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2004 J. Phys.: Condens. Matter 16 S5579

(http://iopscience.iop.org/0953-8984/16/48/014)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) S5579–S5586 PII: S0953-8984(04)81404-8

Spin-dependent transport in ferromagnet/semiconductor/ferromagnet junctions: a fully relativistic approach

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Received 28 May 2004
Published 19 November 2004
Online at stacks.iop.org/JPhysCM/16/S5579
doi:10.1088/0953-8984/16/48/014

Abstract

We present a fully relativistic generalization of the Landauer–Büttiker formalism that has been implemented within the framework of the spin-polarized relativistic screened Korringa–Kohn–Rostoker Green function method.

This approach, going beyond the two-current model, supplies a more general description of the electronic transport. It is shown that the relativistic conductance can be split in terms of individual spin-diagonal and spin-off-diagonal (spin-flip) components, which allows a detailed analysis of the influence of spin–orbit-coupling-induced spin-flip processes on the spin-dependent transport.

We apply our method to calculate the ballistic conductance in Fe/GaAs/Fe magnetic tunnel junctions. We find that, by removing the spin selection rules, the spin–orbit coupling strongly influences the conductance, not only qualitatively but also quantitatively, especially in the anti-parallel alignment of the magnetization in the two Fe leads.

1. Introduction

Ab initio methods developed within the spin density functional theory in its local density approximation (LSDA), using either Kubo–Greenwood or Landauer–Büttiker formalisms, are nowadays a sound basis for investigations on spin-dependent transport between two ferromagnetic electrodes separated by either an insulator or a semiconductor.

The first of these studies were presented by Butler, MacLaren and coworkers [1, 2]. Since then, an impressive theoretical work followed, meant to give a reasonable description of this phenomenon, a comprehensive recent review in this field being given by Tsymbal *et al* [3].

Most of the theoretical investigations done so far have treated the two spin subsystems participating in conductance as being independent of one another (two-current model), introducing in this way a supplementary spin-filter. The fully relativistic calculations that can be found in the literature deal with the transport on the basis of the Kubo–Greenwood formalism [4]. However, a detailed investigation on how spin–orbit coupling, a pure relativistic effect, influences the conductance by mixing the different spin channels is still missing.

It is the purpose of this paper to make a first step in filling this gap. In doing this, we give a fully relativistic formulation of the Landauer–Büttiker expression for conductance. We show that this can be separated, to a good accuracy, into spin-diagonal and spin-off-diagonal (spin-flip) components. This procedure is applied to Fe/GaAs/Fe junctions as a test case. A comparison with previous results for compatible systems, obtained within the two-current model, allows a qualitative and quantitative analysis of the effects induced by spin–orbit coupling.

2. Theoretical framework

The electronic ground state and transport properties have been determined on the basis of the screened Korringa–Kohn–Rostoker Green function method (KKR-GF) combined with the decimation technique for two-dimensional systems [5, 6]. Within this scheme, the one-electron retarded Green function $G^+(\vec{r}, \vec{r}'; E)$ at energy $z = E + \mathrm{i}\varepsilon$ is expressed in terms of the so-called structural Green function matrix $\underline{G}^{nn'}(\vec{k}_\parallel, z)$, which describes the propagation between the sites n and n' located at $\vec{R}_n$ and $\vec{R}_{n'}$. Here n is a compressed index for site α in the two-dimensional unit cell of layer I, $\vec{r} = \vec{R}_n + \vec{\rho}$ and $\vec{R}_n = \vec{R}_I + \vec{\chi}_\nu + \vec{r}_\alpha$. Further details on notation and method of calculation can be found elsewhere [6]. Calculations based on this method are nowadays routinely performed and one can choose either a non- or a fully relativistic representation for the basis functions.

In calculating the electronic transport properties we neglect any nonlinear effects caused by a finite bias voltage applied to the system and restrict ourselves to the linear regime. Within this limit, Baranger and Stone [7] have shown that the ballistic conductance between two leads can be expressed as the flux of the conductivity tensor $\sigma(\vec{r}, \vec{r}')$ into these leads. They also could prove, for the free electron case, that their expression for conductance is equivalent to the Landauer–Büttiker formula [8]. More recently, Mavropoulos *et al* [9] extended the proof to the case of Bloch electrons. Our following discussion is based on this derivation and we are referring to their work for further details.

The two formalisms mentioned above for the calculation of electronic ground state and transport properties have been implemented in a fully relativistic mode in a similar way as was done before for the conventional KKR method [10]. This leads to a very general and flexible scheme which allows one to account for spin polarization and all relativistic effects—including spin–orbit coupling (SOC)—on equal footing.

In the relativistic representation $\Lambda = (\kappa, \mu)$ the conductance between two layers (atomic planes) I and I' of a two-dimensional system is given by ($n \equiv (\alpha, I)$)

$$g = \frac{e^2}{h} \frac{1}{A_{\mathrm{BZ}}} \int_{\mathrm{BZ}} \mathrm{d}^2 k_\parallel \, g(\vec{k}_\parallel)$$

with

$$g(\vec{k}_\parallel) = N_\Lambda^2 \sum_{\substack{\alpha \in I \\ \alpha' \in I'}} \mathrm{Tr}\left[\underline{J}^n(z_\mathrm{F}, z_\mathrm{F}^*) \underline{G}^{nn'}(\vec{k}_\parallel, z_\mathrm{F}) \underline{J}^{n'}(z_\mathrm{F}^*, z_\mathrm{F}) \underline{G}^{nn'*}(\vec{k}_\parallel, z_\mathrm{F})\right] \tag{1}$$

the $\vec{k}_\parallel$-resolved conductance, calculated at the complex energy $z_\mathrm{F} = E_\mathrm{F}+\mathrm{i}0$, with E_F the Fermi energy of the system.

This equation—formally identical with that given by Mavropoulos *et al* [9]—contains the structural Green function matrix, $\underline{G}^{nn'}$, a prefactor depending on several universal constants N_Λ and the matrix of the perpendicular component of the current density operator, $\underline{J}^n$. The latter is calculated within the Wigner–Seitz cell of volume V_n at site n. Here and below, if not otherwise stated, the matrices are labelled by the relativistic quantum numbers, i.e. $(\underline{A})_{\Lambda\Lambda'} = A_{\Lambda\Lambda'}$.

Adopting a fully relativistic treatment means in particular that the single-site problem is solved for the Dirac Hamiltonian (we follow here the notations of [10])

$$\widehat{\mathcal{H}}_\mathrm{D} = c\vec{\alpha}\,\vec{p} + \beta mc^2 + V_\mathrm{eff}(\vec{r}) + \beta\vec{\sigma}\,\vec{B}_\mathrm{eff}(\vec{r}), \tag{2}$$

and that the current density operator has the form $\vec{j} = ec\vec{\alpha}\delta(\vec{r}-\vec{r}')$.

The current density matrix elements can be obtained straightforwardly using this form of the operator. An equivalent formulation, which is more advantageous for a phenomenological interpretation, is obtained using the anti-commutator $[\widehat{\mathcal{H}}_\mathrm{D}, \vec{\alpha}\vec{a}\delta(\vec{r}-\vec{r}')]_+$, with $\vec{a}$ a complex polarization vector normalized to unity. In this way, the perpendicular component of the current density matrix element $\Lambda\Lambda'$ is given by

$$J^n_{\Lambda\Lambda'}(z, z^*) = \frac{1}{V_n}\int_{S_n} \mathrm{d}^2 r\, R^{n\times}_\Lambda(z) a_\perp J_\perp R^n_{\Lambda'}(z^*) \tag{3}$$

with the auxiliary operator $\vec{a}\,\vec{J}$ defined as

$$\vec{a}\,\vec{J} = \overleftrightarrow{\nabla}\,\vec{a} + \frac{\mathrm{i}\,V}{c}\vec{\alpha}\vec{a} - \frac{\mathrm{i}\,B}{c}\beta(\vec{\alpha}\times\vec{a})_\perp \tag{4}$$

and $N_\Lambda = c^2/(E_\mathrm{F}+2mc^2)$. One has to note here that the right-hand and left-hand side solutions R_Λ and $R^\times_\Lambda$ of the Dirac equation need to be considered [11] for both complex energies z and z^* [12].

Within a relativistic representation the electron spin is no longer a constant of motion. The expression above does not treat the scattering region as two independent spin subsystems in which spin-flip processes are *a priori* suppressed and it is therefore far more general. However, especially when investigating spin-dependent phenomena, one might be interested in interpreting the results in the more familiar terms of individual spin contributions. On the other hand, the decomposition into spin-diagonal and spin-off-diagonal terms would also allow one to identify and analyse in detail, within a relativistic treatment, the particular contribution of SOC to the investigated process. We show below that, without leaving the relativistic framework, such an analysis is possible without making use of any severe approximation.

We proceed by recalling that the matrix of the Clebsch–Gordon coefficients $S_{\Lambda\mathcal{L}} = C(l\,\frac{1}{2}\,j;\mu-m_s,m_s)$ provides a unitary transformation between the relativistic $\Lambda = (\kappa,\mu)$ and the non-relativistic $\mathcal{L} = (l, m_l, m_s) = (L, m_s)$ representation [13]:

$$\mathcal{A}_{\mathcal{L}\mathcal{L}'} = \sum_{\Lambda\Lambda'} S_{\Lambda\mathcal{L}} A_{\Lambda\Lambda'} S^\dagger_{\mathcal{L}'\Lambda'}. \tag{5}$$

The matrices $\underline{J}$ and $\underline{G}$ in equation (1) then transform as

$$\underline{J} \mapsto \underline{\mathcal{J}} = \begin{pmatrix} \underline{\mathcal{J}}^{\uparrow\uparrow} & \underline{\mathcal{J}}^{\uparrow\downarrow} \\ \underline{\mathcal{J}}^{\downarrow\uparrow} & \underline{\mathcal{J}}^{\downarrow\downarrow} \end{pmatrix} \qquad \underline{G} \mapsto \underline{\mathcal{G}} = \begin{pmatrix} \underline{\mathcal{G}}^{\uparrow\uparrow} & \underline{\mathcal{G}}^{\uparrow\downarrow} \\ \underline{\mathcal{G}}^{\downarrow\uparrow} & \underline{\mathcal{G}}^{\downarrow\downarrow} \end{pmatrix} \tag{6}$$

with $\uparrow$ and $\downarrow$ representing the two possible m_s values and each of the matrices $\underline{\mathcal{A}}^{m_s m'_s}$ indexed as $\mathcal{A}^{m_s m'_s}_{LL'}$.

The next step is to note that spin-off-diagonal elements in the current density matrices $\underline{\mathcal{J}}$ occur only because of the last term in equation (4). These spin-mixing or spin-flip terms

are, in the local frame of reference of each atom, produced by the SOC alone. For transition metals the spin-flip term $B\sigma_z/c$ is about four orders of magnitude smaller than the first one. Consequently, one can make the following reasonable approximation:

$$\underline{\mathcal{J}} = \begin{pmatrix} \underline{\mathcal{J}}^{\uparrow\uparrow} & \underline{0} \\ \underline{0} & \underline{\mathcal{J}}^{\downarrow\downarrow} \end{pmatrix} \tag{7}$$

and allow spin-flip processes to occur only as a result of the scattering in between the two leads. With this approximation and making use of the properties of the trace, equation (6) allows us to rewrite the sum over α and α' in equation (1) as

$$\sum_{\alpha\alpha'} \mathrm{Tr}\big[\underline{J}^{n}\underline{G}^{nn'}\underline{J}^{n'}\underline{G}^{nn'*}\big] \approx \sum_{\alpha\alpha'}\sum_{m_s,m_s'} \mathrm{Tr}\big[\underline{\mathcal{J}}^{n,m_s m_s}\underline{\mathcal{G}}^{nn',m_s m_s'}\underline{\mathcal{J}}^{n',m_s' m_s'}\underline{\mathcal{G}}^{nn',m_s' m_s *}\big] \tag{8}$$

with the last trace performed over the non-relativistic quantum numbers L. By comparing with equation (1), we can then define the spin-decomposed conductance terms $\widetilde{g}^{m_s m_s'}$ through the following equation:

$$\widetilde{g}^{m_s m_s'} \propto \mathrm{Tr}\big[\underline{\mathcal{J}}^{n,m_s m_s}\underline{\mathcal{G}}^{nn',m_s m_s'}\underline{\mathcal{J}}^{n',m_s' m_s'}\underline{\mathcal{G}}^{nn',m_s' m_s *}\big]. \tag{9}$$

Thus the exact relativistic expression for conductance, equation (1), can be approximated by the sum over individual spin-diagonal and spin-flip contributions $\widetilde{g}^{m_s m_s'}$ in both $\vec{k}_\parallel$-resolved and $\vec{k}_\parallel$-integrated cases

$$g \approx \widetilde{g} = \sum_{m_s,m_s'} \widetilde{g}^{m_s m_s'} \tag{10}$$

which is exactly the formula one would expect if the 'fully relativistic resistor' $R = 1/g$ were replaced by the four parallel 'spin-decomposed' resistors $\widetilde{R}^{m_s m_s'} = 1/\widetilde{g}^{m_s m_s'}$.

3. Computational details

As a case study for our relativistic implementation we have chosen an As-terminated Fe/n(GaAs)/Fe system. The Ga-terminated system, not discussed here, shows the same qualitative behaviour.

In a first step, the electronic structure has been determined self-consistently within the LSDA, with the parametrization for the exchange–correlation potential proposed by Vosko *et al* [14]. For the SCF calculations the junction was modelled by a 6Fe/9(GaAs)/5Fe slab sandwiched between two semi-infinite Fe leads. As has also been found by other authors for similar systems [15, 16], this slab thickness suffices to obtain for the middle GaAs layers an essentially semiconductor bulklike behaviour.

The parent lattice considered was that of the zinc-blende structure, having the lattice constant $a = 5.6536$ Å. All the effects connected with interface interdiffusion, disorder or lattice relaxation have been ignored. While a collinear magnetic configuration has been considered, calculations have been performed for two different cases, a parallel (P) and an anti-parallel (AP) alignment of the magnetization in the two Fe leads.

For the spin-dependent transport investigations the semiconductor thickness has been varied between $n = 21$ and 61 atomic layers. A frozen potential model as used by Mavropoulos *et al* [16] has been used to describe these thick junctions, with the Fermi energy lying in the middle of the gap (occurring in the inner semiconductor layers). In contrast to [16], where the spin injection was studied, an extra potential shift, meant to mimic the gate voltage, has not been applied here. Thus, the results to be presented below correspond to a tunnelling conductance regime. For each of the spacer thicknesses the calculations have been done in the two magnetic configurations P and AP, which allows us to determine the tunnelling magnetoresistance (TMR) ratio.

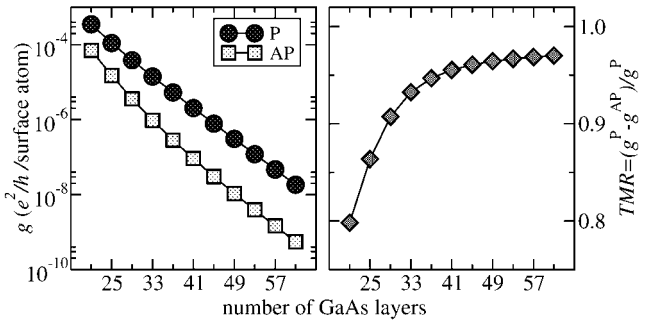

Figure 1. Left, tunnelling conductance for Fe/n(GaAs)/Fe trilayer system as a function of GaAs thickness n, calculated using the relativistic expression, equation (1), for parallel (P) and anti-parallel (AP) alignment of the magnetization in the two Fe leads; right, the corresponding pessimistic TMR ratio $(g^{\mathrm{P}} - g^{\mathrm{AP}})/g^{\mathrm{P}}$. The thickness of one atomic layer is $d = a/4 = 1.4134$ Å.

4. Results and discussion

As deduced from previous investigations, e.g. [2, 17, 18], the main mechanisms governing the ballistic tunnelling are the symmetry of the electronic states of the ferromagnetic leads and how they couple to the evanescent states in the semiconductor, the resonant interfacial states present in the minority spin channels, and the character of chemical bonding at the metal/semiconductor interface. A detailed discussion is beyond the purpose of this paper, so we will restrict ourselves to showing how inclusion of SOC may influence these features.

We present in figure 1 the results of our calculations for the As-terminated Fe/n(GaAs)/Fe junction as a function of the number of semiconductor layers n. In the left-hand panel the relativistic tunnelling conductance is shown (one notes the logarithmic scale), as obtained from equation (1), corresponding to the two different magnetic alignments P and AP. From these two quantities, the (pessimistic) TMR ratio defined by $T = (g^{\mathrm{P}} - g^{\mathrm{AP}})/g^{\mathrm{P}}$ can be determined. The results can be seen in the right-hand panel of figure 1.

Our results are qualitatively comparable with those obtained by MacLaren *et al* [2] for the relatively similar junction Fe/ZnSe/Fe. We refer to their results, but, of course, the main features observed in other calculations dealing with the tunnelling ballistic conductance are the same.

As expected, the conductance decreases exponentially with the semiconductor thickness, for both magnetic alignments. The difference in slope is reflected in the abrupt increase of the TMR ratio for thicker barriers. However, in contrast to the situation presented by MacLaren *et al* [2], the saturation in TMR is far from being reached at comparable thicknesses of the junction (their interval corresponds approximately to the first half of our investigated range).

Qualitative differences can also be observed inspecting the results of figure 2. Here the distribution of conductance over the individual channels around the central point $\bar{\Gamma}$ in the two-dimensional Brillouin zone (2DBZ) is shown for the P (left-hand panel) and AP (right panel) alignment (again on a logarithmic scale).

Several already known characteristics—e.g. the strong peak at the centre of the 2DBZ in the P alignment which becomes narrower for thicker spacer; the resonant peaks out of the normal incidence in the AP alignment—can be recognized in our results. One notes, however, that the structure of $g(\vec{k}_{\parallel})$ in the AP case tends to become the same as for P as the thickness of the semiconductor increases, whereas previous calculations, based on a non-relativistic treatment, always found a local minimum in $g^{\mathrm{AP}}(\vec{k}_{\parallel})$ at the $\bar{\Gamma}$ point.

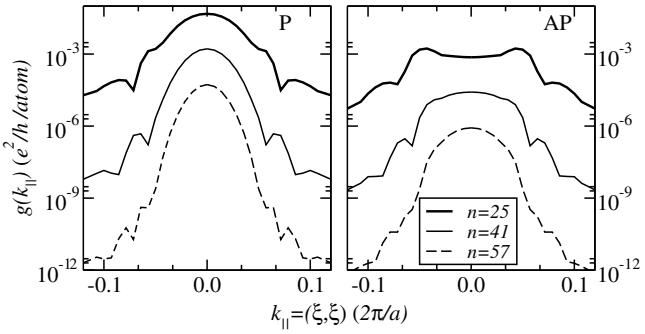

Figure 2. $\vec{k}_{\|}$-resolved relativistic conductance $g(\vec{k}_{\|})$ in Fe/n(GaAs)/Fe along the (110) direction of the zinc-blende structure, for different numbers of layers n. Left- and right-hand panels correspond, respectively, to parallel (P) and anti-parallel (AP) alignments of the magnetization in the two Fe leads.

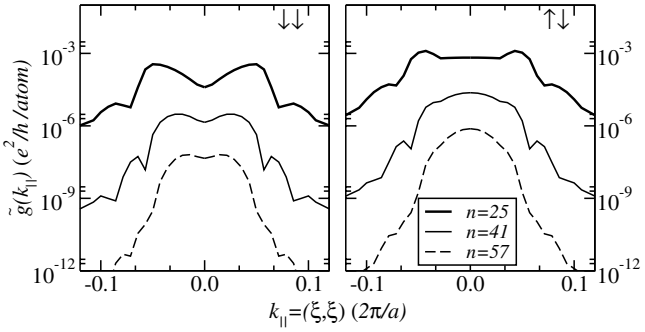

Figure 3. Spin-decomposed terms $\widetilde{g}^{m_s m'_s}(\vec{k}_{\|})$ of the $\vec{k}_{\|}$-resolved conductance in Fe/n(GaAs)/Fe along the (110) direction of the zinc-blende structure, as obtained from equation (9), for several thicknesses n in the AP alignment. Left- and right-hand panels show, respectively, the spin-diagonal—$\widetilde{g}^{\downarrow\downarrow}(\vec{k}_{\|})$—and the spin-flip—$\widetilde{g}^{\uparrow\downarrow}(\vec{k}_{\|}) + \widetilde{g}^{\downarrow\uparrow}(\vec{k}_{\|})$—contributions to the conductance.

Making use of the spin decomposition of conductance as obtained from equations (9) and (10), we can investigate the reason for this behaviour. Figure 3 shows the spin-diagonal $\widetilde{g}^{\downarrow\downarrow}(\vec{k}_{\|})$ (left-hand panel) and spin-flip $\widetilde{g}^{\downarrow\uparrow}(\vec{k}_{\|}) + \widetilde{g}^{\uparrow\downarrow}(\vec{k}_{\|})$ (right-hand panel) terms, corresponding to the relativistic $g^{\mathrm{AP}}(\vec{k}_{\|})$ in the right-hand panel of figure 2 (AP alignment). As one can see, a local minimum at the $\bar{\Gamma}$ point is indeed present, but only in the spin-diagonal term. In the spin-flip term—occurring only as the result of the SOC accounted for—a local maximum is present at the zone centre, that becomes a global maximum as the thickness of the junction increases. Moreover, the spin-flip term is about one order of magnitude bigger than the spin-diagonal one through the whole 2DBZ.

This is also reflected in the integrated conductance $\widetilde{g}$, as can be seen in figure 4. For the P alignment (left-hand panel) the results do not differ too much from what one would get in a non-relativistic calculation: the conductance is overwhelmingly dominant in the majority (spin-down) channel $\widetilde{g}^{\downarrow\downarrow}$, but the spin-flip conductance term (black diamonds) has the second important contribution to the total conductance. In the AP alignment, on the other hand, the main contribution (around 80%) comes from the spin-flip term, that would be missing if one performed a non-relativistic calculation.

We interpret our results in connection with the points mentioned at the beginning of this section. The most important change implied by adopting a fully relativistic treatment is that the

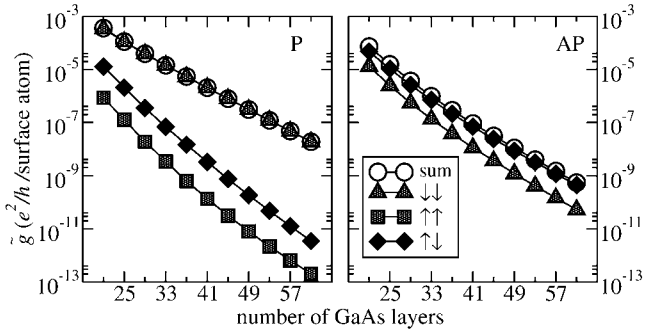

Figure 4. Spin-decomposed components $\widetilde{g}^{m_s m_s'}$ of conductance, as given by equation (9), for the Fe/n(GaAs)/Fe trilayer system as a function of GaAs thickness n. Left- and right-hand panels correspond, respectively, to parallel (P) and anti-parallel (AP) alignments. The label $\uparrow\downarrow$ denotes the sum $\widetilde{g}^{\uparrow\downarrow} + \widetilde{g}^{\downarrow\uparrow}$ of both spin-off-diagonal terms and, for the AP alignment, the term $\widetilde{g}^{\uparrow\uparrow} = \widetilde{g}^{\downarrow\downarrow}$ has been omitted from the right-hand panel of the figure.

symmetry of the states involved in the tunnelling has to be reconsidered on a relativistic level. As the spin is not a good quantum number, the states through the whole junction no longer have a well defined spin character, and thus an electron entering the junction can occupy either a spin-up or a spin-down state on the other side. The effect of SOC is more pronounced in the AP alignment since spin-up and spin-down densities at the Fermi energy have significantly different magnitudes.

We expect not only the interfacial states to be affected by the inclusion of SOC, but also those in the semiconductor. Even for paramagnetic systems, the situation corresponding to the conditions inside the barrier, the inclusion of SOC modifies the electronic structure by lifting the degeneracy of the bands. As a result, the complex band structure of the semiconductor is also changed within a fully relativistic treatment. Within our present formalism, a detailed investigation of the influence of SOC in the different regions of the junction can be straightforwardly done, by selectively modifying the SOC strength in the way was described by Ebert *et al* [19].

To conclude, we found that spin–orbit coupling influences the spin-dependent transport both qualitatively and quantitatively and its inclusion in the calculations is important even for relatively light atoms. Besides, a non-relativistic tunnelling calculation will not distinguish between the magnetization in-plane and out-of plane geometries since there is no coupling between the spin and orbital degrees of freedom.

Acknowledgments

This work was supported by the RT Network of Computational Magnetoelectronics of the European Commission. One of us (VP) gratefully acknowledges the financial support of the Deutsche Forschungsgemeinschaft within the DFG-Förderprojekt FOG 370/2-1 'Ferromagnet-Halbleiter Nanostrukturen: Transport, elektrische und magnetische Eigenschaften'.

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