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Perpendicular transport in Fe/InP/Fe heterostructures

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Abstract

Perpendicular electric transport in Fe/InP/Fe heterostructures with different terminations is investigated within the relativistic spin-polarized version of the screened Korringa–Kohn–Rostoker method and the Kubo–Greenwood formula, and compared to a Landauer-like approach. Both methods show that the magnetoresistance becomes constant with increasing spacer thickness. © 2002 Elsevier Science B.V. All rights reserved.

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In view of spin transport, quantum computers, etc., electric transport properties of metal/semiconductor/metal heterostructures became of quite some technological interest, especially, structures with a reasonable large magnetoresistance (MR) are very much in demand. A systematic search for possible systems, however, is still at the very beginning. In the present work $Fe/(InP)_t/Fe$, where t is the number of repetitions of the spacer material, serves as a model for such a heterostructure. The electronic properties of the system are determined within the fully relativistic spin-polarized screened Korringa–Kohn–Rostoker (SKKR) method for layered systems [1,2] and the local density approximation. The actually investigated systems are of the form $Fe(1\,0\,0)/Fe_s/(AB)_tA/Fe_{(s-1)\pm1}/Fe(1\,0\,0)$, with A and B being either In or P, and $s = 12$. The number of Fe layers in the right lead varies for technical reasons [2]. We assume a BCC-like structure (lattice constant $a = 5.27$ a.u.) instead of the zinc-blende structure of bulk InP. This is a simplification, however, it should be sufficient for small spacer thicknesses. The limitations will be discussed later on.

At present, three different kinds of methods are applied in order to calculate the current perpendicular to the planes, namely in terms of a linearized Boltzmann equation [3], the so-called "Kubo–Landauer" approach [4,5] and the Kubo–Greenwood equation [6]. Here, we adopt the Kubo–Greenwood formalism and compare the results with a Landauer-like approach [7]. Suppose $\mathscr{C}$ denotes the magnetic configuration of the leads, which can be either parallel ($\mathscr{P}$) or antiparallel ($\mathscr{AP}$) and δ is the imaginary part of the complex Fermi energy then $r(\mathscr{C}, n, \delta)$ describes the sheet resistance of a layered system with $n = 2(s+t)\pm 1$ atomic layers. A finite imaginary part of the Fermi energy has to be taken into account because of convergence properties of the k-space integration of the conductivity tensor elements [8]. Therefore, the actual sheet resistance is given by $r(\mathscr{C}, n) = \lim_{\delta\to 0} r(\mathscr{C}, n, \delta)$ [9]. Using the Kubo–Greenwood (KG) equation, the sheet resistance is defined as

$$r_{\mathrm{KG}}(\mathscr{C}, n, \delta) = \sum_{i,j}^{n} \rho_{ij}(\mathscr{C}, n, \delta) = \sum_{i,j}^{n} [\sigma(\mathscr{C}, n, \delta)]_{ij}^{-1}, \qquad (1)$$

where ρ_{ij} is the inverse of the layer-dependent conductivities σ_{ij} [8]. In a Landauer like description, the conductance can be viewed in terms of a two-point conductivity with endpoints situated in the leads [4,5]. The sheet resistance is then given by

$$r_{\mathrm{L}}(\mathscr{C}, n, \delta) = \rho_{1n}(\mathscr{C}, n, \delta) = \frac{1}{\sigma_{1n}(\mathscr{C}, n, \delta)}. \qquad (2)$$

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In both cases the MR is of the form

$$R(m) = \frac{r(\mathscr{AP}, m) - r(\mathscr{P}, m)}{r(\mathscr{AP}, m)} \quad (3)$$

with $m = 2(n_0 + t) + 1$ being the sum of all spacer layers considered including $n_0 = 10$ Fe lead layers. While the sheet resistance in the Kubo–Greenwood formula scans every layer and consequently includes, therefore, the influence of the interior system, the Landauer approach describes the system indirectly as viewed from the leads [4,5]. Therefore, the MR obtained by a Landauer like approach can be understood as an upper limit of the MR.

First of all we will focus on some electronic aspects of the system, especially the charge distribution, which tells us how many layers of the Fe leads do not show bulk-like behavior and have therefore to be included in the actual heterostructure, see Eq. (3). In order to check this layer-resolved Madelung potentials can be used [9], which are shown for a heterostructure with 21 repetitions in Fig. 1. The Madelung potentials for In layers are small and positive, whereas P layers are characterized by much larger but negative Madelung potentials. At the two interfaces, the potentials are disturbed such that P terminated spacers show reduced Madelung potentials and In terminated systems have enhanced Madelung potentials. This is accompanied by strong changes of the Fe Madelung potentials. It is obvious from Fig. 1 that these variations are limited to the region near the interface and vanish rapidly in the leads. Already after six lead layers the Madelung potentials reach the bulk value ($V_{\mathrm{mad}} = 0$). Therefore, the choice of $n_0 = 10$ Fe lead layers is sufficient for the calculation of the sheet resistances and, therefore, for the MR.

The MR (3) is obtained from the calculated sheet resistances as continued to the real axis [10]. The results are presented in Fig. 2. It is found that the product of the number of repetitions t and the sheet resistance varies linearly with t in the Kubo–Greenwood method and quadratic in the Landauer-like approach such as defined in Eq. (2). The MR obtained from this fit reproduces the calculated values quite well (see Fig. 2). Both, the Kubo–Greenwood and Landauer-like method show more or less the same trend for the MR. Only the variation of the data points is smaller in the Landauer like formalism, since only a single matrix element σ_{1n} has to be taken into account, whereas the Kubo–Greenwood equation considers a large number of such elements, see Eqs. (1) and (2). With increasing number of spacer layers, the MR becomes constant for both types of termination. From the Kubo–Greenwood equation (1), a MR of 37% is obtained for the In and 46% for the P terminated spacer. The corresponding values from the Landauer-like approach are 75% (In) and 82% (P), respectively. However, the differences of the MR between an In and a P terminated spacer amount only

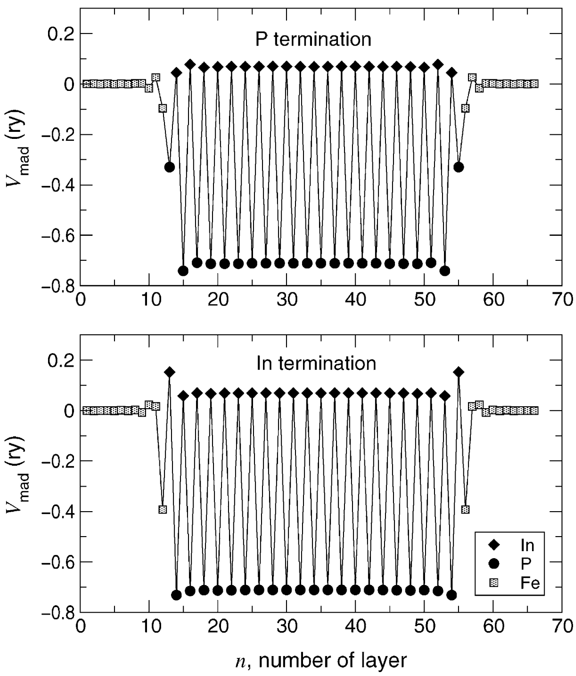

Fig. 1. Layer-resolved Madelung potentials of $Fe_{10}/(InP)_{21}/Fe_{10}$ for different spacer terminations.

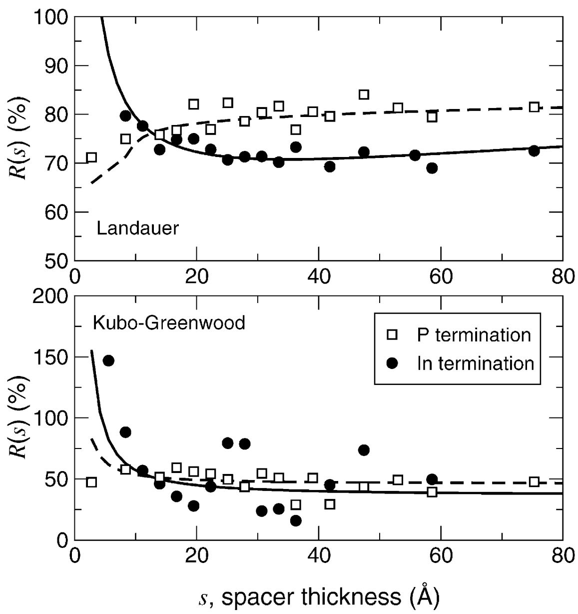

Fig. 2. Magnetoresistance $R(s)$ versus the spacer thickness s for a Landauer-like and the Kubo–Greenwood approach. Lines refer to the fitted sheet resistances, where dashed lines indicate a P termination and full lines mark an In termination of the spacer.

up to 7% or 9% depending on the method. This is obviously much smaller than the asymptotic difference, which we have found in a similar system with a ZnSe spacer [10]. This may be an indication that InP is less suitable as a spacer material in technical devices.

In order to pin-point the origin of the small MR in more detail, it is useful to focus on the difference of the sheet resistances for the $\mathscr{P}$ and the $\mathscr{AP}$ alignment of the leads

$$\Delta r(n,\delta) = r(\mathscr{AP}, n, \delta) - r(\mathscr{P}, n, \delta) \tag{4}$$

which can be partioned into three characteristic parts, namely into contributions from the leads Δr_{L}, from the interface Δr_{I}, and last but not least from the spacer Δr_{S}

$$\Delta r = \Delta r_{\mathrm{Ll}} + \Delta r_{\mathrm{Il}} + \Delta r_{\mathrm{S}} + \Delta r_{\mathrm{Ir}} + \Delta r_{\mathrm{Lr}}, \tag{5}$$

where the indices l and r indicate the left and right side of the system. The interface region is chosen to consist of the actual interface, three lead layers and three layers from the spacer, i.e., is of the form $Fe_3/FeA/BAB$, with A and B being either In or P. In Fig. 3, this partioning is presented for a heterostructure with $t = 21 (\delta = 2\,\mathrm{mRy})$. In contrast to former investigations of a ZnSe spacer [10] the results do not depend significantly on the termination. Both systems show nearly the same kind of contribution to Δr. That underlines what we have already seen in the MR (Fig. 2), where the differences between an In and a P termination are small. The largest contribution to Δr corresponds to the interface region, however, even more interestingly is the fact that the spacer also gives a large, but negative contribution. The $|\Delta r_{\mathrm{S}}|$ amounts to 65% of the interface value, which implies that the spacer material strongly reduces the MR of the system. This in turn explains the relatively small magnetoresistances, which are obtained for the present system as compared with a $Fe/(ZnSe)_t/Fe$ heterostructure.

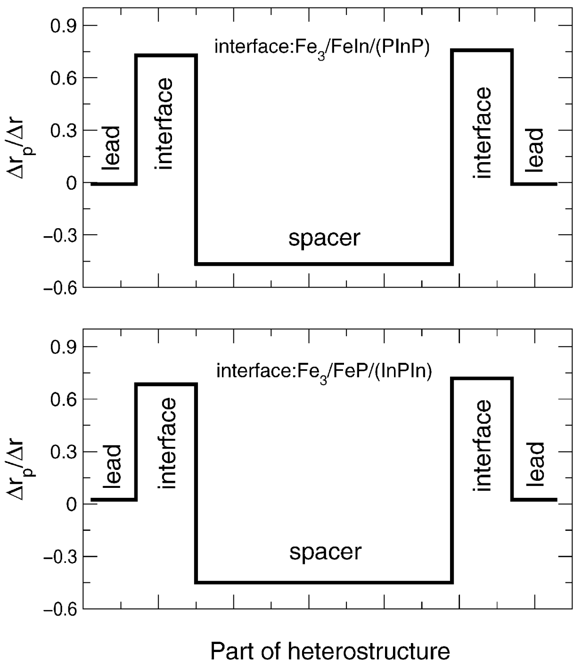

Fig. 3. Normalized fractions of the sheet resistance difference $\Delta r_p/\Delta r$, see Eq. (5), for a heterostructure with 21 repetitions with an In (top) and a P termination (bottom).

Summarizing, we have investigated the MR of $Fe/InP_t/Fe$ heterostructures on the basis of SKKR calculations. We were able to show that both methods give the same trend for the MR, the values from the Landauer-like method being a factor of 2 larger than the Kubo–Greenwood results. It has been found that the type of termination is of minor influence and that the InP spacer strongly reduces the MR. Finally, it should be mentioned that all spacer materials show metallic behavior. This is due to the fact that we have used a BCC structure with the lattice constant of BCC Fe, which is not true for thick spacers. In order to improve our results, we will expand our calculations to complex structures.

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