Interlayer exchange coupling and perpendicular electric transport in Fe/Si/Fe trilayers

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

L. Szunyogh
Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521, Budapest, Hungary and Center for Computational Materials Science, Gumpendorfer Strasse 1a, A-1060 Vienna, Austria

C. Sommers
Laboratoire de Physique des Solides, Université de Paris-Sud, 91405 Orsay, France
(Received 28 January 2002; revised manuscript received 29 May 2002; published 20 August 2002)

The interlayer exchange coupling and the perpendicular magnetoresistance of Fe/Si/Fe systems have been investigated within the fully relativistic screened Korringa-Kohn-Rostoker method and the Kubo-Greenwood equation considering interdiffusion effects, i.e., inhomogeneous Fe-Si alloy formation at the interfaces. It is shown that the experimentally observed strong antiferromagnetic interlayer exchange coupling is caused by the formation of Fe-Si alloys at the interface. Furthermore, our calculations give evidence that the small magnetoresistance, which has been observed experimentally in Fe/Si/Fe trilayers has a similar origin. The results presented here give no evidence for a direct connection between the magnetoresistance and interlayer exchange coupling in Fe/Si/Fe systems.

DOI: 10.1103/PhysRevB.66.064426 PACS number(s): 75.70.Pa, 75.70.Cn, 71.15.Ap

I. INTRODUCTION

Ten years ago Fullerton *et al.*[1] among others discovered that antiferromagnetic (AF) interlayer exchange coupling (IEC) is not necessarily restricted to nonmagnetic metallic interlayers such as Cr or Au,[2] but also exists in systems with so-called semiconducting or insulating spacer materials.[1] In this context, one system, which has been intensively studied, is Fe/Si/Fe. Both trilayers and multilayers have been investigated with nonmetallic amorphous Si,[3] or metallic Fe-Si alloys.[4] The occurrence of an IEC in AF coupled Fe/Si/Fe systems is often attributed to interdiffusion effects causing the spacer to become metallic.[5] Low-energy electron-diffraction and Auger spectroscopy measurements have shown that the existence of an IEC is not restricted to alloying effects at the interface, but an IEC can also be observed in systems with homogeneous Fe-Si alloy spacers[1,6] with a slightly deformed $B2$ structure (c-FeSi).[7,8] All these results suggest that the metallic character of the spacer is the origin of the IEC in Fe/Si/Fe. However, recent results from Gareev *et al.*,[4] jeopardize this conclusion. They examined $Fe/Fe_{1-c}Si_c/Fe$ trilayers with $0.4 \leqslant c \leqslant 1.0$ by using Brillouin light scattering (BLS) and obtained an increase of the coupling constant with increasing Si content in the alloy. This means the IEC is not only present for pure *semiconducting* Si, but it is larger compared to the alloyed system. Up to now the reason for the strong IEC in pure Si spacers is not completely clarified, since two competing effects have been observed for the IEC in Fe/Si/Fe trilayers. As long as the spacer is semiconducting the IEC is expected to show an exponential decay with respect to the thickness of the spacer. Similar behavior was found by de Vries *et al.*[5] for metallic Fe-Si spacers. On the other hand recent results from BLS experiments[7] show that Fe-Si spacers exhibit a typical metallic oscillating behavior. Here we will also address these contradicting results.

Although there exists a large number of experimental results quite a few questions concerning the origin and the strength of the IEC as well as its relation to other effects such as the magnetoresistance[6] (MR) remain open. The last aspect was especially discussed controversially in the literature, because is not clear at all whether or how the existence of the IEC is related to the magnetoresistance of the system.[6,9,10] One aspect of this paper is to give a comprehensive discussion of the IEC in Fe/Si/Fe by varying the number of spacer layers and by taking into account interdiffusion, i.e., formation of disordered alloys at the interfaces. The present calculations complement the results of Robles *et al.*, who examined the interlayer exchange within a k-space tight-binding linear muffin-tin orbital method in the limit of thin Fe-Si spacers.[11] In a recent paper of Pruneda *et al.*[12] the IEC of thicker ordered c-FeSi spacers was examined in the framework of the Bruno model whereas for thin spacers they followed the method from Robles.[11] However, they did not examine the influence of interdiffusion in detail.

The second aspect addressed in this paper is directed to the magnetoresistance of the Fe/Si/Fe trilayers for a current perpendicular to the plane (CPP) geometry. To our knowledge there exist nearly no experimental results concerning CPP transport for such systems, which grow in the (100) direction. Usually the magnetoresistance is investigated for samples grown on a SiO_2 (Refs. 13 and 14) or NaCl (Ref. 15) substrate on which Fe grows in the (110) direction. Furthermore, experimentally a very small MR of at best 2% at low temperatures[13] is recorded, but in most cases values smaller than 1% (Ref. 6 and 14) are obtained. Sometimes even negative MR ratios have been reported.[16] The sign of the MR seems to depend on the growth technique, applied magnetic field, etc.[6,10,16] Additional problems can arise from

the fact that the epitaxial growth is hindered because of island formation.[13] Furthermore, Fe and Si easily form nonmagnetic metallic alloys, which also occur at the interfaces of a Fe/Si/Fe heterostructure.[5] Due to the existence of Fe-Si alloys the interface to the spacer is no longer properly defined, i.e., the question arises whether the small measured MR is the MR ratio of the Fe/Si/Fe trilayer or only due to an FeSi alloy at the interface.[16] In this paper we will demonstrate that the reason for this small MR is the formation of Fe-Si alloys at the interface and/or in the spacer.

Only very little theoretical work is devoted to the magnetoresistance of Fe/Si/Fe trilayers or multilayers. Mavropoulos *et al.*[17] have used complex band structures in order to explain the tunneling in Fe/Si/Fe and other metal/I/metal systems (I = insulator), but a systematic study of Fe/Si/Fe trilayers is lacking. In this paper we will present a first-principles study of CPP transport in Fe(100)/Si/Fe(100) trilayers in terms of the Kubo-Greenwood equation.[18] Our investigations especially include a discussion of the spacer thickness dependence and of interdiffusion effects. Additional calculations were performed for systems with homogeneously alloyed Fe-Si spacers, which allow a more detailed discussion of the alloying effects on the MR.

II. METHOD OF CALCULATION AND COMPUTATIONAL DETAILS

A. Self-consistent calculations

We have performed *ab initio* calculations within the fully relativistic spin-polarized version of the screened Korringa-Kohn-Rostoker method for layered systems[19,20] in order to investigate the electronic structure and magnetic properties of bcc Fe/Si/Fe trilayers with the (100) growth direction. The local-density approximation (LDA) in the parametrization of Ref. 21 has been used to describe the exchange-correlation potential. The trilayers have been modeled by systems of the type

$$\mathrm{Fe}(100)/\mathrm{Fe}_{12}\mathrm{Si}_s\mathrm{Fe}_{12\pm1}/\mathrm{Fe}(100), \quad 1\leqslant s\leqslant 24,$$

with 12 layers of Fe serving as a buffer to the left substrate and 12 ± 1 Fe buffer layers to the right substrate. This variation of the number of right buffer layers results from the special properties of the screened structure constants, implying that the total number of considered layers has to be a multiple of three, see, e.g., Ref. 20. In all calculations a bcc parent lattice[22] has been assumed with a lattice constant of 5.27 a.u., which corresponds to the bulk lattice constant of bcc Fe in the LDA, i.e., no layer relaxation is considered. The interlayer distance obtained from Bragg reflection experiments is about $d_\perp = 1.4331$ Å,[8] which reflects closely the experimental bcc Fe lattice constant, i.e., the mismatch between the experimental and theoretical lattice spacing amounts only to 3%.

In order to determine self-consistently within the LDA the effective potentials and effective exchange fields for each particular system under consideration a minimum of 45 $\mathbf{k}_\parallel$ points in the irreducible wedge of the surface Brillouin zone (ISBZ) was used. All self-consistent calculations refer to a ferromagnetic configuration with the orientation of the magnetization parallel to the surface normal.

B. Interlayer exchange energy and magnetic anisotropy energy

Suppose $\mathcal{C}_0$ and $\mathcal{C}$ denote two different magnetic configurations, which differ in total energy by

$$\Delta E = E(\mathcal{C}) - E(\mathcal{C}_0), \tag{1}$$

where $\mathcal{C}_0$ usually is termed the magnetic reference configuration. If we suppose further that $\mathcal{C}_0$ refers to a ferromagnetic and $\mathcal{C}$ to an antiferromagnetic configuration then this energy difference corresponds to an interlayer exchange-coupling (IEC) energy. In here the ferromagnetic reference configuration ($\mathcal{C}_0$) refers to a ferromagnetic configuration in which the magnetization in all layers is oriented perpendicular to the surface. Furthermore, a symmetric antiferromagnetic configuration has been considered in which the orientation of the magnetization was switched in one lead and in half of the spacer layers simultaneously.

If in Eq. (1) $\mathcal{C}$ refers to a ferromagnetic configuration with a uniform in-plane orientation of the magnetization, then ΔE is said to be the total-energy part of the magnetic anisotropy energy E_a which also includes the shape anisotropy. The latter one is the energy difference corresponding to the magnetic dipole-dipole interaction ΔE_{dd}. Since for a trilayer system with semi-infinite leads on both sides a definition of the shape anisotropy is somewhat ambiguous, in this paper we restrict ourselves to the investigation of ΔE.

The energy difference in Eq. (1) is evaluated by making use of the magnetic force theorem which implies that only the reference configuration is determined self-consistently within the LDA and ΔE is replaced by the respective difference in the grand canonical potentials,

$$\Delta E \sim \Delta E_b = \sum_{p=1}^{n} \Delta E_b^p, \tag{2}$$

$$\Delta E_b^p = \int_{\epsilon_b}^{\epsilon_F} [n^p(\epsilon;\mathcal{C}) - n^p(\epsilon;\mathcal{C}_0)](\epsilon - \epsilon_F)\, d\epsilon, \tag{3}$$

which as indicated in Eq. (3) can be written in terms of layer-dependent quantities ΔE_b^p. Here, n denotes the total number of layers and $n^p(\epsilon;\mathcal{C})$ is the layer-resolved density of states for a given magnetic configuration $\mathcal{C}$. The values ϵ_b and ϵ_F are the valence-band bottom and the Fermi energy of the substrate, respectively. It should be noted that according to Eq. (1) $\Delta E_b > 0$ means that $\mathcal{C}_0$ is the energetically preferred magnetic configuration. In the present paper all ΔE_b are evaluated by using 990 $\mathbf{k}_\parallel$ points in the ISBZ, which was shown to be sufficient in the case of magnetic anisotropy energies.[20] A detailed discussion of this method based on the formalism developed by Jansen[23] is given in Ref. 20.

C. Transport perpendicular to the planes

The electric transport properties of the Fe/Si/Fe trilayers have been investigated within the fully relativistic spin-polarized Kubo-Greenwood equation.[18] A complete descrip-

tion of this method can be found elsewhere.[24,25] Here, we focus only on some aspects that are important for the present calculation. By implying that a current at layer q causes a resistivity ρ_{pq} at layer p, this resistivity ρ_{pq} is defined[24] as the inverse of the layer-resolved conductivity σ_{pq},

$$\sum_{q=1}^{n} \rho_{pq}\sigma_{qp'} = \delta_{pp'}, \tag{4}$$

with n being the total number of layers in the system. For a given magnetic configuration $\mathcal{C}$ the resistance of the trilayer—the so-called sheet resistance—can then be defined as sum over these resistivities ρ_{pq},

$$r(\mathcal{C},n,\delta) = \sum_{p,q}^{n} \rho_{pq}(\mathcal{C},n,\delta), \tag{5}$$

where δ is the imaginary part of the complex Fermi energy $\epsilon_F + i\delta$. For practical purposes δ is usually chosen to be between 1 and 3 mRy. Here, $\delta = 2$ and 3 mRy have been used. The actual sheet resistance is then determined from Eq. (5) in the limit of $\delta \to 0$ by numerical continuation to the real axis. However, it was shown in a preceding paper[25,26] that for a given system of size $n = 2n_0 + s$ (n_0 is the number of Fe layers on each side) the sheet resistance varies linearly with δ provided that the number of Fe buffer layers is large enough, see Sec. II A. Therefore, the sheet resistance $r(\mathcal{C},n,\delta=0)$ can be obtained from calculations for finite values of δ. Using the definition of the sheet resistance in Eq. (5) the magnetoresistance of a particular trilayer can then be written in the form

$$R(n) = \frac{r(\mathcal{AP},n) - r(\mathcal{P},n)}{r(\mathcal{AP},n)}, \quad R(n) \leqslant 1, \tag{6}$$

where $\mathcal{P}$ and $\mathcal{AP}$ denote the magnetic configuration of the layers. Here, $\mathcal{P}$ refers to the ferromagnetic (FM) reference configuration $\mathcal{C}_0$ and $\mathcal{AP}$ to the antiferromagnetic configuration, see Sec. II B.

The number of Fe buffer layers n_0 was 11 for all systems, which is sufficient to reflect even very tiny oscillations in the layer-resolved Madelung potentials, see Ref. 25. Furthermore, for a magnetic configuration $\mathcal{C}$ a sheet resistance of a single layer p can be defined for illustrative purposes as

$$r_p(\mathcal{C},n,\delta) = \sum_{q=1}^{n} \rho_{pq}(\mathcal{C},n,\delta). \tag{7}$$

This allows us to detect in detail, which part of the trilayer actually contributes to the sheet resistance. Starting from the sheet resistances of the two magnetic configurations we define

$$\Delta r(n,\delta) = r(\mathcal{AP},n,\delta) - r(\mathcal{P},n,\delta) \tag{8}$$

and use Eq. (7) to analyze $\Delta r(n,\delta)$ for different parts of the system. Here, we suppose that the heterostructure consists of three characteristic parts marked by Roman numbers: leads (I, V), interfaces (II, IV) and the spacer (III). The interface regions contain the real interface and three additional layers from the leads, for details see Ref. 26. It should be noted, however, that only the sum over all layer-resolved sheet resistances $r_p(\mathcal{C},n,\delta)$ is well defined.

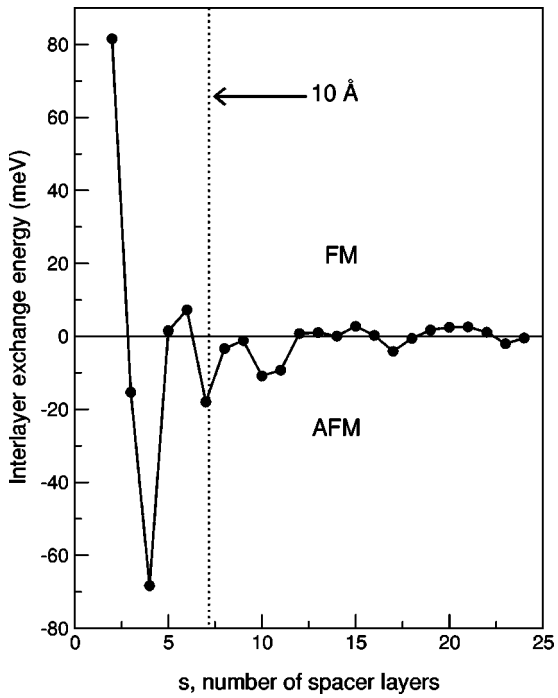

FIG. 1. Interlayer exchange energy (IEC) of Fe/Si/Fe trilayers vs the number of spacer layers s.

III. RESULTS AND DISCUSSION

A. Interlayer exchange coupling and magnetic anisotropy energy

The IEC as obtained from Eq. (1) is displayed in Fig. 1 versus the number of spacer layers s. As can be seen from this figure the IEC shows enormous oscillations especially for thin spacers, which for increasing spacer thickness decrease. Furthermore, from Fig. 1 it is obvious that these oscillations refer to permanent changes from FM to AF coupling, whereby FM coupling is preferred in the case of very thin spacers <3 ML. Characteristic periods of oscillations, however, are not visible within the investigated range of spacer thicknesses. In most heterostructures interdiffusion effects at the interfaces are of crucial importance for the IEC, the magnetic anisotropy energy, but also for transport properties.[7,16] Here a two-layer interdiffusion is considered, meaning that for a system with s Si layers the following cases have been investigated:

$$\ldots \mathrm{Fe/Fe}_{1-c_d}\mathrm{Si}_{c_d}/\mathrm{Fe}_{c_d}\mathrm{Si}_{1-c_d}/\mathrm{Si}_{s-2}/\mathrm{Fe}_{c_d}\mathrm{Si}_{1-c_d}/\mathrm{Fe}_{1-c_d}\mathrm{Si}_{c_d}/\mathrm{Fe}\ldots,$$

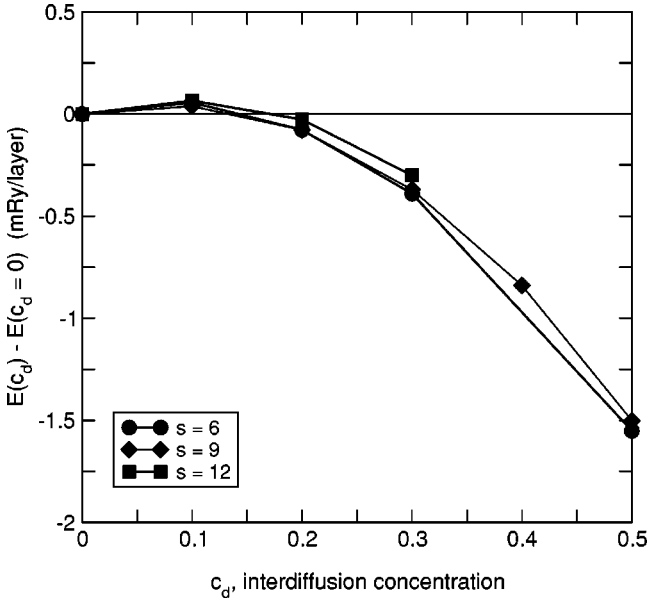

FIG. 2. Total-energy differences, $E(c_d)-E(c_d=0)$, with respect to the interdiffusion concentration c_d. The number of spacer layers s is marked explicitly.

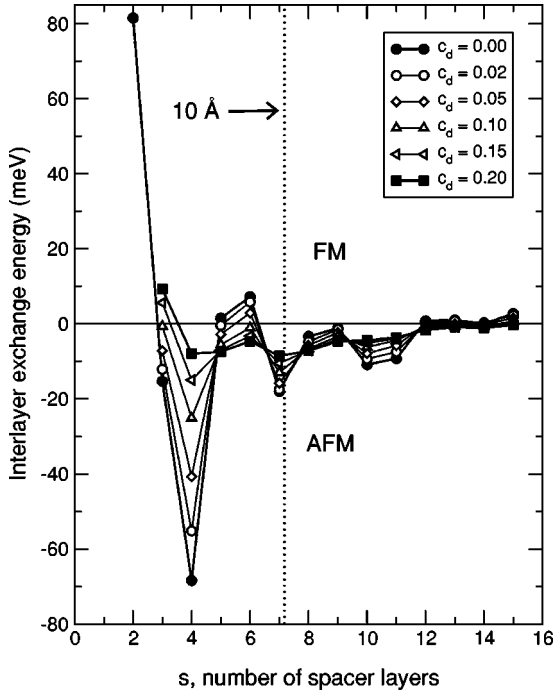

FIG. 3. Changes of the IEC with respect to the number of spacer layers for different interdiffusion concentrations c_d.

with c_d denoting the interdiffusion concentration and replacing the experimentally suggested $B2$ structure[7,8] by an inhomogeneously disordered alloy. Experimental studies with Mössbauer and photoemission spectroscopy have shown that the Fe/Si and Si/Fe interfaces are not equivalent with respect to the Fe-Si formation.[8,27] The compositions on the top and bottom of the sample are different, because more Fe diffuses from the top into the spacer.[8] In the present paper this has been neglected and the two interfaces have been chosen to be identical.

From a comparison of total energies it can be seen that trilayers with a sufficiently large interdiffusion concentration are energetically favored as compared to the system with ideal interfaces. In Fig. 2 the total-energy differences $E(c_d)-E(c_d=0)$ are shown for particular spacer thicknesses with respect to the interdiffusion concentration c_d. If the interdiffusion concentration exceeds 20% interface alloys are preferred by the majority of the systems. For interdiffusion concentrations below 20% the solution without interdiffusion seems to be stable. However, the energy difference is rather small ($\leqslant 0.07$ mRy), which means that the two states are almost degenerated. The results shown in Fig. 2 suggest that for thicker spacers higher interdiffusion concentrations are needed to stabilize the system. From this figure, however, it is clear that Fe/Si/Fe trilayers are stabilized by interdiffusion. Since the calculations refer to zero temperature, these arguments apply only for sufficiently low temperatures.

In Fig. 3 the IEC is presented for a variety of interdiffusion concentrations as a function of the number of Si layers. From this figure it can be seen that with increasing interdiffusion the large oscillations for small spacer thicknesses are reduced dramatically, while for larger spacer thicknesses interdiffusion effects seem to be less important. It should be noted, however, that for $c_d>0.15$ the regime of antiferromagnetic coupling is considerably enlarged extending for $c_d=0.2$ from $s=4$ to $s=12$. Thus strong interdiffusion at the interfaces helps to stabilize the antiferromagnetic coupling.

A similar oscillating behavior was observed in recent experiments from Gareev *et al.*[7] They used a somewhat different system with an epitaxial $Fe_{1-c}Si_c$ spacer, which cannot directly be compared to our results. However, the occurrence of oscillations suggests that the mechanism of the IEC in this system is the same as in usual metallic trilayers. Earlier results from de Vries *et al.*,[5] who examined systems with an ordered *c*-FeSi spacer, cannot be confirmed. They found an exponential decay of the IEC with respect to the spacer thickness and therefore predicted a new type of coupling for metallic Fe/FeSi/Fe trilayers. This seemingly was confirmed by recent *ab initio* and molecular-dynamics calculations from Pruneda *et al.*[12] One possible reason for the two types of results can be ordering of the alloy. We always use disordered alloys and so did Gareev *et al.*,[7] whereas de Vries *et al.*[5] and Pruneda *et al.*[12] investigated systems with ordered *c*-FeSi spacers. In general an exponential decay of the IEC is expected[4] to occur if the spacer becomes semiconducting and alloy formation is mainly suppressed. Such an exponential decrease cannot be observed in our results for the ideal system (Fig. 1), because for the chosen parent lattice even without interdiffusion Si this system turns out to be a poor metal. It is important to note that semiconducting Si in such heterostructures is amorphous, which cannot be described within the present theoretical framework. Furthermore, we have seen that the oscillating behavior is strongly influenced by interdiffusion. Experimental data for the IEC with varying Si thicknesses, obtained for Fe/Si multilayers,[6] also show a kind of oscillations. For spacers thicker than 10 Å AF coupling is preferred, which is in agreement with the results from Gareev *et al.*[4] for Si and Fe-Si spacers. From our calculations

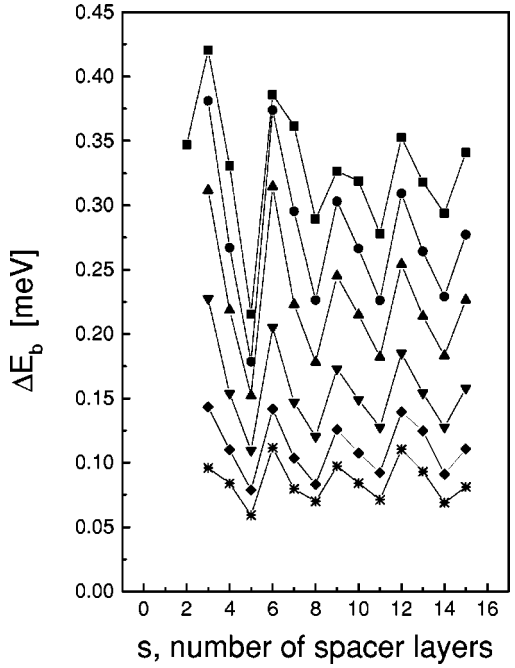

FIG. 4. Band energy part of the magnetic anisotropy energy ΔE_b for Fe/Si/Fe systems with two-layer interdiffusion at the interfaces vs the number of spacer layers. The results are shown for different interdiffusion concentrations c_d, whereby c_d increases from the top $c_d=0.0$ (squares) to the bottom $c_d=0.2$ (stars).

we can conclude that the AF coupling is stabilized by interface alloying (Fig. 3), whereas in the case of a pure metallic Si spacer the IEC alternates between FM and AF coupling (Fig. 1). It should be mentioned that experimental results are available only for spacers thicker than 6 Å[4] or even 10 Å.[6] Furthermore, Inomata *et al.*[6] simply assumed that the system stays FM below this thickness, which of course must not be the case. The present results give rise to the assumption that additional oscillations exist for thinner spacers (Fig. 1). In principle, it is plausible that a sufficiently large interdiffusion concentration suppresses the FM coupling completely, which is in accordance with existing experimental[4] and theoretical[11,12] work.

In Fig. 4 the band energy part of the magnetic anisotropy energy, see Eq. (3), is displayed considering a two-layer interdiffusion at the Fe/Si interfaces. The curves for different interdiffusion concentrations c_d seem to differ in size only by a rigid shift. With increasing interdiffusion concentration ΔE_b is reduced and shows an oscillation period of 3 ML. Since ΔE_b remains positive for all spacer thicknesses and interdiffusion concentrations, it favors a perpendicular orientation of the magnetization, a fact that of course is important for the transport properties, which will be discussed below.

The mentioned reduction of ΔE_b with increasing interdiffusion concentration essentially occurs at the interfaces (Fig. 5, top). In this figure the concentration-dependent changes of the layer-resolved ΔE_b for the system with nine Si layers prove to be restricted to about three layers at the interface. In the bottom part of Fig. 5 a comparison between the effect of interdiffusion and of homogeneous alloying in the spacer is presented for the band energy part of the magnetic anisotropy energy in the same system (nine Si layers). As can be seen for $c \leqslant 0.05$ both cases of disorder show about the same reduction in ΔE_b, whereas for $c>0.05$ homogeneous alloying causes a much slower reduction of ΔE_b with increasing c.

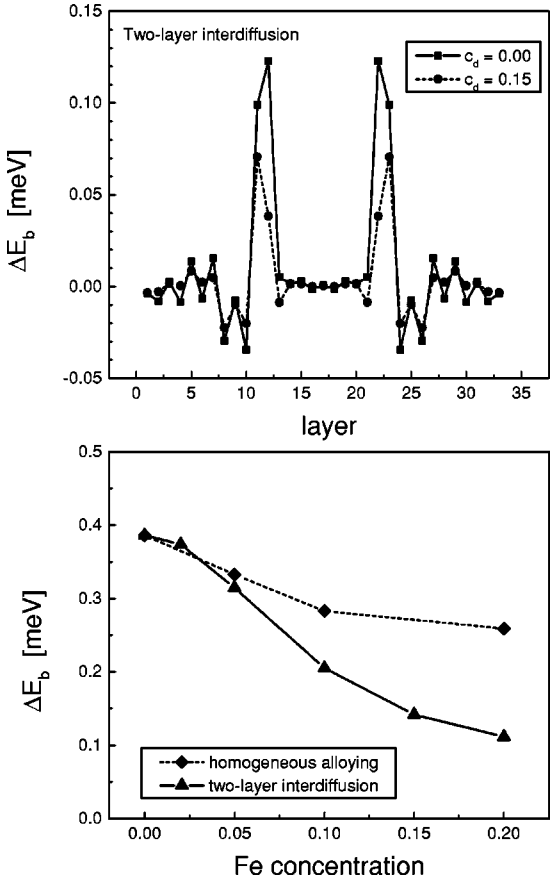

FIG. 5. Upper panel:The layer-resolved band energy part of the magnetic anisotropy energy ΔE_b^p for Fe(100)/Si_9/Fe(100) for a clean interface (squares) and a finite interdiffusion concentration (circles). Lower panel: ΔE_b^p vs the Fe concentration. The dashed line marks the results for the homogeneously alloyed spacer Fe_cSi_{1-c}.

B. Perpendicular electric transport

The dependence of the MR on the Si thickness was studied first for the ideal system, i.e., for clean interfaces and no alloying in the spacer (Fig. 6). The spacer thickness varies again between 2 and 24 ML, that is, between 2.79 and 33.45 Å. The black line in Fig. 6 represents a fourth-order fit to the data points. The MR oscillates around this fit with a small amplitude. This can be seen from the inset of Fig. 6, where the difference between the calculated points and the fit is displayed. These oscillations show no characteristic period. Since an oscillating behavior was obtained for the IEC and the magnetic anisotropy energy, see Sec. III A, it is tempting to assume common periods for all three properties. Concerning the IEC this cannot be confirmed. The oscillating behavior of the MR is different from what we have obtained for the IEC. The oscillations for the magnetic anisotropy energy

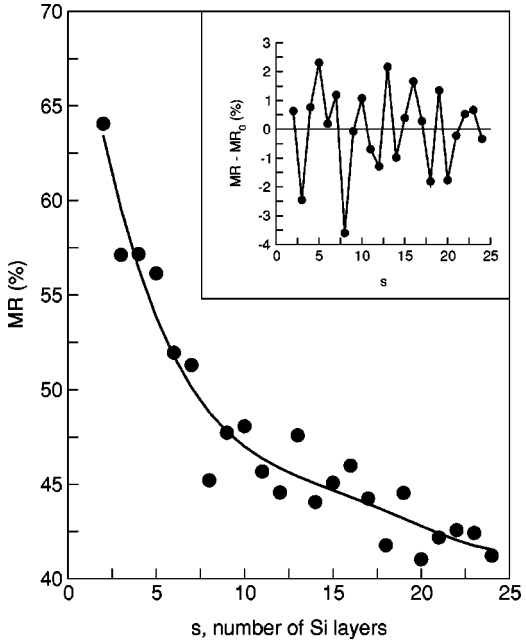

FIG. 6. Magnetoresistance for $Fe/Si_s/Fe$ trilayers versus the number of Si spacer layers *s*. The full line is a fourth-order fit MR_0 to the data points. Inset: Difference between the calculated points and the fit MR_0 depending on the number of Si layers.

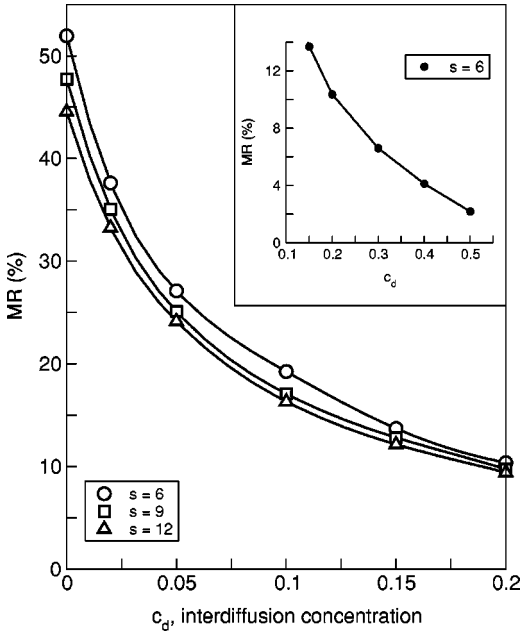

FIG. 7. Dependence of the magnetoresistance on the interdiffusion concentration for $Fe/Si_s/Fe$ systems.

(Fig. 5) appear to be of the same type as for the MR as long as the spacer is thin enough ($s \leqslant 12$ ML). However, this similarity does not give sufficient evidence for a common origin of the oscillations in the magnetic anisotropy energy and the electric properties.

In viewing Fig. 6 it can be seen that the MR slightly decreases with the number of Si layers. Previous investigations have shown that for a sufficient large number of spacer layers the MR becomes constant.[25,26] Here, at 24 ML this asymptotic value of the MR is not yet reached and the MR of the trilayer still decreases, but, nevertheless, it is obvious that a reasonably large MR exists even for thick spacers. The largest system with 24 ML Si still shows a MR of 41%, which is comparable in value to previous results for Ge spacers[25] and Fe/[Zn-Se]/Fe trilayers with Se termination.[26]

However, such large MR's have not been reported experimentally for Fe/Si/Fe systems. We presumed that the differences may arise from the fact that we used a perfect trilayer with clean interfaces. Therefore, the calculations have been repeated for three particular systems with 6, 9, and 12 ML Si taking into account a two-layer interdiffusion, see Sec. III A. The MR for finite interdiffusion concentrations c_d is shown in Fig. 7. Independently from the number of spacer layers the MR immediately is lowered if Fe diffuses into the spacer. With respect to the MR for $c_d = 0.0$ the concentration-dependent curves are more or less rigidly shifted. An interdiffusion concentration of about 20% is sufficient to reduce the MR to a fifth of the value for $c_d = 0$. Since all systems show the same trend, in order to examine the MR at larger interdiffusion concentrations the 6 ML Si systems serve as an example, see inset of Fig. 7. As expected a further increase of c_d leads to even smaller values of the MR. From the literature it is known that a $Si_{0.5}Fe_{0.5}$ alloy is quite likely to occur at the Fe/Si interfaces.[5,8] From the present investigations a MR of about 2.2% is obtained for an interdiffusion concentration of 50% (Fig. 7). This means if realistic interdiffusion concentrations are considered the calculated MR is rather small ($\approx 2\%$). This is in quite a good agreement with the experimental findings, which lie between 0.1 (Ref. 6) and 2.2%,[13,14] depending on the preparation technique, the substrate, and the structure of the sample. In comparing these results one should keep in mind that most of the experimental results were obtained for systems grown in the [110] (Ref. 6 and 14) direction. Therefore, a direct comparison of absolute values must be handled with care. Nevertheless, the calculated results already show the right trend.

Up to now interdiffusion was assumed to be restricted to the vicinity of the interfaces, which surely is a simplification, because Mössbauer experiments have shown that in Fe(60 Å)/Si(30 Å)/Fe systems the average spatial regime of interdiffusion comprises 3.3 Å Fe and 8 Å Si.[8] This means approximately eight layers are affected by interdiffusion, whereby the actual compositions are layer dependent. Instead of such a complicated interdiffusion profile we have studied a somewhat different system, namely, replacing the whole spacer by a homogeneous bcc Fe_cSi_{1-c} alloy with the Fe concentration varying between 0 and 40%. From Fig. 8 it can be seen that the MR rapidly decreases with increasing *c*. For a $Fe_{0.2}Si_{0.8}$ alloy the remaining MR amounts only to 5%. At a first glance the MR seems to drop faster than in the case of the interface alloy, but a direct comparison of the two cases is somehow difficult, because in contrast to the interface alloy in the homogeneous alloy a nominal amount of Si changes with *c*.

The smallest MR was obtained for 30% Fe. From Fig. 8 it is obvious that with a further increase of the Fe concentration in the spacer the MR grows again. This is an artifact since the $Fe/(Fe_{0.4}Si_{0.6})_6/Fe$ system contains only 3.6 ML Si in

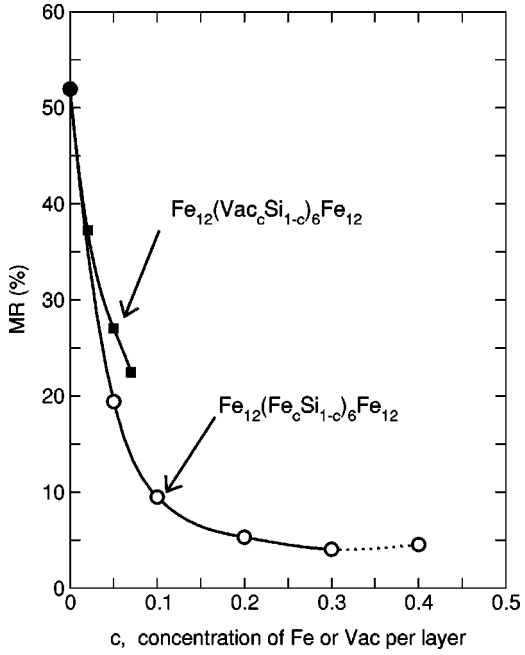

FIG. 8. Magnetoresistance for systems with homogeneous Fe_cSi_{1-c} spacers (circles) or Vac_cSi_{1-c} (squares) depending on the Fe or Vac content c per layer.

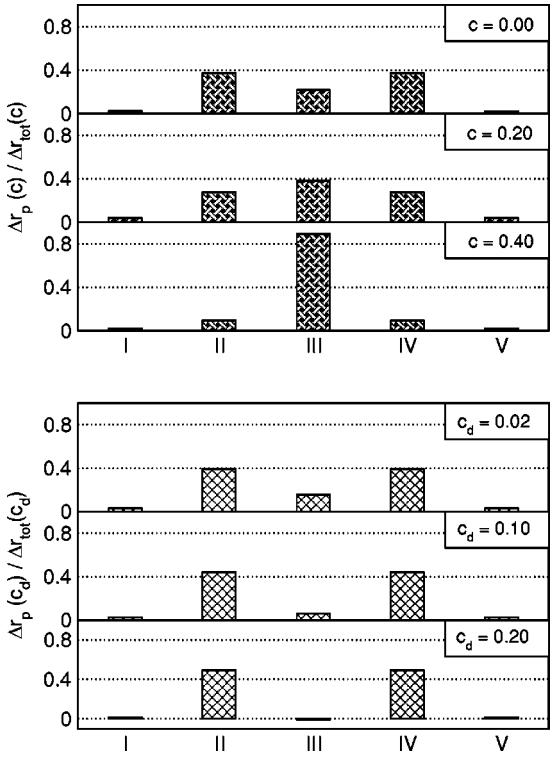

FIG. 9. Normalized fractions of the layer-resolved sheet resistance differences Δr_p for characteristic regions p of a trilayer with six spacer layers. In the upper panel the results for homogeneous alloying of the spacer are shown. The results for interface alloying are displayed in the bottom panel. Roman numbers mark particular regions of the system: I left lead, II left interface, III spacer, IV right interface, and V right lead.

total. Therefore, the character of the system is mainly determined by Fe and the $\mathcal{P}$=FM magnetic configuration is preferred. This means that the sheet resistance of the $\mathcal{P}$ configuration vanishes, whereas the sheet resistance of the $\mathcal{AP}$ configuration grows, which in turn leads to an enhancement of the MR, see Eq. (6).

Furthermore, additional calculations have been performed for a homogeneous silicon-vacancy alloy, which simulates a larger average volume of the Si atoms. If Si in the spacer is replaced by vacancies the MR also drops with increasing vacancy concentration; however, the decrease is smaller as compared to the homogeneous Fe-Si alloy (Fig. 8). The MR of $Vac_{0.1}Si_{0.9}$ is of the same size as the MR of an Fe-Si interface alloy with 10% Fe.

The above presented results nicely demonstrate that the formation of Fe-Si alloys at the interface is the main reason for the extremely small MR obtained in experimental measurements: the presence of Fe or vacancies in the spacer is responsible for the observed low value of the MR.

In order to demonstrate which parts of the heterostructure contribute mostly to the MR the sheet resistance fractions defined in Eq. (8) can be used. Again the 6 ML Si system was chosen as an example. Previous investigations on Fe/ZnSe/Fe systems have shown that for not too thin spacers the main contribution to the MR stems from interfaces.[26] This fact is confirmed by the present calculations for the nonalloyed system and for interdiffusion (Fig. 9), although a reasonably large contribution (20%) arises from the spacer. An increase of the interdiffusion concentration c_d causes a decrease of the spacer contribution to Δr (Fig. 9, bottom), which means the MR ratio is mainly determined by the interfaces.

A completely different picture applies for the systems with a homogeneous Fe-Si alloy (Fig. 9, top). Fe in the spacer region not only lowers the MR ratio, but, in addition, also the importance of the different regions changes. In the case of homogeneous alloying (Fig. 9, top) the interfaces lose their importance. With increasing Fe concentration the main contribution to the MR comes from the Fe-Si spacer. If the Fe concentration in the spacer amounts to 40% the spacer contributes 85% of the total MR. Furthermore, from Fig. 9 it is obvious that in any case the outer Fe layers—the leads—do not give a sizable contribution. The above-described results show that except for the ideal system the main contribution to Δr stems from that part of the system that contains Fe-Si alloys.

IV. SUMMARY

In this paper we have presented an *ab initio* study of the IEC and electric transport properties of Fe/Si/Fe trilayers with respect to the spacer thickness and the influence of two different types of interdiffusion. In accordance with recent experimental findings[7] the IEC shows an oscillating behavior, which is typical for metallic spacers. It has been shown that two-layer interdiffusion damps the amplitude of the oscillations and with increasing interdiffusion concentration the AF coupling is preferred. This is, in principle, agreement

with previous investigations from Robles *et al.*[11] However, in contrast to their results we obtain FM coupling for very thin spacers, which is essentially due to the fact that we have used disordered FeSi alloys and smaller interdiffusion concentrations than Robles *et al.*[11] The present results show more or less the same trend as the experimental findings.[4,6,7] It has been mentioned before that the results from de Vries *et al.*[5] could not be reproduced. The exponential decay reported in this paper is possibly caused by their preparation technique. A comparison of our present results with the mentioned theoretical and experimental findings seems to provide the conclusion that the two different types of IEC are caused by the degree of order of the spacer alloy, at least when considering homogeneously alloyed spacers.

Although the MR also oscillates with spacer thickness, like the IEC, no direct connection between these two properties can be observed. It was shown that the calculated MR is of the same size as the experimental one, if we allow for interdiffusion. Without interdiffusion the MR would amount to $\approx 50\%$. An interdiffusion concentration at the interfaces of only about 50%, which corresponds to *c*-FeSi, leads to a MR of about 2%. If a homogeneous Fe-Si spacer alloy is used, the decrease of the MR is even faster. In this case a Fe concentration of 30% is sufficient to reduce the MR to below 5%. From this we can conclude that the small MR of Fe/Si/Fe trilayers is essentially caused by the formation of metallic Fe-Si in the spacer and/or at the interfaces. In conclusion, it can be predicted that the MR of Fe/Si/Fe trilayers can only be enhanced if the interdiffusion of Fe into the spacer is considerably suppressed.

ACKNOWLEDGMENTS

This work has been partially funded by the RTN network ''Magnetoelectronics'' (Contract No. RTN1-1999-00145) and by the Austrian science ministry (Contract No. BM:bwk GZ45.504). Financial support was provided by the Hungarian National Science Foundation (Contract Nos. OTKA T030240 and T038162). In addition, we wish to thank the computing center IDRIS at Orsay where a part of the calculations was performed on a Cray T3E computer.

[1] E.E. Fullerton, J.E. Mattson, S.R. Lee, C.H. Sowers, Y.Y. Huang, G. Felcher, S.D. Bader, and F.T. Parker, J. Magn. Magn. Mater. **117**, L301 (1992).
[2] P. Grünberg, R. Schreiber, Y. Pang, M.B. Brodsky, and H. Sowers, Phys. Rev. Lett. **57**, 2442 (1986).
[3] S. Toscano, B. Briner, H. Hopster, and M. Landolt, J. Magn. Magn. Mater. **114**, L6 (1992).
[4] R.R. Gareev, D.E. Bürgler, M. Buchmeier, R. Schreiber, and P. Grünberg, J. Magn. Magn. Mater. **240**, 235 (2002).
[5] J.J. de Vries, J. Kohlhepp, F.J.A. de Broeder, R. Jungblut, R. Coehoorn, A. Reinders, and W.J.M. de Jonge, Phys. Rev. Lett. **78**, 3023 (1997).
[6] K. Inomata, K. Yusu, and Y. Saito, Phys. Rev. Lett. **74**, 1863 (1995).
[7] R.R. Gareev, D.E. Bürgler, M. Buchmeier, D. Olligs, R. Schreiber, and P. Grünberg, Phys. Rev. Lett. **87**, 157202 (2001).
[8] G.J. Strijkers, J.T. Kohlhepp, H.J.M. Swagten, and W.J.M. de Jonge, Phys. Rev. B **60**, 9583 (1999).
[9] K. Inomata, K. Yusu, and Y. Saito, J. Appl. Phys. **33**, L1670 (1994).
[10] F.J.A. den Broeder and J. Kohlhepp, Phys. Rev. Lett. **75**, 3026 (1995).
[11] R. Robles, J.M. Pruneda, S. Bouarab, J. Ferrer, and A. Vega, Surf. Sci. **481-485**, 994 (2001).
[12] J.M. Pruneda, R. Robles, S. Bouarab, J. Ferrer, and A. Vega, Phys. Rev. B **65**, 024440 (2002).
[13] R.J. Highmore, K. Yusu, S.N. Okuno, Y. Saito, and K. Inomata, J. Magn. Magn. Mater. **151**, 95 (1995).
[14] L. Tong, M. Pan, X. Wu, M. Lu, and H. Zhai, J. Magn. Magn. Mater. **198-199**, 101 (1999).
[15] C.L. Foiles, M.R. Franklin, and R. Loloee, Phys. Rev. B **50**, 16 070 (1994).
[16] N. Ihara, S. Narushima, T. Kijima, H. Abeta, T. Saito, K. Shinagawa, and T. Tsushima, Jpn. J. Appl. Phys., Part 1 **38**, 6272 (1999).
[17] P. Mavropoulos, N. Papanikolaou, and P.H. Dederichs, Phys. Rev. Lett. **85**, 1088 (2000).
[18] P. M. Levy, *Solid State Physics* (Academic Press, Cambridge, 1994), Vol. 47.
[19] L. Szunyogh, B. Újfalussy, and P. Weinberger, Phys. Rev. B **51**, 9552 (1995).
[20] P. Weinberger and L. Szunyogh, Comput. Mater. Sci. **17**, 414 (2000).
[21] S.H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).
[22] P. Weinberger, Philos. Mag. B **75**, 509 (1997).
[23] H.J.F. Jansen, Phys. Rev. B **59**, 4699 (1999).
[24] P. Weinberger, P.M. Levy, J. Banhart, L. Szunyogh, and B. Újfalussy, J. Phys.: Condens. Matter **8**, 7677 (1996).
[25] P. Weinberger, L. Szunyogh, C. Blaas, and C. Sommers, Phys. Rev. B **64**, 184429 (2001).
[26] H.C. Herper, P. Weinberger, A. Vernes, L. Szunyogh, and C. Sommers, Phys. Rev. B **64**, 184442 (2001).
[27] R. Kläsges, C. Carbone, W. Eberhardt, C. Pampuch, O. Radar, T. Kachel, and W. Gudat, Phys. Rev. B **56**, 10 801 (1997).