Perpendicular electric transport in Fe/X/Fe model heterostructures

H. C. Herper and P. Weinberger
Center for Computational Materials Science TU-Vienna, Gumpendorferstr. 1a, A-1060 Vienna, Austria

L. Szunyogh
Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521, Budapest, Hungary

C. Sommers
Laboratoire de Physique des Solides, Université de Paris-Sud, 91405 Orsay, France

The electric transport properties of $Fe/X_s/Fe$ model systems have been investigated for current perpendicular to the plane geometry. Three different spacer materials X=Ge, [In, P], [Zn, Se] have been used in order to examine the dependence of the magnetoresistance with respect to the spacer thickness. In the case of binary spacer materials the influence of the termination of the spacer material is also investigated. In addition, some important technical aspects like the variation of the sheet resistance with the number of lead layers are discussed. The investigations have been performed in the framework of the relativistic spin-polarized version of the screened Korringa–Kohn–Rostoker method, and the Kubo–Greenwood formula has been used to describe the transport properties. It has been observed that for all three systems the magnetoresistance becomes constant with increasing spacer thickness, the absolute value depending on the material and the termination of the spacer. Furthermore, we can demonstrate that the dominant contributions to the magnetoresistance arise from the Fe/X and X/Fe interfaces. [DOI: 10.1063/1.1452653]

I. INTRODUCTION

The possibility of spin dependent transport in ferromagnet-semiconductor heterostructures has inflamed the discussion of future applications like spin electronics and magnetic data storage. In this connection amorphous Ge and ZnSe semiconductors have been discussed.[1] Iron layers, which were separated by an amorphous spacer show a reversible exchange coupling at temperatures lower than 200 K (ZnSe), which means the coupling switches between FM and AFM coupling if the temperature is changed. If the temperature goes beyond this temperature the system becomes FM. From this point on renewed cooling does not lead back to AFM coupling.[1] Furthermore, Fe/X/Fe junctions with X being a semiconducting material usually show a small tunnel magnetoresistance (MR$\leqslant$0.1%).[2] In addition, a finite positive MR can be observed in presence of a magnetic field.[2] In the case of ZnSe experiments have shown that the conductivity of the system shows a remarkable dependence on the Fe thickness.[3] If the thickness of the Fe layer reaches 18 Å the conductivity shows metallic contributions, whereas for thinner magnetic layers the semiconducting behavior prevails. However, nearly no quantitative values for the MR are available. In this paper we have investigated the dependence of the MR on the spacer thickness for three planar model systems of the type Fe/X/Fe, in which bcc Fe is separated by Ge, [Se, Zn], and [In, P] spacers. We have used the Kubo formula[4] for calculating the electric properties. The experimental structures of the spacer material, being zinc-blende, diamond or even amorphous, have been replaced by a bcc parent lattice.[5]

II. THEORETICAL DETAILS

The electronic structure calculations were performed within the spin-polarized local density approximation of the density functional theory by using a fully relativistic version of the screened Korringa–Kohn–Rostoker method (SKKR).[6,7] For the description of the electric transport we employed a fully relativistic form of the Kubo formula.[4] In order to keep the two-dimensional translational symmetry, which is necessary for the *k*-space calculations we chose a bcc parent lattice ($a=5.27$ a.u.) for all systems, which means in the case of binary spacer materials that each layer contains only one type of atom. This is a strong restriction, but for thin spacers it should be valid (see Sec. III).

It was shown by Levy[4] that the Kubo formalism is not only sufficient for current in-plane geometry but can also be used if the current flows perpendicular to the planes, if we assume that we are in the steady state.[8] We can then define the sheet resistance as a sum of layer dependent resistivities ρ_{ij} at site i caused by a current at site j,

$$r(\mathcal{C},n,\delta)=\sum_{i,j}^{n}\rho_{ij}(\mathcal{C},n,\delta). \tag{1}$$

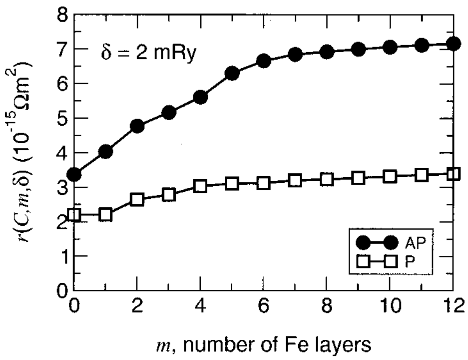

FIG. 1. Variation of the sheet resistance $r(C,n,\delta)$ with the number of Fe lead layers n for $Fe_n/Ge_{15}/Fe_n$. The results are given for parallel and antiparallel alignment of the leads and the imaginary part of the Fermi energy is chosen to be 2 mRy.

Here, n is the total number of layers and δ is a small but finite imaginary part of the complex Fermi energy $e_F + i\delta$, which is necessary for the k-space integration.[9] Furthermore, the sheet resistance depends on the magnetic configuration $\mathcal{C}$. In order to determine the magnetoresistance MR two different lead configurations are needed. Here, the parallel ($\mathcal{P}$) and the antiparallel ($\mathcal{AP}$) alignment of the lead magnetic moments is considered. The magnetoresistance can then be written in the form:

$$R(n) = \frac{r(\mathcal{AP},n) - r(\mathcal{P},n)}{r(\mathcal{AP},n)}. \qquad (2)$$

Two problems arise from the above description of the MR. First, the Fe layers near the interface between the bulk material and the multilayer do not show bulk behavior and have to be included in the active part of the multilayer. For a sufficient large number of buffer layers, however, the sheet resistance varies linearly with the number of layers m

$$r(\mathcal{C},m,\delta) = r_0(\mathcal{C},\delta) + m k_1(\mathcal{C},\delta), \qquad (3)$$

where $r_0(\mathcal{C},\delta)$ is the value of Eq. (3) for $m=0$ and k_1 is the slope. A typical example is shown in Fig. 1 for the $Fe_m/Ge_{15}/Fe_m$ system and $\delta = 2$ mRy.[10] From this it is obvious that the sheet resistance varies linearly with the number of layers if $m \geqslant 8$. Here, all calculations were performed

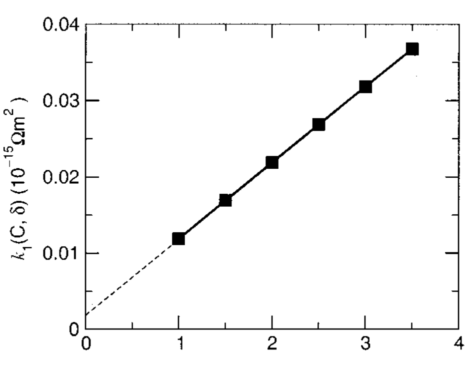

FIG. 2. Variation of $k_1(C,\delta)$ with respect to the imaginary part of the Fermi energy δ for $Fe(100)/Fe_{45}/Fe(100)$.

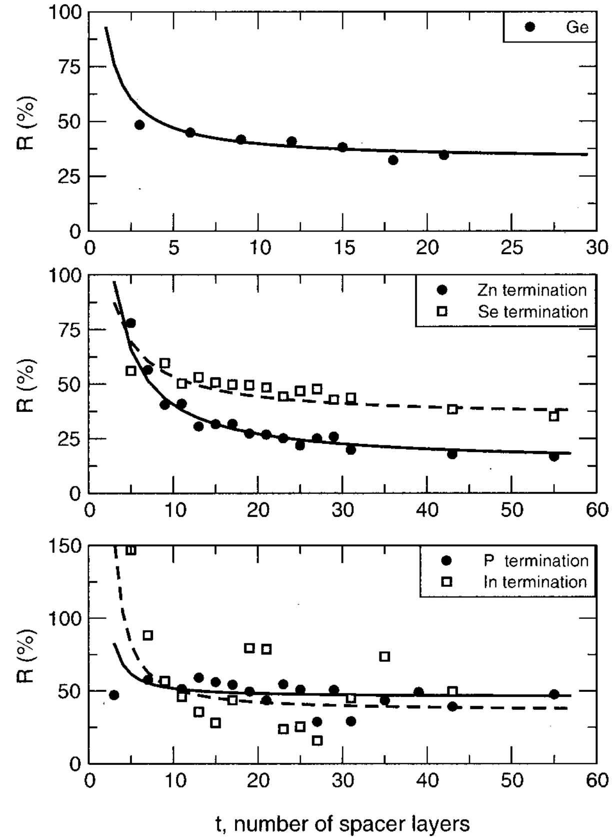

FIG. 3. Magnetoresistance $R(s)$ vs the number of spacer layers s for $Fe/X_s/Fe$, with X = Ge, [In, P] and [Zn, Se]. Lines refer to the fitted sheet resistances, full lines indicate a P or Zn termination and dashed lines an In or Se termination of the spacer.

with $m \geqslant 10$, which surely lies in the linear regime. Second, because of Eq. (3), k_1 tends to zero for $\delta \rightarrow 0$, because the true sheet resistance does not depend on the number of lead layers, which were taken into account. This was checked for a $Fe(100)/Fe_{45}/Fe(100)$ system, where the semiconductor was replaced by pure Fe and the sheet resistances were calculated for imaginary parts δ between 1 and 3.5 mRy (Fig. 2). It can be seen that k_1 indeed tends to zero, if the imaginary part of e_F goes to zero. The tiny remaining part is probably due to computational errors.

III. RESULTS AND DISCUSSION

The magnetoresistance [Eq. (2)] for the three heterostructures was obtained from the sheet resistances [Eq. (1)] as a function of the spacer thickness. The results are summarized in Fig. 3. In order to reduce the computational effort the MR of the $Fe/Ge_m/Fe$ system was only calculated for δ (2 mRy). Due to the Eq. (3) this curve is rigidly shifted such that the MR is reduced compared to the MR for $\delta = 0$. In the case of the binary spacer materials we calculated the sheet resistances for several values of δ and were able to continue the sheet resistances to the real axis; see Eq. (3). Therefore, the MR refers to $\delta = 0$ mRy. The corresponding result is shown in Fig. 3. The MR of all three systems shows the same trend. It becomes constant if the system contains a sufficient large number of spacer layers. Systems with a Ge spacer

TABLE I. Normalized fractions of the sheet resistance difference $\Delta r_p/\Delta r$ for the regions p of the system, defined in the text. The present system consists of 43 spacer layers with an Se and a Zn termination.

Termination	$\Delta r_p/\Delta r$		
	Lead	Interface	Spacer
Se	0.0049	0.4912	−0.0089
Zn	0.0034	0.6030	−0.1959

reach an asymptotic value of 37% already after 15 spacer layers. If the spacer contains more than one type of atomic species, the MR can depend on the termination of the spacer. Therefore, we have investigated the MR for both types of termination, assuming equal termination for both interfaces. The MR of the Fe/[Se, Zn]/Fe system shows a distinct dependence on the termination. The Se terminated system has a twice as large MR (38%) as compared to the system with Zn termination (18%). In contrast to that the system with an [In, P] spacer is less sensitive to the termination and the asymptotic values are similar to each other (Fig. 3). In addition, the MR does not decrease smoothly with growing number of layers, but seems to oscillate, which may be caused by interlayer exchange coupling effects. However, all investigated systems show the same asymptotic behavior. This is in accordance with recent experiments from Hunziker *et al.*,[3] who examined Fe/ZnSe heterostructures depending on the Fe thickness (4–18 Å). They found that the conductivity does not change much with the thickness of the spacer material.

In order to understand where the MR locally comes from and why it depends on the termination of the spacer, we analyzed the difference between the $\mathcal{AP}$ and $\mathcal{P}$ sheet resistance

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

A multilayer can be thought to consist of the three characteristic parts

$$\Delta r=\Delta r_{\mathrm{L_l}}+\Delta r_{\mathrm{I_l}}+\Delta r_{\mathrm{S}}+\Delta r_{\mathrm{I_r}}+\Delta r_{\mathrm{L_r}}, \tag{5}$$

namely the leads L, interfaces I, and the spacer S. In Eq. (5) the indices l and r mark the left and right side of the system. In our case the interface is chosen to consist of the actual interface plus three additional layers from the leads and the spacer. One typical result is given in Table I for the Fe/[Zn, Se]/Fe system with 43 spacer layers (≈60 Å), which is in the middle of the regime experimentally studied.[2] The main contribution to the MR comes from the two interfaces, whereas the MR of the leads is negligible. The contribution of the spacer depends on the termination of the spacer. Here, a Se terminated system shows nearly no MR inside the spacer, on the other hand Zn termination shows there a MR of about 20% but with negative sign. This explains why the asymptotic value of the Zn terminated system is much smaller as compared to the system with Se termination (Fig. 3). In contrast to that the [In, P] system has similar sheet resistance fractions for both terminations, which has already been discussed elsewhere.[11] Therefore, in this system the MR is nearly independent of the termination of the spacer and the asymptotic values of the MR for In and P termination are similar.

Finally, the influence of the structure should be discussed. As mentioned at the beginning all systems were treated within a bcc parent lattice, which does not correspond to the bulk structure of the spacer materials. Therefore, all the systems remain metallic even for large spacer thicknesses and the tunneling regime cannot be well described. However, experiments with Fe on ZnSe show some metallic contributions even if the semiconductor is rather thick,[3] in which case a reduction of the density of states at the Fermi level and a possibly band gap in the middle of the spacer should be expected. Butler *et al.* have investigated a Fe/Ge/Fe heterostructure with nine Ge layers using the diamond structure of Ge, they also obtained metallic behavior in the inner Ge layer.[12]

Financial support has been received from the RTN Network Magnetoelectronics (Contract No. HPRN-CT-2000-00143) and the Hungarian National Science Foundation (Contract No. OKTA T030240). We also wish to thank the CNRS IRIS Computing Center at Orsay for calculations done on their T3E Cray.

[1] P. Walser, M. Hunziker, T. Speck, and M. Landolt, Phys. Rev. B **60**, 4082 (1999).
[2] D. H. Mosca, J. M. George, J. L. Maurice, A. Fert, M. Eddrief, and V. H. Etgens, J. Magn. Magn. Mater. **226–230**, 917 (2001).
[3] M. Hunziker and M. Landolt, Surf. Sci. **468**, 187 (2000).
[4] P. M. Levy, *Solid State Physics* (Academic, Cambridge, 1994), Vol. 47.
[5] P. Weinberger, Philos. Mag. B **75**, 509 (1997).
[6] L. Szunyogh, B. Újfalussy, and P. Weinberger, Phys. Rev. B **51**, 9552 (1995).
[7] P. Weinberger and L. Szunyogh, Comput. Mater. Sci. **17**, 414 (2000).
[8] H. C. Herper, P. Weinberger, A. Vernes, L. Szunyogh, and C. Sommers, Phys. Rev. B **64**, 184442 (2001).
[9] P. Weinberger, P. M. Levy, J. Banhart, L. Szunyogh, and B. Újfalussy, J. Phys.: Condens. Matter **8**, 7677 (1996).
[10] P. Weinberger, L. Szunyogh, C. Blaas, and C. Sommers, Phys. Rev. B **64**, 184429 (2001).
[11] H. C. Herper, P. Weinberger, L. Szunyogh, and C. Sommers, J. Magn. Magn. Mater. **240**, 180 (2002).
[12] W. H. Butler, X.-G. Zhang, X. Wang, J. V. Ek, and J. M. Maclaren, J. Appl. Phys. **81**, 5518 (1997).