

Influence of the interlayer exchange coupling on the electric transport in Fe/Cr/Fe and Fe/Cr/T/Fe ($T = \text{Mn, V}$): An *ab initio* study

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The electronic and magnetic properties of the Fe/Cr/Fe systems are studied within the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method by performing calculations for varying spacer thickness. The obtained interlayer exchange coupling shows a 2 ML period as well as phase slips due to the spin-density wave (SDW). In agreement with experimental findings we are able to prove that Mn impurities destroy the spin-density wave, whereby a statistically disordered Cr-Mn alloy spacer exhibits substantially larger effects than an atomic Mn layer separating the Cr spacer from the Fe leads. Using for such a layer V instead of Mn the SDW survives, but leads to a phase shift. The 2 ML period remains if an in-between layer of Mn or V is considered, whereas in the case of alloy formation in the spacer a superposition of different periods occurs. Further effort has been devoted to investigate the transport properties of the Fe/Cr/Fe sandwiches in the current perpendicular to the plane geometry in order to examine possible differences in the giant magnetoresistance due to the above-mentioned changes in the interlayer exchange coupling. From the present investigations we are able to show that the changes in the magnetic coupling, e.g., periods of oscillations or shifts, can directly be observed in the giant magnetoresistance.

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I. INTRODUCTION

The resistance of two magnetic layers that are separated by a nonmagnetic material is extremely sensitive to the magnetic configuration of the magnets, whereby the resistance is usually strongly decreased by applying an electric field.¹⁻³ Today, the giant magnetoresistance (GMR) effect is already technologically used in reading media, e.g., recording heads and magnetic sensors (see the review of Maekawa and Shinjo¹ and references therein). Quite some theoretical and experimental effort has been undertaken during the last one and a half decades to understand this effect and its relevance for technical applications.^{1,4-7} Most frequently it was suggested that the GMR is directly related to the interlayer exchange coupling (IEC).^{8,9} As the IEC depends on the constitution of the specimen, e.g., substrate temperature⁹ and structure of the interfaces,¹⁰ and it is influenced by transition metal impurities or “overlayers,”^{10,11} these effects should also be reflected in the GMR. Only very few papers, however, deal with both effects simultaneously in order to study the influence of the IEC on the GMR.¹²⁻¹⁴ Two systems turned out to be of special interest, namely Co/Cu and Fe/Cr multilayers, mainly because of the oscillating antiferromagnetic (AF) IEC depends on the spacer thickness.^{15,16} The IEC of both systems has been frequently studied especially as a function of the spacer thickness.^{10,11,17-20}

In Fe/Cr/Fe sandwiches two different oscillation periods have been observed by scanning electron microscopy¹⁷ (SEMPA), Brillouin light scattering¹⁰ (BLS), and the magneto-optic Kerr effect²¹ (MOKE). For spacers thicker than 4 monolayers (ML) a short period of 2 ML has been observed, which leads to AF coupling for even numbers of

spacer layers and to ferromagnetic (FM) coupling for odd numbers, whereby the sequence of order is reversed in the presence of interface alloying.^{10,22} This short period can only be observed for substrate temperatures higher than room temperature¹⁷ and under special experimental conditions.¹⁰ Nearly independent from the growth technique or temperature a second, much larger period with 10–12 ML of Cr exists in Fe/Cr systems. Due to the spin-density wave (SDW) of Cr,¹⁷ phase slips occur every 20 ML, whereby the first one occurs at 24 ML of Cr. It has been shown that the long period can also be observed in the GMR of (100)-oriented Fe/Cr superlattices at least at room temperature,^{23,24} which implies a direct connection of the GMR and the IEC. To our knowledge no indication of the short period has yet been found in GMR measurements, because of unavoidable interdiffusion effects.²³

Here, we investigate the GMR of Fe/Cr/Fe trilayers for the current perpendicular to the planes geometry (CPP) as a function of the thickness of the Cr spacer. The GMR is calculated in the (100) direction, although in GMR experiments often the (110) or (211) directions are preferred. However, Fullerton *et al.*²⁴ showed that the main properties are the same.

From Auger spectroscopy²⁵ and scanning tunneling microscopy (STM) measurements²⁶ it is known that at the Fe/Cr interfaces alloy formation takes place, whereby the interdiffusion concentration varies with the thickness of the Cr layer.^{25,27,28} In addition, it has been confirmed recently by Santamaria *et al.*²⁹ that the GMR of Fe/Cr multilayers is mostly determined by the structure and the width of the interface. Therefore, interface alloying is included in the present calculations using the coherent potential approximation (CPA). Although the IEC was already discussed in sev-

TABLE I. Structure of the investigated trilayers.

Type	Description	Structure of the spacer and interfaces	
A	Ideal interfaces	Fe/Cr _s /Fe	1 ≤ s ≤ 42
B	Finite interdiffusion	Fe/Fe _{1-c} Cr _c /Fe _c Cr _{1-c} /Cr _{s-2} /.../Fe	0 ≤ c ≤ 0.2
C	Homogeneous Cr-Mn alloy	Fe/(Cr _{1-x} Mn _x) _s /Fe	0 ≤ x ≤ 0.1
D	Mn “overlayer”	Fe/Cr _{s-1} /Mn ₁ /Fe	3 ≤ s ≤ 22

eral papers in view of the origin of the oscillation periods¹¹ or the magnetic moments at the interface,^{19,22} we have calculated the IEC for Fe/Cr/Fe trilayers for varying spacer thickness examining the influence of interdiffusion and its relation to the GMR. These investigations are different from those of Vernes *et al.*¹³ because they used trilayers with vacuum on top and examined solely systems with ideal interfaces. Furthermore, in contrast to the present paper the GMR there was discussed for the current in-plane geometry (CIP).

In the second part of this paper we refer to recent investigations by Heinrich *et al.*,¹⁰ who studied the changes in the phase and size of the IEC if a small amount of Mn is added to the Cr spacer, because Mn is known to destroy the SDW of Cr.³⁰ They restricted their measurements to sandwiches with 11 ML of Cr and 1–3 ML Mn on top of the Cr layers and concluded that Mn does not change the phase, but enhances the strength of the coupling by a factor of 2.5. Possible changes due to the thickness of the Cr layer were neglected. Here, investigations have been carried out for 3d transition metal impurities, such as Mn and V. The calculations have been performed for two different configurations: (1) a monolayer of Mn or V on top of the Cr spacer and (2) a homogeneous Cr_{1-x}Mn_x (x ≤ 0.1) spacer. It should be noted that a stabilization of the second case fails in experiment (at least at those temperatures needed to get layer by layer growth) because of the strong tendency of Mn to segregate to the surface during the growth process.¹⁰ Furthermore, we investigated the GMR for systems with Mn and V impurities. Our calculations show that in accordance with the experiments by Baumgart *et al.*³¹ small Mn or V concentrations do not affect the size of the GMR. We are also able to demonstrate that the oscillation periods are influenced by Mn. In order to understand in more detail the changes in the magnetic coupling and the GMR caused by interdiffusion and impurities, a separate section is devoted to the magnetic moments of the above mentioned systems.

II. COMPUTATIONAL DETAILS

A. Systems

The trilayers considered consist of s monolayers of a non-ferromagnetic spacer embedded between two semi-infinite bcc Fe(001) bulk systems. In addition, a buffer of m additional Fe layers between the spacer and the bulk material is used in order to account for the charge transfer at the interfaces.³² The actual systems considered are therefore of the form

$$\text{Fe}(001)/\text{Fe}_m/\text{S}_s/\text{Fe}_m/\text{Fe}(001),$$

$$s \leq 42, \quad 9 \leq m \leq 11. \quad (1)$$

All systems are two-dimensional translational invariant. Due to the properties of the screened two-dimensional structure constants³³ the total number of layers $2m+s$ has to be a multiple of three, therefore, the number of buffer layers m slightly varies [see Eq. (1)]. No attempt was made to account for lattice relaxations, i.e., the interlayer distance is assumed to be $d = 2.635$ a.u. [FM bcc Fe in the local density approximation (LDA)] for the whole system, which is 2.5% smaller than the experimental bulk value of Fe.³⁴

We have investigated Fe/Cr/Fe trilayers with four different types of spacers and interfaces; three of them deviate from the simple structure in Eq. (1) (see Table I). Besides systems with ideal interfaces (case A), trilayers with finite interdiffusion at the interfaces are studied (case B). In this case, the interdiffusion region extends over two layers with an interdiffusion concentration of 20%, which is close to the value given experimentally.³⁵ Further calculations have been done with Mn contamination, which is expected to suppress the SDW of Cr. This situation was modeled by assuming a disordered spacer Cr_{1-x}Mn_x alloy with 0 ≤ x ≤ 10% and a Cr spacer that is covered on one side with a monolayer of Mn, a case that can be realized in experiment at low substrate temperatures.¹⁰ Additional calculations have been performed with V monolayers on the Cr spacer, which seems not to destroy the SDW. We have assumed that the interface alloys and the Cr_{1-x}Mn_x spacer are disordered, and therefore can be described in terms of the inhomogeneous CPA.

B. Electronic structure and interlayer exchange energy

The electronic and magnetic properties of the Fe/Cr/Fe trilayers presented in Sec. II A have been calculated by means of the fully relativistic spin-polarized version of the screened Korringa-Kohn-Rostoker (SKKR) method for layered systems^{32,36} using the atomic sphere approximation (ASA) and the LDA.³⁷ It should be noted that the use of the LDA instead of a generalized gradient approximation (GGA) is adequate, although in the case of bcc Fe the GGA leads to a better agreement of calculated equilibrium geometries with respect to experimental data, since we use a fixed geometry and determine only magnetic energy differences within this structure. Furthermore, since transport properties depend only on the Fermi energy, it is not necessary at all to use the GGA. The interlayer exchange coupling can be defined by the total energy difference

$$\Delta E = E(\text{AF}) - E(\text{FM}), \quad (2)$$

where FM and AF denote a parallel (ferromagnetic) and an antiparallel (antiferromagnetic) relative coupling of the two semi-infinite Fe systems. In order to determine the interlayer exchange coupling from these calculations we made use of the magnetic force theorem,³⁸ which allows us to determine only one of the two configurations self-consistently and replace the difference of the total energies (2) by the band energy difference

$$\Delta E \sim \Delta E_b = \sum_{p=1}^n \Delta E_b^p, \quad (3)$$

where n denotes the total number of layers $n=2m+s$ and ΔE_b^p is the layer-dependent band energy (for details see Refs. 32 and 39). In the present investigations the FM configuration with the magnetic orientation perpendicular to the planes is calculated self-consistently, whereby it is assumed that the spacer layers show the same magnetic orientation as the nearest Fe bulk system.

C. Magnetoresistance

The magnetoresistance R can be defined in terms of the difference between the sheet resistances for zero field (assumed to be AF) $r(\text{AF})$ and with applied field $r(\text{FM})$:

$$R = \frac{r(\text{AF}) - r(\text{FM})}{r(\text{AF})}, \quad 0 \leq R \leq 1. \quad (4)$$

Here, we focus on the electric transport perpendicular to the planes and the $r(\mathcal{C})$ ($\mathcal{C}=\text{FM,AF}$) are obtained from the Kubo-Greenwood equation^{40,41} employing a fully relativistic spin-polarized version.⁴² For a sandwich of n layers and a magnetic configuration \mathcal{C} the sheet resistance can be written as

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

whereby the resistivity ρ_{pq} connects the current in layer p to the electric field in layer q . Due to numerical reasons the Fermi energy has to be complex, $\epsilon_F + i\delta$, and the sheet resistance is calculated for a finite imaginary part δ . Throughout this paper we have used $\delta=2$ mRy. It has been shown in our previous works^{43,44} that the sheet resistance varies linearly with δ . The calculated magnetoresistance (4) is systematically shifted to higher values for $\delta=0$, and therefore Eq. (4) serves as a lower limit for the GMR ratio at $\delta=0$.

One should be aware of the fact that in Fe and Cr systems noncollinear structures can occur—especially at the Fe-Cr interfaces—but it should be noted that in terms of electric transport such effects only matter for the size of possible anisotropic parts of the resistance, i.e., anisotropic magnetoresistance (AMR) effects. Furthermore, as noncollinearity can comprise both noncollinear spin structures with respect to the planes and within these planes, the magnetoresistance ratio no longer simply relates parallel and antiparallel resistivities to each other. In that case the MR ratio has to be redefined. In principle, noncollinearity can be taken into account, e.g., in discussing domain wall resistivities,⁴⁵ but in

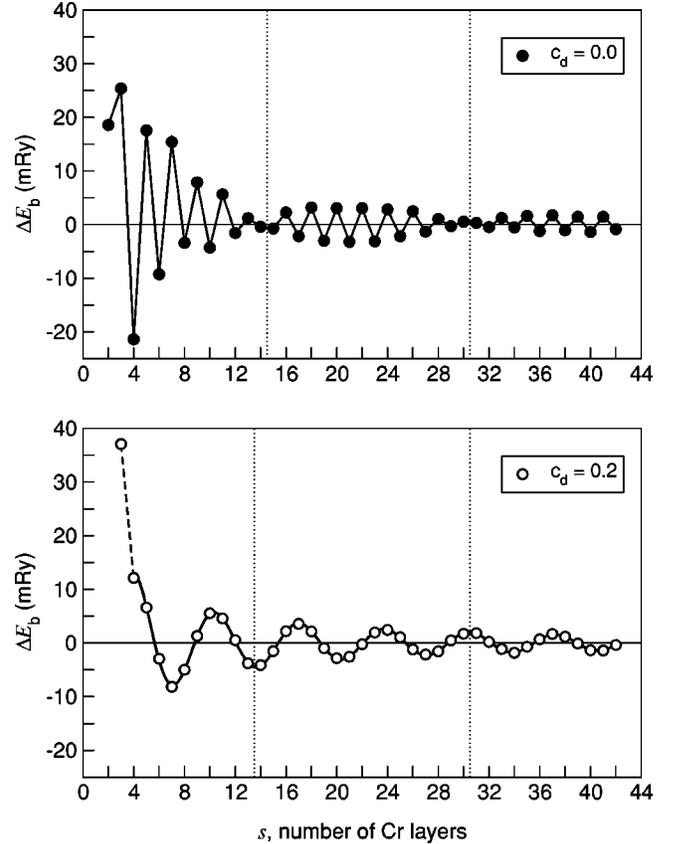


FIG. 1. Interlayer exchange energy ΔE_b of Fe/Cr/Fe trilayers versus the number of spacer layers s without interdiffusion ($c_d=0$, top) and with a two-layer interdiffusion ($c_d=0.2$, bottom). In the latter case the full line corresponds to a RKKY-type fit [Eq. (6)]. Vertical lines mark the nodes of the SDW, see text.

the present case such a study of noncollinearity would give only qualitative results due to the huge number of possible magnetic configurations.

III. RESULTS AND DISCUSSION

A. Fe/Cr/Fe with interdiffusion

1. Interlayer exchange coupling

We have used Eq. (3) to calculate the IEC of the Fe/Cr/Fe trilayers. The results for the systems A and B are summarized in Fig. 1, whereby some general aspects of the systems of type A have already been discussed in the literature.^{11,13,22} Therefore, in this paper we will focus on the those features that are important for matters of comparison to the IEC of the systems B–D. Two different periods are observed in the case of the ideal Fe/Cr/Fe system (Fig. 1, top). The short 2 ML period has been found for spacer thicknesses s larger than 2 ML, whereby for thinner spacers the coupling becomes FM, which in turn is in good agreement with experiment.^{10,46} However, in experiment this short period has been observed only for $s \geq 9$ (see Ref. 46), whereas most calculations show an onset of the short period for $s \geq 3$ or for even thinner films.^{11,13} This difference is most likely caused by interface roughness, which occurs during the growth of

the system and is neglected in all theoretical calculations up to now. In agreement with the results by Freyss *et al.*²² and Vernes *et al.*¹³ we obtained AF coupling for even numbers of spacer layers and $s \leq 15$ or $s \geq 32$, whereby this order is reversed for systems with $15 < s < 32$. A second, longer period is usually observed in magnetization measurements with a period of 10–12 ML.^{17,24} This period was already discussed in several theoretical papers by fitting the energy differences of Eq. (2) to RKKY-type expressions.^{11,20}

Furthermore, the calculated IEC (Fig. 1) shows phase slips at every 16 ML, which are related to the incommensurability of the Cr SDW;⁴⁶ the first slip occurs at 14 ML of Cr. In experiment these phase slips have a period of 20 ML at room temperature, the first slip can be observed at 24 ML.^{46,47} This large deviation of the calculated period from the experimental result has been observed also in previous calculations [a phase slip after 14 (Ref. 48) or 29 ML (Ref. 11)] and seems to be sensitive to the theoretical technique used, i.e., whether a supercell method was applied or not. The main difference between a supercell approach and the present calculations is that in supercell calculations the Fermi energy changes with the thickness of the Cr spacer and is not related to the Fermi energy of the leads. It should also be mentioned that the calculations refer to $T=0$, whereas the measurements were performed above the Néel temperature. Since we are able to investigate relatively thick spacers with more than 40 ML of Cr and since as in Ref. 13 no slab geometry is used, the phase slip can directly be seen in Fig. 1.

However, usually Fe/Cr interfaces are not as perfect as described above. Interdiffusion effects lead to the formation of Fe-Cr alloys, the roughness of the interface being determined by the growth temperature. For growth temperatures well above room temperature T_R the interface roughness is relatively small and the short period can be recorded. In Fe/Cr whiskers it has been observed by BLS experiments¹⁰ that the short period also exists for finite interdiffusion. In this case the layer dependence becomes reversed (even numbers of spacer layers are now coupled ferromagnetically), which was also confirmed theoretically.²² Similar results are reported in Ref. 47 in terms of SEMPA experiments.

In our calculations we have assumed a randomly disordered alloy at the two interfaces of the trilayer (case B) (see Table I), which corresponds to the experimental situation of frozen disorder due to low growth temperatures. In agreement with the experimental findings the short period vanishes with the onset of disorder. As can be seen from Fig. 1 the 2 ML period is replaced by a longer period of about 7 ML, which, however, has not been observed in experiments. In order to exclude that the oscillations in Fig. 1 refer to a superposition of oscillations with two different periods, we used a RKKY-type expression to fit the calculated data points with respect to the number of Cr layers s ,

$$J(s) = A_0 \frac{\sin(2\pi s/T_0 + \phi_0)}{s^2} + A_1 \frac{\sin(2\pi s/T_1 + \phi_1)}{s}, \quad (6)$$

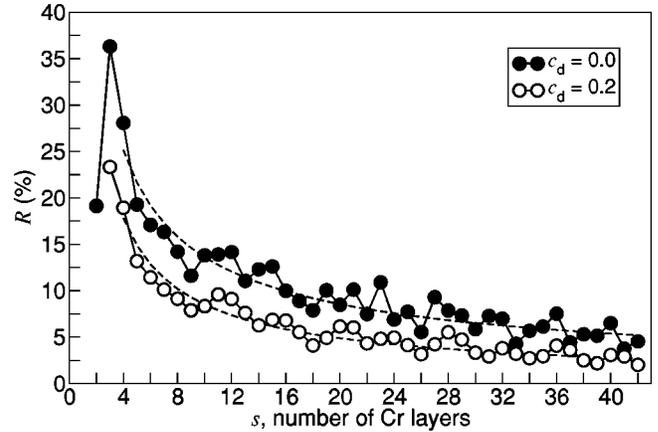


FIG. 2. Giant magnetoresistance R of Fe/Cr_{*s*}/Fe trilayers with ideal interfaces (filled circles) and for a finite interdiffusion of 20% (open circles) as a function of the number of Cr layers s . The broken lines are cubic splines as guide to the eyes.

whereby the $1/s^2$ term corresponds to the usual RKKY interaction, which describes the asymptotic limit $s \rightarrow \infty$. The $1/s$ term occurs in the case of fully planar nesting, which in turn has to be related to the short period.¹¹ In the present case, however, there seems to be no short period. The fit gives only one period of $T_0 = T_1 = 6.74$ ML. Comparing the present results with the experimental data it turns out that the assumption of total disorder (CPA) at the interfaces provides the right trend for destroying the short period. The results indicate that the 7 ML period is strongly related to disorder at the interface. Furthermore, it should be mentioned that the phase slips occurring at 13 and 30 ML can hardly be seen.

2. Giant magnetoresistance

It is well known from literature that the switching between AF and FM coupling is reflected in the GMR. A famous example is the Co/Cu multilayer (see Ref. 49). The question of how far the different oscillation periods caused by interdiffusion can be observed in the CPP GMR will be addressed in this section. The GMR for the two types of systems, $c_d = 0.0$ and 0.2 , has been calculated using Eq. (4) (Fig. 2). In both cases the shape of the GMR curve looks similar: It decreases slowly with an increasing number of spacer layers. The alloying at the interfaces leads to an additional decrease of approximately 5%, which becomes less important for thicker Cr layers (Fig. 2). This is in agreement with previous model calculations by Hood *et al.*⁵⁰ They also observed a decrease of the GMR if the roughness of the interface becomes larger than 2 Å, whereby the absolute value depends on the choice of the model parameters. However, Rensing *et al.*⁵¹ reported an enhancement of the GMR due to Cr doping of the Fe layers. This result does not contradict our results, because they deposited thin Cr layers on the Fe layer and avoid interdiffusion by annealing. For very thick spacers the GMR is still finite, namely between 5% and 2.5% at 42 ML of Cr. This is different from previous calculations within the Kubo-Greenwood formalism by Vernes *et al.*¹³ for the CIP GMR in similar trilayers with vacuum on one side. In the CIP case the GMR oscillates around zero if

TABLE II. Algorithm used to detect the local extrema of the GMR (R) and the IEC (ΔE_b) depending on the number of the spacer layers s . Local maxima of the IEC (GMR) are described by $x=0$ ($x=1$) and local minima by $x=-1$ ($x=0$), respectively.

Ascent of R and ΔE	x
$(s) < R(s+1)$	1
$R(s) > R(s+1)$	0
$\Delta E_b(s) < \Delta E_b(s+1)$	-1
$\Delta E_b(s) > \Delta E_b(s+1)$	0

the spacer becomes thicker than 30 ML of Cr. As compared to the CPP GMR the CIP values are always smaller, a fact that has also been observed experimentally at low temperatures.^{52,53} Furthermore, from Fig. 2 it is obvious that the decrease is accompanied by small oscillations, for which the period seems to depend on the structure of the interface. In the CIP case¹³ such oscillations could be observed in the resistances, but not in the GMR because of the small differences between the AF and FM resistivities. In order to make the relation between the IEC and GMR visible, we have made use of the model presented in Table II. We have already discussed in detail in a previous paper the system without interdiffusion that the 2 ML period of the IEC is directly related to local maxima and minima in the GMR:⁵⁴ The GMR shows the same short 2 ML period as the IEC; even the phase slips can be observed although being slightly shifted and smeared out (inset in Fig. 3). It should be noted that the maxima always correspond to AF coupling and the minima to FM coupling, respectively. However, until now only the long period has been found in experiments.¹⁵

In order to check whether this correlation also applies to a finite interdiffusion, we used the same algorithm as in Ref. 54, namely, the one summarized in Table II. The corresponding results are displayed in Fig. 3 with respect to the number of Cr layers. For a finite interdiffusion the phase matching between the IEC and the GMR seems to be destroyed. The maxima and minima in the GMR are no longer directly re-

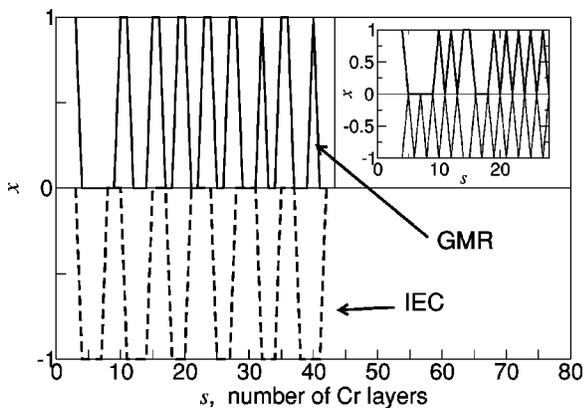


FIG. 3. Comparison of the oscillations in the GMR and the IEC for $c_d=0.2$. Local maxima in the IEC (GMR) are described by $x=0$ ($x=1$) and local minima by $x=-1$ ($x=0$), respectively, s is the number of spacer layers. The inset shows the results for $c_d=0$.

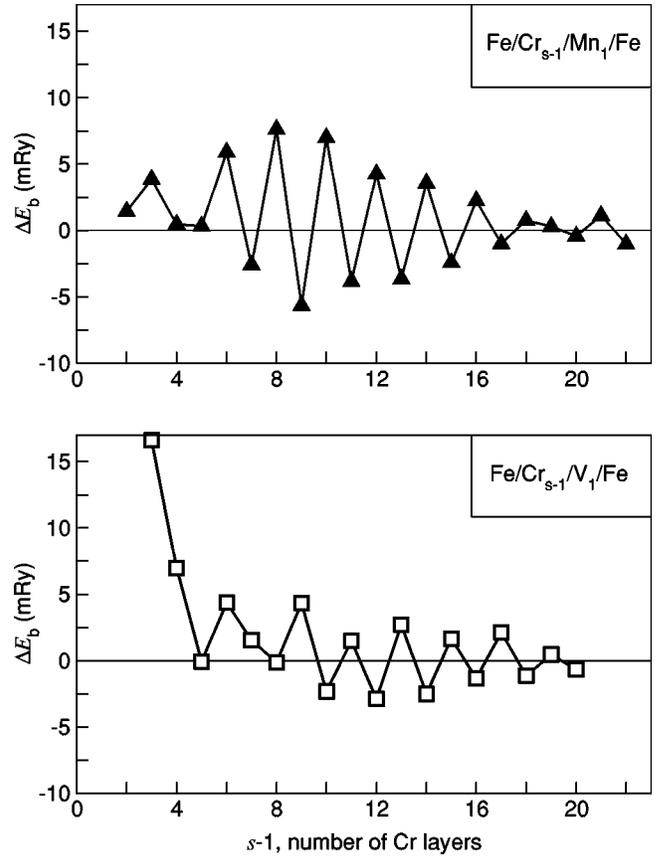


FIG. 4. Interlayer exchange coupling energy ΔE_b of $\text{Fe}/\text{Cr}_{s-1}/T_1/\text{Fe}$ sandwiches with $T=\text{Mn}, \text{V}$ versus the number of Cr layers $s-1$.

lated to FM or AF coupling, which in turn is confirmed by the fact that the oscillation period of the GMR is smaller (5 ML) than that of the IEC (7 ML).

B. Fe/Cr/Fe with Mn and V impurities

1. Interlayer exchange coupling

The coupling behavior of Fe/Cr multilayers or sandwiches seems to be very sensitive to the incommensurability of the magnetic configuration of Cr. Therefore, it is interesting to examine how the IEC changes, if the magnetic configuration transforms to a commensurate AF configuration. Here, the magnetic configuration has been varied by adding 3d transition metal impurities into the spacer or as a separate layer between the spacer and the leads. The results for Cr spacers covered by a single monolayer of V or Mn (case C) are displayed in Fig. 4. In both cases the 2 ML period can be observed for systems with more than 4 ML of Cr, whereby an “overlayer” of Mn leads to a shift of the phase, e.g., even numbers of Cr layers are ferromagnetically coupled. It should be recalled that in the case of pure Fe/Cr/Fe, odd layers are ferromagnetically coupled up to the first phase slip. The same type of coupling has been found in experiments with $\text{Fe}/\text{Cr}_{11}/\text{Mn}_1/\text{Fe}$ sandwiches.¹⁰ It is also reported in the same paper that an “overlayer” of Mn leads to a much stronger coupling. This, however, is not supported by the

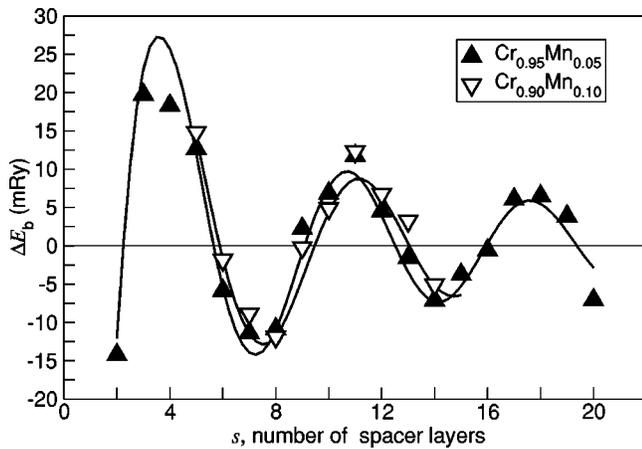


FIG. 5. Interlayer exchange coupling energy ΔE_b of trilayers with $\text{Cr}_{1-x}\text{Mn}_x$ spacers versus the number of spacer layers s for 5% (filled triangles) and 10% (open triangles) of Mn. Solid lines mark fits to the RKKY-type expression in Eq. (6).

present results. Due to the fact that experimentally only one particular Cr thickness has been examined, it is questionable whether this statement applies to all thicknesses. Here, the magnitude of the IEC of $\text{Fe}/\text{Cr}_{10}/\text{Mn}_1/\text{Fe}$ is 1.4 times larger as compared to the $\text{Fe}/\text{Cr}_{10}/\text{Fe}$ system, whereas for 9 ML of Cr the IEC decreases when inserting an atomic plane of Mn atoms.

From Fig. 4 it is obvious that the IEC is rapidly damped if the spacer layer becomes thicker than 17 ML, a behavior that is different from cases A and B. For very thin (≤ 4) Cr layers the IEC is FM. In this limit of film thicknesses the strength of the coupling for systems with V “overlayers” is comparable to the coupling without impurities, whereas Mn strongly reduces the FM coupling in the thin spacer limit. This most likely can be attributed to frustration effects, because Cr always couples AF to Fe, while the coupling between Fe and Mn is reversed in the case of even numbers of Cr layers. Furthermore, in the case of AF coupling the magnitude of the IEC is reduced by a layer of V atoms, whereas Mn seems not to influence significantly the magnitude of the IEC.

As compared to case A no phase slips are visible with the exception of perhaps such a slip between 4 and 5 ML of Cr for systems with Mn “overlayers.” From the present calculations we are not able to exclude the existence of phase slips completely, it may still be possible that such slips occur for thicker spacers. It will be demonstrated below that the SDW survives in the case of an V “overlayer,” while Mn transforms the SDW into an commensurate AF phase (see Sec. III C).

Up to now it was assumed that the impurities are located at the boundary of the Cr spacer to the Fe leads, which at least is known for Mn to be the experimental situation at elevated temperatures.¹⁰ Nevertheless, it is interesting to know what happens if the impurities form alloys with the spacer material. For this reason we have replaced the Cr spacer by a statistically disordered Cr-Mn alloy with a Mn concentration of 5% and 10%. As can be seen from Fig. 5, the results are nearly independent from the impurity concen-

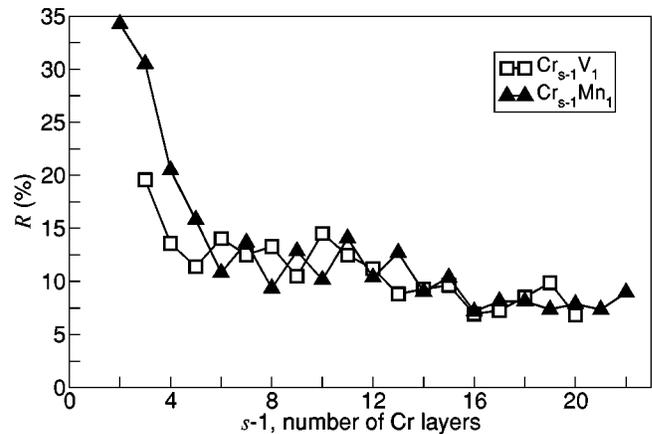


FIG. 6. Giant magnetoresistance R of $\text{Fe}/\text{Cr}_{s-1}/T_1/\text{Fe}$ sandwiches, $T = \text{Mn}, \text{V}$, as a function of the number of Cr layers s .

tration, i.e., there are only minor differences between the two curves. The IEC for systems with $\text{Cr}_{1-x}\text{Mn}_x$ spacers, however, is completely different from that of case C (“overlayer”) (see Fig. 5). In contrast to the previously discussed systems with Mn on top of the Cr layers no 2 ML period can be seen. As it seems likely that the IEC is a superposition of two oscillations, we have used the same RKKY expression as before [Eq. (6)] in order to determine the periods for the system with 5% of Mn. We found an oscillation of $T_0 = 6.9$ ML just as in the case of interdiffusion and alloy formation at the interfaces (case B). This has been expected due to the fact that this period can be related to disorder in the spacer. However, in the present case this period of approximately 7 ML seems to be superposed by a short 2 ML ($T_1 = 2.005$ ML) period, although the latter is less pronounced in systems with impurity “overlayers.” This is confirmed also by the analysis of the systems with 10% of Mn (see Fig. 5). In summary the 2 ML period is not completely destroyed by disorder or interdiffusion, but damped with respect to the actual composition of the alloyed spacer.

2. Giant magnetoresistance

Although impurities have an enormous influence on the coupling of the Fe layers the changes in the GMR due to additional Mn or V layers are less pronounced. Neither impurity “overlayers” nor a Cr-Mn alloy spacer lead to significant changes of the size of the GMR (Figs. 6 and 7). The GMR ranges between 7.5% and 15% for spacer layers thicker than 4 ML. This agrees with the experimental findings reported in Ref. 31 for Fe/Cr multilayers with impurity layers of V and Mn. It should be noted that it has been observed that thicker impurity layers can enhance the GMR.³¹ In systems with very thin Cr spacers (≤ 4 ML) the size of the GMR depends on the type of impurity. Sandwiches with V “overlayers” have slightly smaller GMR values than a corresponding pure $\text{Fe}/\text{Cr}/\text{Fe}$ trilayer; the size of the GMR is not changed by Mn impurities.

For systems with more than 4 ML of Cr the different periods, which have been discussed in the preceding section, are clearly reflected in the GMR. The GMR shows a zigzag behavior due to the short period; the amplitude decreases

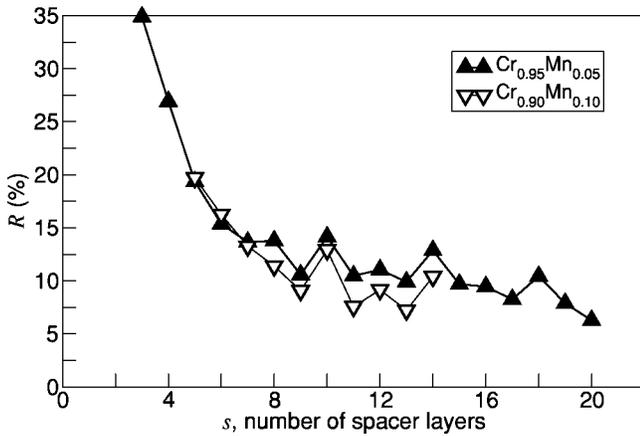


FIG. 7. Giant magnetoresistance R of $\text{Fe}/(\text{Cr}_{1-x}\text{Mn}_x)_s/\text{Fe}$ sandwiches as a function of the number of spacer layers s for 5% (filled triangles) and 10% (open triangles) of Mn.

rapidly with an increasing number of Cr layers. Especially, for the case of a Mn “overlayer” it is obvious that maxima corresponding to AF coupling occur at odd numbers of Cr layers and minima at FM coupling, whereas in the case of V the trend is less clear. From Fig. 6 it seems that the meaning of the maxima and minima is reversed (i.e., odd numbers of Cr layers couple AF), but there are deviations from this behavior, e.g., for systems with 15–17 ML of Cr. This can be understood from the fact that V does not destroy the SDW of Cr (see Sec. III C). The above investigations for systems with V and Mn “overlayers” have confirmed what has been suggested for case A: the 2 ML oscillations in the IEC are indeed mapped in the GMR. This also applies to the phase slips in the SDW.

It has been shown in the preceding section that distributing the Mn atoms in the spacer (case D) instead of on top of the Cr layers (case C) leads to significant changes in the IEC. These changes are also reflected in the GMR (Fig. 7). For small numbers of spacer layers the behavior is comparable to that of $\text{Fe}/\text{Cr}/\text{Fe}$. With an increasing number of spacer layers the GMR starts to oscillate—as before—with the number of spacer layers. Just as in case B the period can be roughly estimated to be 5 ML. In contrast to the IEC the indications of the short 2 ML period can directly be seen in Fig. 7, because for the systems with 12 and 16 ML there are small additional maxima, which can be related to the short 2 ML period. Finally, it should be mentioned that the GMR slightly decreases with an increasing amount of Mn impurities, which is in agreement with results from resistance measurements.³¹

C. Magnetic moments

In the above discussion of the GMR and the IEC of $\text{Fe}/\text{Cr}/\text{Fe}$ sandwich structures it has been stated that, due to interdiffusion or impurities, these properties are strongly related to respective changes in the magnetic moments. In order to discuss the magnetic properties of the Fe/Cr systems under investigation, we have performed additional calculations for systems with 39 and 40 ML of Cr. With the excep-

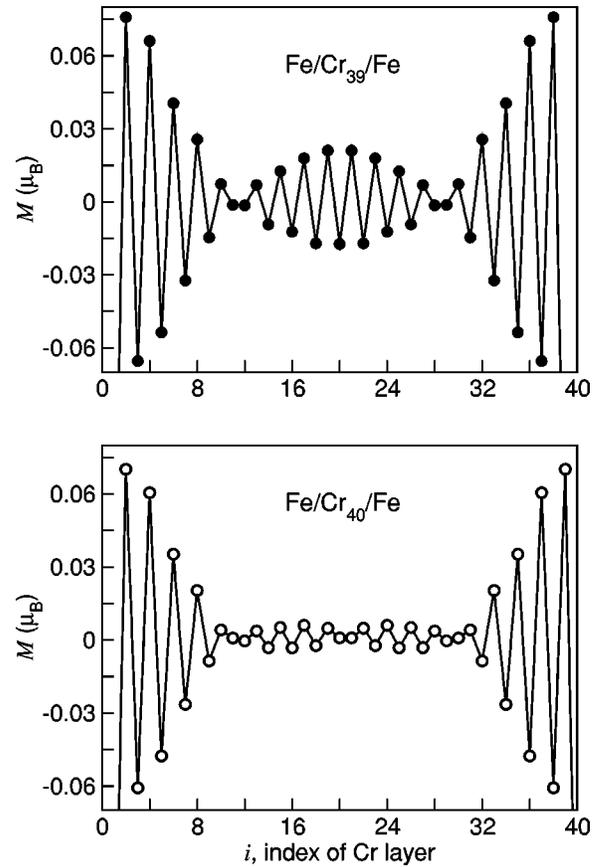


FIG. 8. Magnetic moments of Cr in $\text{Fe}/\text{Cr}_s/\text{Fe}$ trilayers with $s = 39$ (filled circles) and $s = 40$ (open circles) layers of Cr versus the index of the Cr layer i .

tion of one example, all magnetic moments shown here have been calculated for the FM configuration of the leads. The AF configuration leads only to an interchange of parity, i.e., magnetic configurations that are for even numbers of Cr layers are switched to odd numbers and vice versa. The size of the Cr magnetic moments is rather small ($< 0.1\mu_B$); however, they show a clear trend. In agreement with previous investigations of Vernes *et al.*¹³ the typical 2 ML period is observed for $\text{Fe}/\text{Cr}/\text{Fe}$ sandwiches without interdiffusion (see Fig. 8). In a sufficient distance from the interfaces a modulation of the amplitude of the magnetic moment occurs, whereby odd numbers of Cr layers lead to one belly with two nodes, whereas even numbers exhibit a third node in the middle of the Cr spacer. Systems with odd numbers of Cr layers show the same long period as the IEC, while in the case of even numbers of spacer layers the period is halved: A thicker spacer would be needed to reach the long period.

Although, interdiffusion at the Fe-Cr interface (case B) leads to significant changes in the GMR and IEC, the magnetic moments are very similar to the undisturbed case (see Fig. 9). The amplitudes of the induced moments are, however, smaller by a factor of 2 as compared to the results shown in Fig. 8. Furthermore, the long periods are slightly larger than for $\text{Fe}/\text{Cr}/\text{Fe}$, which can also be seen in the IEC. From Fig. 9 it is obvious that the number of Cr layers is *a priori* decisive for the nodes and periods, whereby the inter-

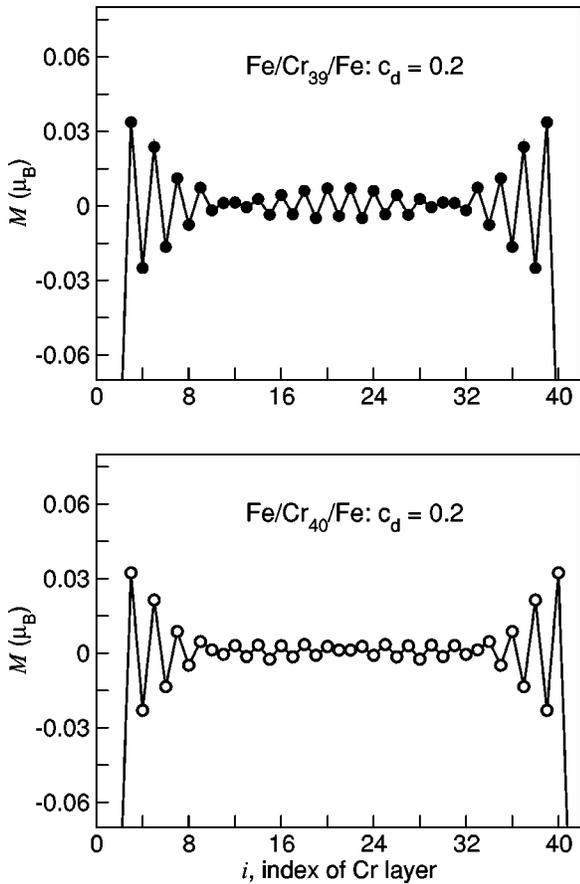


FIG. 9. Magnetic moments of Cr in $\text{Fe}/\text{Cr}_s/\text{Fe}$ trilayers with $s = 39$ (filled circles) and $s = 40$ (open circles) Cr layers for a finite interdiffusion of 20% versus the index of the Cr layer i .

diffusion plays only a minor role. That seems to be in contradiction to the results for the IEC, compare Sec. III A 1. The magnetic moments themselves show no indication for a 7 ML period and what is even more important, the magnetic moments do show the 2 ML period (Fig. 9). These two facts suggest that a 2 ML period exists, which is suppressed in the IEC.

As discussed in Section III B 3d transition metal “overlayers” lead to significant changes in the IEC. The magnetic moments for a thick Cr spacer with V or Mn on top are displayed in Fig. 10. In both cases the 2 ML period can be observed, but with respect to the SDW of Cr these two systems behave differently. An “overlayer” of Mn destroys the SDW and the magnetic moments decrease continuously with the distance from the Mn-covered Fe lead. However, the SDW has not completely vanished, which is indicated by the node on the left side of the spacer. This node arises from the Fe-Cr interface, which is not covered by Mn. If the Mn atoms are distributed in the Cr spacer (case D) instead of forming an atomic plane on top of the Cr spacer, the SDW vanishes completely (Fig. 11). This is in agreement with experimental observations.³⁰

An “overlayer” of V on the contrary does not destroy the SDW of Cr (Fig. 10). Due to the V “overlayer” the moments are no longer symmetrically distributed; nevertheless two nodes can clearly be seen. The behavior of the moments is

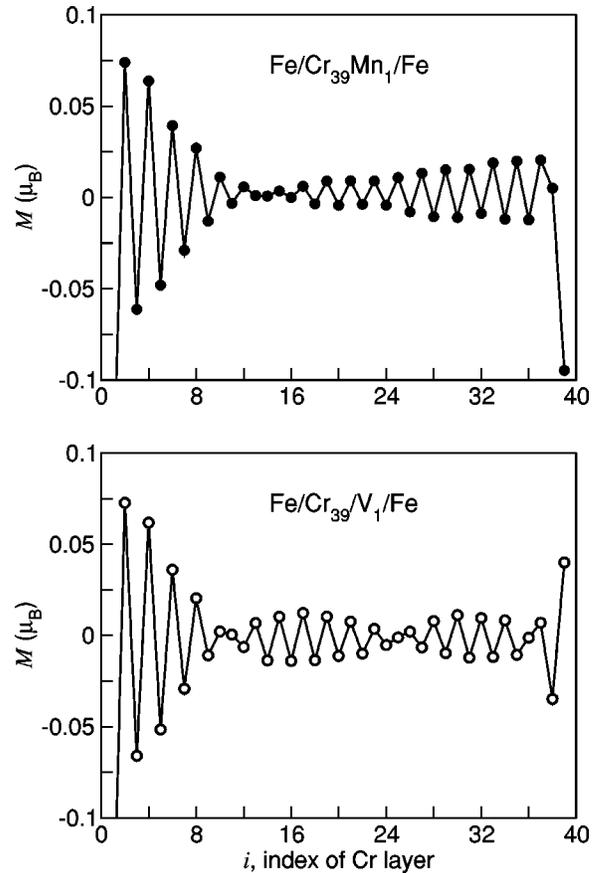


FIG. 10. Magnetic moments of Cr for a $\text{Fe}/\text{Cr}_{39}/T_1/\text{Fe}$ sandwich with $T = \text{Mn}$ (filled circles) and $T = \text{V}$ (open circles) versus the index of the Cr layer i .

comparable to the $\text{Fe}/\text{Cr}/\text{Fe}$ system with 40 ML of Cr. This agrees with the results for the GMR and IEC (see Secs. III B 2 and III B 1), which are shifted by one monolayer as compared to the $\text{Fe}/\text{Cr}/\text{Fe}$ or $\text{Fe}/\text{Cr}/\text{Mn}/\text{Fe}$ systems. This difference is caused by the Fe-V coupling. The V atoms couple antiferromagnetically to Fe and Cr, which induces a rearrangement in the spacer. In the case of Mn this problem does not occur, because Mn also couples antiferromagnetically to Cr, but the coupling between Fe and Mn is ferromagnetic.

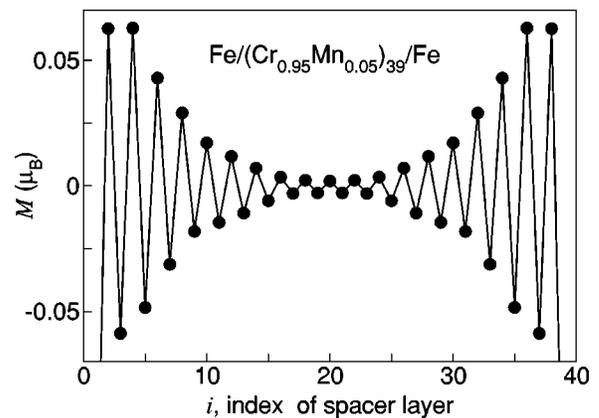


FIG. 11. Magnetic moments of a $\text{Fe}/(\text{Cr}_{1-x}\text{Mn}_x)_{39}/\text{Fe}$ trilayer versus the index of the spacer layer i .

IV. CONCLUSIONS

Using the SKKR method and the Kubo-Greenwood equation we have investigated the interlayer exchange coupling and the CPP GMR of Fe/Cr/Fe trilayers, which contain planes of $3d$ transition metal impurities or form alloys at the Fe-Cr interfaces. Although the size of the GMR and IEC depends only weakly on these effects, the oscillation periods of the IEC and the GMR are strongly influenced by the type of impurities and interdiffusion. In agreement with experiments and other theoretical investigations a short 2 ML period has been found for Fe/Cr/Fe trilayers and due to the SDW of Cr phase slips every 15 ML.

From the present results it is obvious that the periods of oscillations in the IEC and the GMR are the same for trilayers with undisturbed interfaces and $3d$ metal “overlayers.” If interdiffusion occurs at the interfaces or a disordered Cr-Mn spacer applies, the period of the IEC seems to be slightly larger as compared to the GMR. This can be explained by a superposition of two oscillations with different periods as follows from a RKKY-type fit for the alloyed spacers. The case of interdiffusion turns out to be more complicated: the results for the IEC and GMR gave no indication for a superposition of different periods, but the magnetic moments of a thick Cr spacer did. From investigations of spacers with more than 39 ML of Cr it can be seen that, besides a pronounced 7 ML period, a 2 ML period still exists. It has to be mentioned that this 7 ML period was not observed in experiment up to now and may be an artifact of using the concept of statistical disorder (CPA).

As mentioned above covering the Cr spacer with an “overlayer” does not change the 2 ML period. In the case of

Mn, however, the phase slips vanish at least on the side where the “overlayer” has been placed. If Mn atoms are distributed randomly in the spacer the phase slips vanish completely and the SDW transforms into a commensurate AF structure. This transformation has also been observed experimentally. Further investigation of V monolayers on the Cr spacer have shown that, in contrast to Mn, V does not destroy the SDW. The magnetic moments of the Cr spacer are of course no longer symmetric, but still show typical nodes. As previously discussed⁵⁴ for the ideal system the extrema are related to AF or FM coupling. For a sufficiently large number of spacer layers, Mn “overlayers” lead to FM coupling for even numbers of Cr layers, whereas odd numbers couple antiferromagnetically. If V is used instead of Mn, the sequence is reversed. This most likely is caused by the fact that V prefers AF coupling with Fe and Cr, whereas Mn couples antiferromagnetically to Cr and ferromagnetically to Fe.

In summary, it has been shown that most of the changes in the transport properties or the magnetic coupling can be correlated to respective changes in the magnetic configuration of the Cr spacer. However, modifications of the spacer and of the interfaces strongly vary the periods of the GMR, or IEC, but not their size: The GMR, therefore, is not enhanced.

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