AB INITIO STUDY OF ELECTRIC TRANSPORT AND INTERLAYER EXCHANGE COUPLING IN Fe/Si/Fe SYSTEMS

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Abstract

We present a first principles study of the magnetoresistance (MR) perpendicular to the planes of atoms and the interlayer exchange coupling (IEC) in Fe/Si/Fe trilayers. In both cases the dependence on the number of spacer layers is investigated, whereby the spacer thickness ranges between 3 and 21 Å for the IEC and extends to 33 Å for the MR in order to obtain the asymptotic behavior. Additionally, the influence of alloy formation at the interfaces on the MR and the IEC is examined. The calculations of the electronic structure are performed

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within the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method and the transport properties are derived from the Kubo-Greenwood equation. Our results give evidence that interdiffusion is one of the origins of the small magnetoresistance, which is observed experimentally in Fe/Si/Fe trilayers. AFM coupling occurs for spacers thicker than 4 Å which is in accordance with the experimental findings. It seems that interdiffusion stabilizes AFM coupling in Fe/Si/Fe trilayers.

1 Introduction

Multilayer systems consisting of Fe/Si or Fe/FeSi are candidates for new electronic devices, because it is possible to change the size of the magnetic coupling by light [Mattson *et al.* (1993)] or heat [Briner and Landolt (1994); Inomata *et al.* (1995); Highmore *et al.* (1995)]. Therefore, it is necessary to understand which features influence the associated variables. The present paper focuses on two important properties – the interlayer exchange coupling (IEC) and the magnetoresistance (MR).

The existence of AFM coupling in Fe/Si/Fe trilayers or multilayers is already known for quite a long time [Fullerton *et al.* (1992); Toscano *et al.* (1992); de Vries *et al.* (1997)], however there are still some unsolved questions concerning the influence of interdiffusion and the asymptotic behavior of the IEC. In the case of ordered c-FeSi spacers an exponential decay has been observed if the spacer thickness becomes larger than 12 Å [de Vries *et al.* (1997)], which is supported by recent *ab initio* calculations [Pruneda *et al.* (2002)]. In that work the IEC is obtained from TB-LMTO calculations; in the region of thick spacers ($>$ 13 Å $\approx$ 10 ML), however, in which the exponential decay occurs, only the Bruno model [Bruno (1995)] was used. For disordered $Fe/Fe_{0.56}Si_{0.44}/Fe$ spacers on the other hand an oscillating coupling has been observed up to 34 Å spacer thickness [Gareev *et al.* (2002)]. This oscillating behavior is known to be a characteristic feature of metallic systems [Parkin *et al.* (1990); You *et al.* (1999)]. Similar observations have been reported in the case of pure Si spacers. For sufficiently thick spacers ($\geq$ 15Å) an exponential decrease of the IEC has been observed [Gareev *et al.* (2002)]. It was suggested that these seemingly controversial results are due to the fact that the outer spacer layers try to form iron silicides [Strijkers *et al.* (1999)], whereby the structure and concentration are determined by the deposition procedure. In the present paper we concentrate of the latter case investigating the influence of interdiffusion on pure Si spacers using *ab initio* methods.

In the second part we focus on the magnetoresistance, which is of crucial importance for the discussion of new devices. All MR ratios of Fe/Si multilayers or trilayers determined experimentally are rather small as compared to systems with metallic spacers [Mosca *et al.* (1991); Parkin *et al.* (1990); Mosca *et al.* (2001)] or even insulating spacers like Al_2O_3 [Miyazaki and

Tezuka (1995)]. Independent of the substrate which determines the growth direction the MR in Fe/Si systems ranges between 0.3 and 2.2 % [Highmore *et al.* (1995); Tong *et al.* (1999); Ihara *et al.* (1999)]. At room temperature also negative values of the MR have been found [Inomata *et al.* (1995); Ihara *et al.* (1999)]. Only very little theoretical work is devoted to the magnetoresistance of Fe/Si/Fe trilayers or multilayers in order to explain these extremely small values. Two years ago the tunneling behavior of Fe/Si/Fe sandwiches has been investigated by using complex bandstructures [Mavropoulos *et al.* (2000)], but systematic investigations of the MR of Fe/Si/Fe trilayers – to our knowledge – do not exist. In this paper we present an *ab initio* study of the MR of Fe/Si/Fe trilayers in the current perpendicular to the plane (CPP) geometry in terms of the Kubo-Greenwood equation [Levy (1994)] taking into account in particular the influence of interdiffusion at the interfaces on the MR.

2 Computational techniques

2.1 Self-consistent calculations and interlayer exchange coupling

The electronic structure and the magnetic properties of Fe/Si/Fe trilayers have been investigated in the framework of the fully relativistic spin-polarized version of the screened Korringa-Kohn-Rostoker (SKKR) method for layered systems [Szunyogh *et al.* (1995); Weinberger and Szunyogh (2000)] using the local density approximation (LDA) in the parameterization of Ref. [Vosko *et al.* (1980)]. Assuming a bcc-like lattice and (100) growth direction we have used trilayers of the type $\mathrm{Fe}(100)/\mathrm{Fe}_{12}\mathrm{Si}_s\mathrm{Fe}_{12\pm1}/\mathrm{Fe}(100)$, with $1 \leq s \leq 24$.

As mentioned at the beginning usually alloy formation occurs at the interfaces of such trilayers [de Vries *et al.* (1997); Strijkers *et al.* (1999)]. In most systems these interdiffusion effects at the interfaces are important for the IEC and as well as for the transport properties [Gareev *et al.* (2001); Ihara *et al.* (1999)]. In order to study the influence of interdiffusion additional investigations have been carried out for systems of the type

$$\mathrm{Fe}_{11}/\mathrm{Fe}_{0.8}\mathrm{Si}_{0.2}/\mathrm{Fe}_{0.2}\mathrm{Si}_{0.8}/\mathrm{Si}_{s-2}/\mathrm{Fe}_{0.2}\mathrm{Si}_{0.8}/\mathrm{Fe}_{0.2}\mathrm{Si}_{0.8}/\mathrm{Fe}_{11\pm1},$$

where s is the total number of Si layers. The experimentally suggested $\mathrm{c}-\mathrm{Fe}_{1-x}\mathrm{Si}$ alloy, which crystallizes in the B2 structure [Gareev *et al.* (2001); Strijkers *et al.* (1999)] has been replaced by a disordered alloy. In here, we assume that the alloy composition is identical at both interfaces. This is of course a simplification, because from photo-emission spectroscopy and Mössbauer experiments [Strijkers *et al.* (1999); Kläsges *et al.* (1997)] it is known that Fe preferentially diffuses from the top into the spacer [Strijkers *et al.* (1999)].

Twelve (eleven in the case of interdiffusion) and 12 ± 1 (11 ± 1) layers of Fe serve as a buffer to the left and right substrate, respectively. The number of Fe layers on the right side is not fixed, because due to the special properties of the screened structure constants the total number of layers must be a multiple of three [Weinberger and Szunyogh (2000)]. These buffer layers are included in the multilayer system in order to account for the charge transfer at the Fe/spacer interface. From the Madelung potentials (Fig. 1) it is obvious that the charge transfer region extends over at least ten layers. Beyond, the Madelung potentials reach the bulk value ($V_{\rm mad}^{\rm bulk} = 0$) within an accuracy of $6 * 10^{-6}$ Ry/layer, thus, in our calculations we have always chosen the number of Fe layers ≥ 10.

Throughout all calculations a bcc parent lattice [Weinberger (1997)] has been used, in which the lattice constant corresponds to the bulk lattice constant of bcc FM Fe in LDA (5.27 a.u.). The lattice spacing in Fe/Si/Fe systems is close to the value of bcc Fe and amounts to $d_\perp = 1.4331$ Å [Strijkers *et al.* (1999)]. Therefore, the mismatch between the experimental and theoretical lattice spacing is restricted to the difference between the experimental and LDA interlayer distance which amounts to $\approx 3\,\%$.

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

The interlayer exchange coupling energy corresponds to the difference between the energy of the FM reference state and an AFM configuration

$$\Delta E \;=\; E(\mathcal{AFM}) - E(\mathcal{FM}). \tag{1}$$

In here the interlayer exchange energy (1) has been evaluated in terms of layer resolved band energies making use of the magnetic force theorem [Weinberger and Szunyogh (2000); Jansen (1999)], which implies that only the FM state has to be calculated selfconsistently. A detailed discussion concerning the magnetic force theorem can be found in the review article [Weinberger and Szunyogh (2000)]. The interlayer exchange energy for a system with n layers can then be written as

$$\Delta E \sim \Delta E_b = \sum_{p=1}^{n} \int_{\epsilon_b}^{\epsilon_{\rm F}} \left[n^p(\epsilon; \mathcal{AFM}) - n^p(\epsilon; \mathcal{FM}) \right] (\epsilon - \epsilon_{\rm F}) d\epsilon, \tag{2}$$

where the right hand side corresponds to the energy difference in the grand canonical potentials. The values ϵ_b and ϵ_F denote the valence band bottom and the Fermi energy of the substrate, respectively, the $n^p(\epsilon; \mathcal{C})$ refer to layer-resolved densities of states for a given magnetic configuration $\mathcal{C}$. In this description a positive ΔE_b refers to FM coupling.

2.2 CPP transport

The fully relativistic spin-polarized Kubo-Greenwood equation [Weinberger *et al.* (1996)] has been used to investigate the electric transport properties of the Fe/Si/Fe trilayers. In this scheme ρ_{pq} is the resistivity which is caused at layer q by a current at layer p and ρ_{pq} is defined as the inverse of the layer resolved conductivity σ_{pq} [Weinberger *et al.* (1996)] such that

$$\sum_{q=1}^{n} \rho_{pq}\sigma_{qp'} = \delta_{pp'}, \tag{3}$$

with n being the total number of layers in the system. For a given magnetic configuration $\mathcal{C}$ the sum over these resistivities ρ_{pq} corresponds to the resistance (sheet resistance) of the trilayer

$$r(\mathcal{C}, n, \delta) \;=\; \sum_{p,q}^{n} \rho_{pq}(\mathcal{C}, n, \delta). \tag{4}$$

Due to the k-space integration the energy has to be complex and δ is the imaginary part of the complex Fermi energy $\epsilon_{\mathrm{F}} + i\delta$. Throughout this paper we have used two different values for δ being 2 and 3 mRy. Using the fact that for a given system size the sheet resistances vary linear with δ the actual sheet resistances can be determined by continuation to the real axes [Weinberger *et al.* (2001); Herper *et al.* (2001)]. Using the definition of the sheet resistance in Eq. (4) and the two magnetic configurations ($\mathcal{C} = \mathcal{FM}, \mathcal{AFM}$) described in the previous section, the magnetoresistance of a particular trilayer can then be written in the form

$$R(n) \;=\; \frac{r(\mathcal{AFM}, n) \;-\; r(\mathcal{FM}, n)}{r(\mathcal{AFM}, n)}, \quad R(n) \;\leq\; 1, \tag{5}$$

3 Results and discussion

3.1 Interlayer exchange coupling

We have investigated the IEC of two different types of trilayers as a function of the spacer thickness. In the case of ideal interfaces we observe huge oscillations of the IEC with respect to the number of spacer layers s (Fig. 2). With increasing number of spacer layers the amplitude of these oscillations becomes smaller. However, the system seems to change permanently between FM and AFM coupling, whereby FM coupling is preferred in trilayers with very thin spacers ($s \leq 4\,\mathrm{ML}$). The switching of the coupling from FM to AFM and vice versa is in disagreement with the experimental data. All experiments report a transition from FM to AFM somewhere below 10 Å spacer thickness [Inomata *et al.* (1995); Gareev *et al.* (2001)], but from there on the coupling remains AFM. Furthermore, in the case of pure Si spacer the IEC should decrease exponentially at least for thick spacers [Gareev *et al.*

(2002)]. This is not observed in the present investigations (Fig. 2). Consequently, the system with ideal interfaces is not a suitable model for realistic Fe/Si/Fe trilayers. The reasons are twofold, firstly Si in such heterostructures is often amorphous, which cannot be described within the present theoretical framework. Instead a bcc parent lattice has been assumed (see Sec. 2.1), in which Si is at least a poor metal instead a semiconductor. Secondly, perfect interfaces usually do not exist in Fe/Si systems [Strijkers *et al.* (1999)].

If interface diffusion is taken into account the AFM coupling is stabilized (Fig. 2). Only systems with very thin spacers ($s \leq 3\,\mathrm{ML}$) still prefer FM coupling. In principle, it is plausible that FM coupling is completely suppressed by a sufficiently large interdiffusion concentration. Compared to the system with ideal interfaces therefore still some oscillations exist, but with a much smaller amplitude (Fig. 2). The occurrence of oscillations suggests that the mechanism of the IEC in this system is the same as in usual metallic trilayers. An exponential decay as observed in systems with ordered FeSi spacers [de Vries *et al.* (1997)] does not exist in the present systems, where alloying is restricted to a small interface region. One should keep in mind that a direct comparison of our results and these experimental findings is somewhat difficult. Nevertheless, it is obvious that the oscillations of the IEC are similar to the experimental results for $Fe_{0.2}Si_{0.8}$ [Gareev *et al.* (2002)] or $Fe_{0.56}Si_{0.44}$ [Gareev *et al.* (2001)]. Therefore, it seems that the coupling is crucially influenced by the structural order in the spacer. From the present investigations, however, we can conclude that the AFM coupling observed in experiment [Inomata *et al.* (1995)] is stabilized by interdiffusion.

According to the majority of the experimental results for Si and FeSi spacers [Gareev *et al.* (2001); de Vries *et al.* (1997)] for $s > 12\,\mathrm{ML}$ the IEC tends to zero. Only Inomata *et al.* reported a renewed increase of the IEC for very thick spacers [Inomata *et al.* (1995)], which can not be compared to our results, because it occurs beyond the calculated spacers thicknesses.

3.2 Perpendicular electric transport

We now discuss the results for the MR of the two types of trilayers as obtained using Eq. (5). The MR of the Fe/Si/Fe system without interdiffusion ($c_\mathrm{d} = 0.0$) is calculated for spacer thicknesses ranging between 2 and 24 ML. The results are displayed in Fig. 3 together with a fourth order fit to the data points (black line). In viewing Fig. 3 it can be seen that the thickness dependence of the MR is rather weak, which is in contrast to former results for Fe/[Zn,Se]/Fe trilayers [Herper *et al.* (2001)], but is quite similar to the results obtained for trilayers with Ge spacers [Herper *et al.* (2002)]. The MR decreases from 64 % for the 2 ML spacer system to 41 % for the largest system taken into consideration. Previous investigations [Weinberger *et al.* (2001); Herper *et al.* (2001)] have shown that the MR becomes constant in the limit of thick spacers. After 24 ML the MR still decreases with growing number of Si layers. It is obvious, however, that a reasonably large MR

remains even for thick spacers, which is in disagreement with the known experimental findings [Tong *et al.* (1999); Ihara *et al.* (1999); Inomata *et al.* (1995)]. It is suggested that the origin of this discrepancy is similar to what has been discussed in the case of the IEC. Since, it has been shown in the previous section that the results are in agreement with experiment if the interfaces are described more realistic, additional transport calculations have been performed for two particular systems with 6 and 9 ML Si taking a two-layer interdiffusion into account, compare Sec. 2.1. Independent of the spacer thickness the MR rapidly decreases for finite interdiffusion concentrations c_d, see Fig. 4. An interdiffusion concentration of 10 % reduces the MR to one third of the value for $c_d = 0$. From the literature it is known that the interdiffusion rate can be much higher and $SiFe_{1-x}$ ($0 \leq x \geq 0.5$) alloys are likely to be formed [de Vries *et al.* (1997); Strijkers *et al.* (1999)] at Fe/Si interfaces. Further increase of c_d still leads to smaller values of the MR. In the case of a 50 % interdiffusion concentration the MR is of about 2.2 % (Fig. 4).

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 extends over approximately 8 ML [Strijkers *et al.* (1999)], whereby the actual composition of the alloy is layer dependent. In order to gain information of how the size of the interface region influences the MR we have studied a somewhat different system by using a four-layer interdiffusion and eight ML Si, namely

$$Fe_{0.98}Si_{0.02}/Fe_{0.92}Si_{0.08}/Fe_{0.08}Si_{0.92}/Fe_{0.02}Si_{0.98}/Si_4/...,$$

where the average interdiffusion amounts to 5 %. Quite obviously, a broadening of the interdiffusion region leads to a faster drop of the MR. As compared to the systems with two-layer interdiffusion with a MR of 5 % the MR is now much smaller, see Fig. 4.

This means if realistic interdiffusion concentrations are considered the *ab initio* determined MR is rather small ($\approx$ 2 %), which agrees well with the experimental data, which lie in turn between 0.1 [Inomata *et al.* (1995)] and 2.2 % [Tong *et al.* (1999); Highmore *et al.* (1995)]. The spread of the experimental MRs is due to different preparation techniques, substrates and structure of the sample. It should be mentioned that in experiments often SiO_2 substrates are used, on which the Fe/Si/Fe systems grow in (110) direction [Inomata *et al.* (1995); Tong *et al.* (1999)]. In here, the trilayers are oriented in (100) direction. Therefore, a comparison of absolute values must be handled with care. However, the calculated MR shows already the right trend.

Finally, in viewing Fig. 3 it can be seen that the MR oscillates around a 4th order fit, with a rather small amplitude. Since, similar oscillations have been observed in the IEC (see Sec. 3.1) it is tempting to assume a common driving force for the MR and the IEC. From the present investigations, however, it is not possible to prove the existence of a direct connection between

these oscillations and therefore between the IEC and MR.

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, which means that the presence of Fe in the spacer is most likely responsible for the reduced MR.

4 Summary

The IEC and MR of Fe/Si/Fe trilayers have been discussed with respect to the spacer thickness and the influence of interdiffusion. The calculations have been performed within the SKKR approach and the Kubo-Greenwood equation. In both cases it has been shown that interdiffusion improves the agreement with the experimental findings. The IEC oscillates with the spacer thickness; a two-layer interdiffusion is already sufficient to stabilize the AFM coupling seen in the experimental results. From our calculations the exponential decrease reported for thick Si and ordered FeSi spacers could not be observed. A possible explanation for the behavior of the IEC for ordered FeSi spacers can be found in Ref. [Pruneda *et al.* (2002)].

The transport calculations have shown that similar oscillations with respect to the number of spacer layers occur for the MR, but no direct connection between the MR and the IEC could be established. A possible relation of the IEC and the magnetic anisotropy energy has already been discussed elsewhere [Herper *et al.* (2002)]. Again, the experimental results are well reproduced if the interfaces are interdiffused. Furthermore, it has been demonstrated that a broadening of the interdiffusion region monitors the decrease of the MR. Without any interdiffusion the MR is too large as compared to the measured data. From these two findings we can conclude that interdiffusion effects and alloying are the origins of the small MR reported in Fe/Si/Fe trilayers.

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Figure 1: Layer-resolved Madelung potentials for $Fe_{12}Si_9Fe_{12}$ versus the number of layers n. Inset: Madelung potentials versus the number of Fe buffer layers n_{Fe}.

Figure 2: Interlayer exchange energy (IEC) of Fe/Si/Fe trilayers versus the number of spacer layers s

Figure 3: Magnetoresistance for $Fe/Si_s/Fe$ trilayers versus the number of Si spacer layers s. The full line refers to a fourth order fit to the data points.

Figure 4: Dependence of the magnetoresistance on the interdiffusion concentration c_d for $Fe/Si_s/Fe$ systems. The triangle refers to the result for a system with a four-layer interdiffusion region and eight Si layers in total, for details see text.

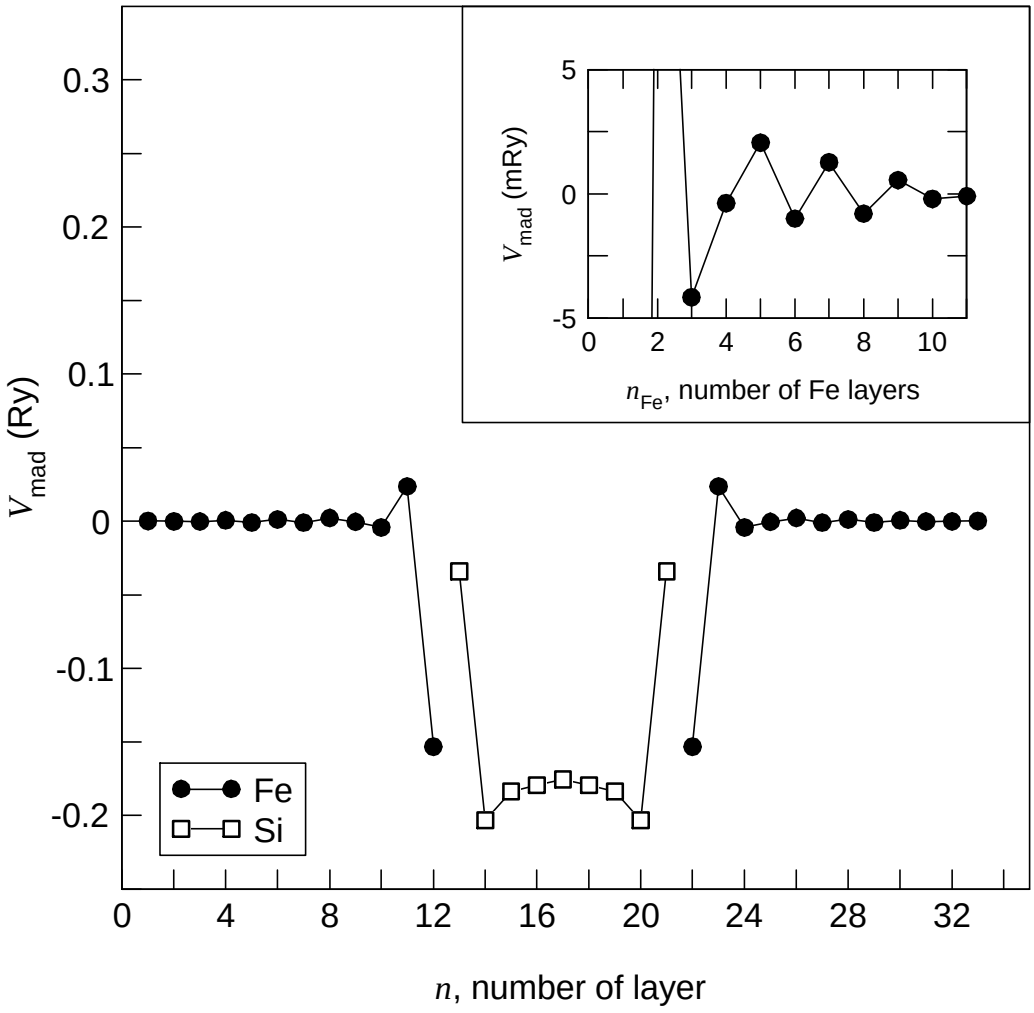
0.3
0.2
0.1
0
-0.1
-0.2
V_{mad} (Ry)
0
4
8
12
16
20
24
28
32
n, number of layer
Fe
Si
5
0
-5
V_{mad} (mRy)
0
2
4
6
8
10
n_{Fe}, number of Fe layers

Fig. 1

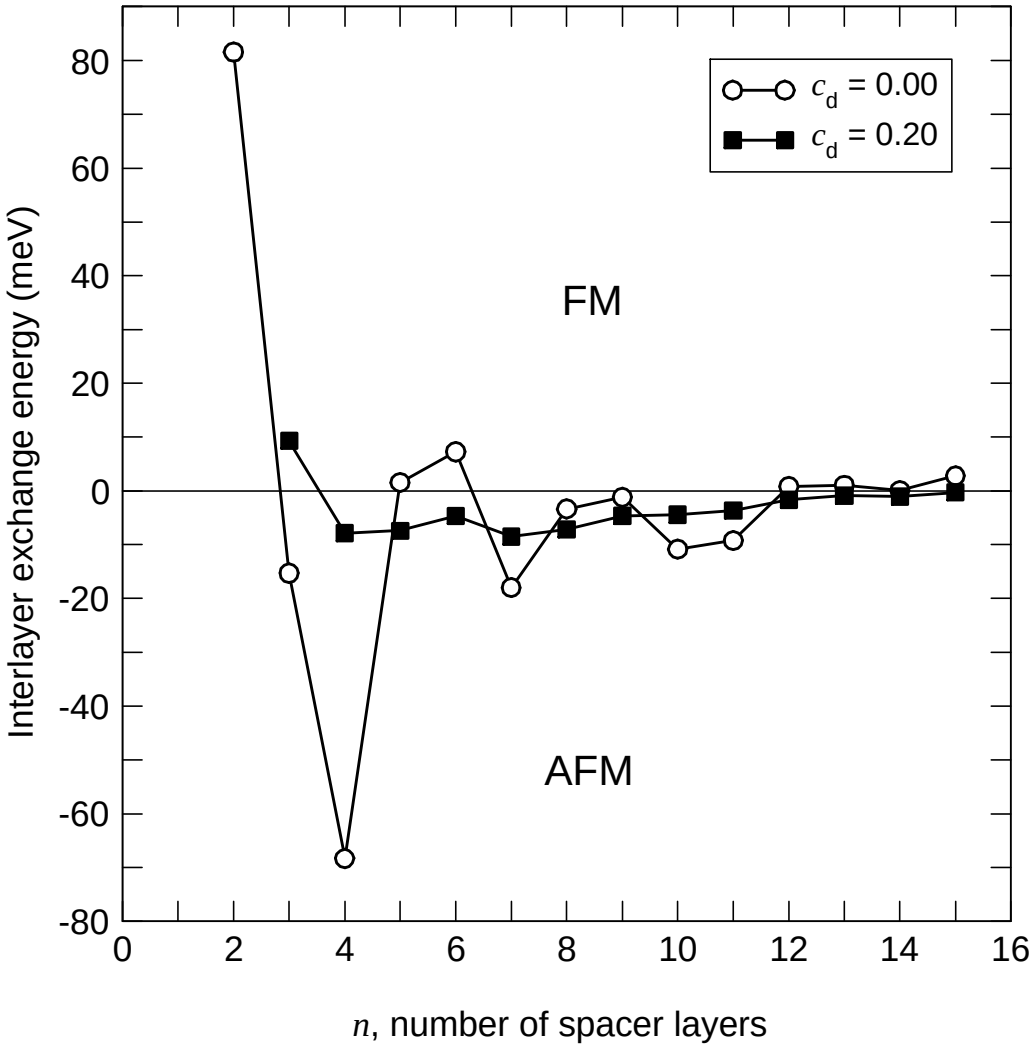
c_d = 0.00
c_d = 0.20
FM
AFM
Interlayer exchange energy (meV)
n, number of spacer layers
80
60
40
20
0
-20
-40
-60
-80
0
2
4
6
8
10
12
14
16

Fig. 2

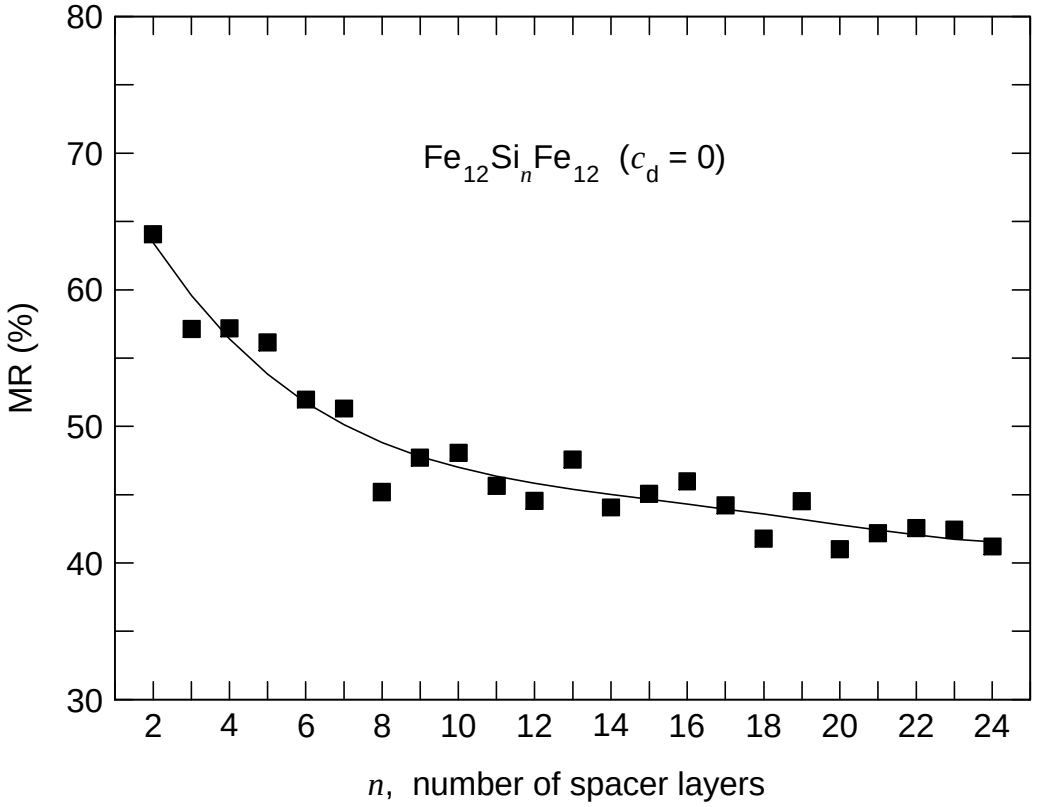
80
70
60
50
40
30
MR (%)
Fe12Sin Fe12 (cd = 0)
2
4
6
8
10
12
14
16
18
20
22
24
n, number of spacer layers

Fig. 3

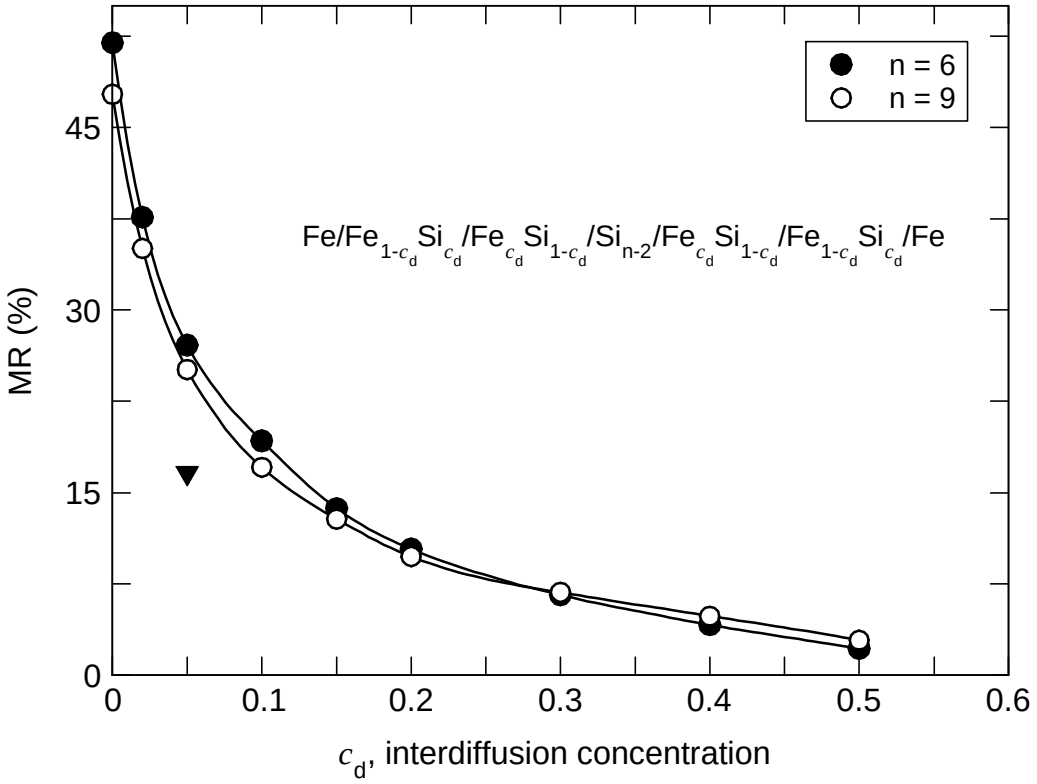
n = 6
n = 9
Fe/Fe1-cdSicd/Fecd Si1-cd/Sin-2/Fecd Si1-cd/Fe1-cd Sicd/Fe
MR (%)
0
15
30
45
0
0.1
0.2
0.3
0.4
0.5
0.6
cd, interdiffusion concentration

Fig. 4