needed to verify the validity of the series resistor model [12] for this system.

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References

[1] M.A.M. Gijs, G.E.W. Bauer, Adv. Phys. 46 (1997) 285.
[2] J. Bass, W.P. Pratt Jr., J. Magn. Magn. Mater. 200 (1999) 274.
[3] D. Bozec, M.A. Howson, B.J. Hickey, S. Shatz, N. Wiser, E.Y. Tsymbal, D.G. Pettifor, Phys. Rev. Lett. 85 (2000) 1324.
[4] J. Kudrnovský, V. Drchal, C. Blaas, P. Weinberger, I. Turek, P. Bruno, Phys. Rev. B 62 (2000) 15084.
[5] K. Xia, P.J. Kelly, G.E.W. Bauer, I. Turek, J. Kudrnovský, V. Drchal, Phys. Rev. B 63 (2001) 064407.
[6] I. Turek, V. Drchal, J. Kudrnovský, M. Šob, P. Weinberger, Electronic Structure of Disordered Alloys, Surfaces and Interfaces, Kluwer Academic Publishers, Boston, 1997.
[7] A. Oswald, R. Zeller, P.J. Braspenning, P.H. Dederichs, J. Phys. F 15 (1985) 193.
[8] A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, V.A. Gubanov, J. Magn. Magn. Mater. 67 (1987) 65.
[9] J. Bass, K.H. Fisher, (Eds.) Landolt–Börnstein, New Series, Vol. III(15a), Springer, Berlin, 1982, p. 177.
[10] A. Vernes, H. Ebert, J. Banhart, unpublished.
[11] K.M. Schep, P.J. Kelly, G.E.W. Bauer, Phys. Rev. B 57 (1998) 8907.
[12] T. Valet, A. Fert, Phys. Rev. B 48 (1993) 7099.