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CPP TRANSPORT IN Fe/Cr/Fe TRILAYERS WITH Mn IMPURITIES: AN *AB INITIO* STUDY

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The influence of Mn impurities on the electric transport properties of Fe/Cr/Fe sandwiches has been investigated as a function of the thickness of the Cr layer by employing the Kubo–Greenwood equation. The electronic and magnetic properties of the Fe/Cr sandwich-structures have been evaluated within the screened Korringa–Kohn–Rostoker method for layered systems. In this article, two types of impurities are studied: atomic layers of Mn placed on top of the Cr layers, and spacers consisting of disordered CrMn alloys. In agreement with experimental findings it is found that the size of the giant magnetoresistance (GMR) is not much affected by Mn impurities. However, Mn is known to transform the spin density wave (SDW) of Cr into a commensurate antiferromagnetic structure. These kinds of changes in the magnetic coupling are reflected in the GMR. The present results show that 5% of Mn in the spacer is sufficient to destroy the SDW.

Keywords: Electric transport; Giant magnetoresistance; Kubo–Greenwood equation; Magnetic multilayers

1. INTRODUCTION

Fe/Cr/Fe trilayers and Fe/Cr multilayers show an antiferromagnetic (AF) interlayer exchange coupling (IEC) in a wide range of Fe and Cr thicknesses (Grünberg *et al.*, 1986). At elevated substrate temperatures a short 2 monolayer (ML) period is observed if the spacer thickness becomes larger than 9 ML (Unguris *et al.*, 1991; Heinrich *et al.*, 1999). Due to the spin density wave (SDW) of Cr phase slips occur at every 20 ML (Unguris *et al.*, 1991). Transition metal impurities, e.g. Mn, influence the magnetic structure of the Cr spacer (Fawcett *et al.*, 1994) and the IEC (Heinrich *et al.*, 1999; Herper *et al.*, 2003c). Here, the influence of Mn impurities on the magnetic configuration of Fe/Cr/Fe trilayers has been investigated for Fe/Cr/Fe sandwiches, whereby the investigation of very thick (≥ 39 ML) systems allows a detailed analysis of the long-range magnetic structure. The impurities have been added in two different ways. First, a monolayer of Mn has been placed on top of the Cr spacer. Second, the Mn atoms are distributed in the spacer by using a statistically disordered CrMn alloy as

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spacer material with 5% of Mn. It will be shown that the SDW of Cr tends to transform into a commensurate AF structure, whereby a complete transformation only takes place in the case of a disordered CrMn spacer.

Fe/Cr multilayers show a giant magnetoresistance (GMR) effect, which means that the resistance depends on the relative magnetic configuration of the Fe layers. It is assumed that the changes in the magnetic configuration of Cr will be also present in the GMR. Though Fe/Cr systems have been heavily studied, most of the experiments or calculations are devoted only to the coupling behavior (Fert *et al.*, 1995; Pierce *et al.*, 1999). The GMR has been studied (Fullerton *et al.*, 1993; Fawcett *et al.*, 1994) mostly in the CIP geometry; only a few papers deal with the GMR in the current perpendicular to the plane (CPP) geometry (Gijs *et al.*, 1993). The CPP GMR is usually larger than the CIP GMR; its measurement, however, is more complicated. In this article results for the CPP GMR depending on the spacer thickness are presented. The resistances are calculated via the Kubo–Greenwood equation (Kubo, 1957; Greenwood, 1958; Weinberger, 2003). In the present study it will be shown that the changes in the magnetic coupling due to the impurities can also be observed in the GMR.

2. COMPUTATIONAL METHOD

The investigated systems consist of two semi-infinite bulk systems, i.e. bcc Fe sandwiching a number of spacer layers. In order to take into account charge accumulation effects at the interfaces it is necessary to include ≈ 10 additional Fe lead layers in the self-consistent calculation (Herper *et al.*, 2003a). In this article, three different types of spacers are studied, see Table I. Impurities of Mn have been included as single monolayers on top of the Cr spacer and in the form of disordered CrMn alloys with 5% of Mn. For comparison, the results for ideal Fe/Cr/Fe trilayers are included. The fully relativistic spin-polarized screened Korringa–Kohn–Rostoker (SKKR) method (Szunyogh *et al.*, 1995; Weinberger and Szunyogh, 2000) and the inhomogeneous coherent potential approximation (Weinberger *et al.*, 1996) have been employed in order to obtain the electronic and magnetic properties of the systems described in Table I. The present calculations have been performed within the atomic sphere approximation (ASA) and the local density approximation (LDA) for the exchange correlation functional.

The electric conductivity has been obtained using the Kubo–Greenwood equation (Kubo, 1957; Greenwood, 1958; Weinberger *et al.*, 1996). Suppose the system grows in the z-direction (Fig. 1), then the in-plane components of the electric field are assumed to be constant. Unfortunately, the calculation of the conductivity in CPP geometry is not as straightforward as in the CIP case, because the electric field perpendicular to the layers, $E(z)$, is not constant in space. However, it has been shown that these problems can be overcome by assuming steady-state conditions (Levy, 1994). This means that the electronic density is time-independent which implies that the continuity equation is only fulfilled for a constant current. In this case the electric field can be described by the generalization of Ohm's law

$$E(z) = j \int dz' \rho_{\perp}(z, z'), \tag{1}$$

TABLE I Description of the spacer structures used in the present article

Type	*The spacer and the interfaces*
Ideal interfaces	$Fe/Cr_s/Fe$
CrMn alloy	$Fe/(Cr_{1-x}Mn_x)_s/Fe$
Mn overlayer	$Fe/Cr_s/Mn_1/Fe$

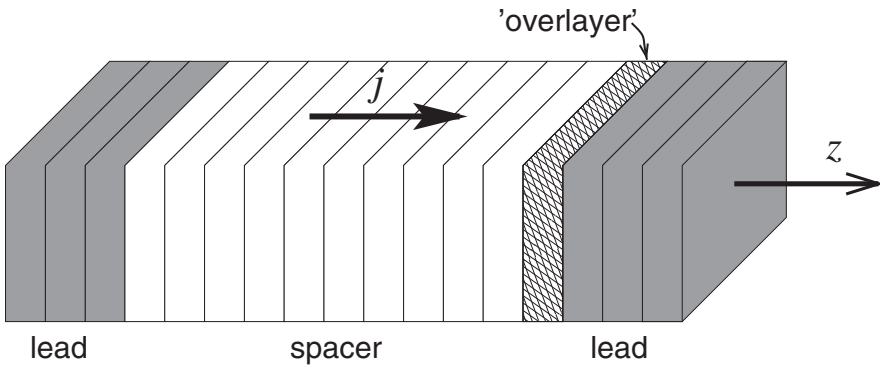

FIGURE 1 Schematic drawing of a trilayer consisting of two semi-infinite leads (bulk Fe), a particular number of spacer layers, and optionally an 'overlayer' of Mn on top of the Cr spacer. Here, it is assumed that the system grows in the z-direction. In the case of CPP transport the current is parallel aligned to the z-axis.

with z and z' being continuous variables and $\rho_\perp$ being the inverse of the conductivity matrix. The measured quantities can be derived by using the average of Eq. (1) divided by the size of the system L

$$\langle E \rangle = j \frac{1}{L} \int dz\, dz' \rho_\perp(z, z') = j\, \rho_{\mathrm{CPP}}, \tag{2}$$

whereby ρ_{CPP} corresponds to the measured resistivity.

The Kubo–Greenwood equation (Weinberger *et al.*, 1996) yields directly the conductivity, therefore the following integral equation has to be solved to obtain the resistivity ρ_{CPP} (Eq. (2)) of the system,

$$\int dz'' \sigma_\perp(z, z'') \rho_\perp(z'', z') = \delta(z - z'). \tag{3}$$

For practical purposes sheet resistances are used, which are defined as the resistivity multiplied by the length of the system

$$r = L\rho_{\mathrm{CPP}} = \int dz\, dz' \rho_\perp(z, z'). \tag{4}$$

Under certain conditions the continuous variables can be mapped onto a system of discrete variables, i.e., planes of atoms. The sheet resistance of n layers can then be rewritten as

$$r(n) = \sum_{p,q=1}^{n} \rho_{pq}(n), \tag{5}$$

where $\rho_{pq}(n)$ stands for the layer-dependent, nonlocal resistivities. For details see also Herper (2003).

For a detailed investigation of the resistance in a layered system it can be useful to define a layer-resolved sheet resistance,

$$r_p(\mathcal{C}, n) = \sum_{q=1}^{n} \rho_{pq}(\mathcal{C}, n). \tag{6}$$

The quantity of particular interest is the GMR, i.e., the difference of the resistances due to an applied magnetic field. Therefore, $r(n)$ has to be calculated for an AF and FM alignment of the magnetic moments in the two leads, which in turn correspond to the case of zero field and applied field, respectively. By using Eq. (5) the GMR can be defined by

$$R(n) = \frac{r\,(\mathrm{AF}, n) - r\,(\mathrm{FM}, n)}{r\,(\mathrm{AF}, n)}. \tag{7}$$

Because of the fact that $r\,(\mathrm{AF}, n) > r\,(\mathrm{FM}, n)$ this definition yields $R(n) \leq 1$.

Finally, it should be mentioned that the Kubo–Greenwood equation is always evaluated for a complex Fermi energy $\epsilon_{\mathrm{F}} + i\delta$, due to the use of the surface Green's function techniques in the calculations. Throughout this article the imaginary part δ amounts to 2 mRy. Previous investigations (Herper *et al.*, 2003b; Weinberger *et al.*, 2001) have shown that the sheet resistance varies linearly with δ provided the number of buffer lead layers is large enough. The GMR for finite imaginary parts of the Fermi energies can then be viewed as a lower limit of the actual GMR.

3. MAGNETIC CONFIGURATIONS

The resistances of Fe/Cr multi- or trilayers are strongly related to the interlayer exchange coupling and, therefore, to the magnetic configuration of the spacer. It has been suggested that even a small amount of Mn impurities can transform the SDW of Cr into a commensurate AF structure (Fawcett *et al.*, 1994). In Fig. 2 the magnetic moments for the three different spacer structures (Table I) are displayed for 11 and 12 spacer layers, respectively. The magnetic moments of the Fe atoms have the same size as in the bulk system, only at the interfaces they are slightly changed. In the case of ideal interfaces, the Cr moments couple AF from layer to layer. Replacing 5% of the Cr atoms by Mn, the magnetic moments of the Cr layers seem not to be influenced (Fig. 2, middle) and the magnetic moments of the Mn atoms match with the magnetic moments of the Cr atoms except for the coupling to the Fe lead layers. In contrast to Cr, Mn couples FM to Fe. This agrees with results for bulk Mn, which show that Mn in

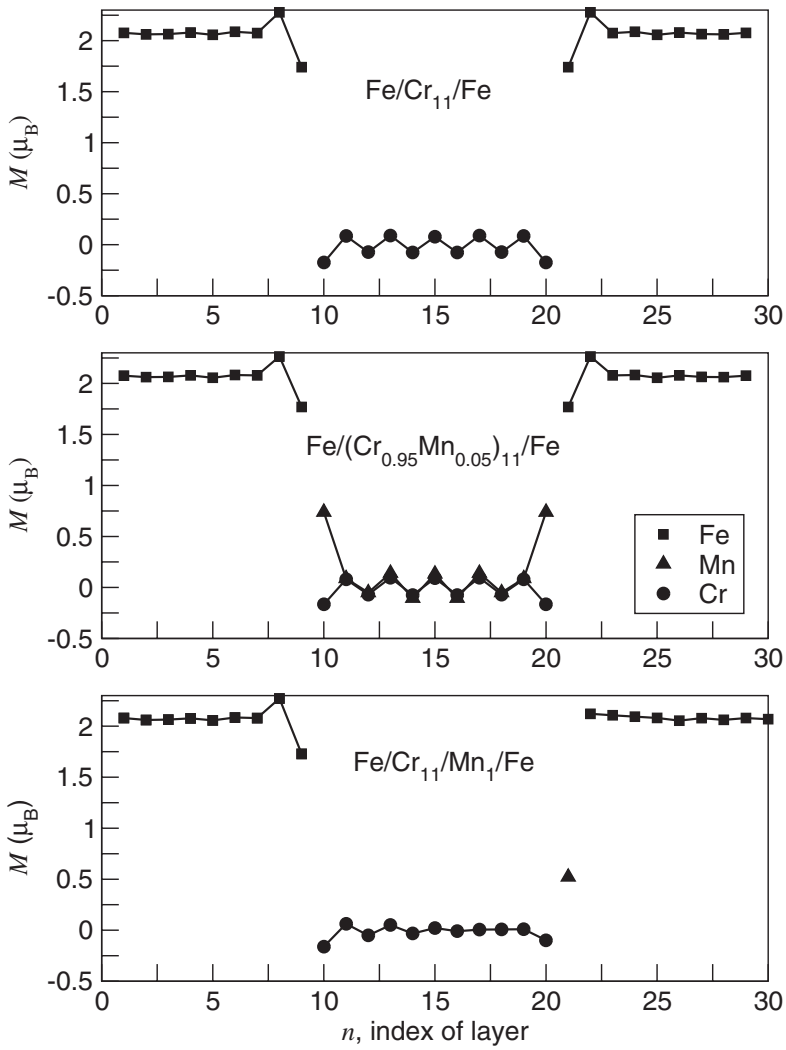

FIGURE 2 Layer- and component-dependent magnetic moments of Fe/Cr/Fe trilayers for different spacer structures. The magnetic moments of the Fe atoms are marked by squares, triangles denote the Mn and open circles the Cr magnetic moments.

its bcc phase prefers FM for small volumes (Herper, 2000). The situation becomes different if an Mn layer is used on top of the Cr spacer as then the oscillations in the magnetic moments are damped on the Mn side (Fig. 2). Because of the long wavelength of the SDW, systems with very thick spacers, i.e., ≈ 39 spacer layers, have to be taken, in order to examine the influence of the SDW. Systems without impurities show the typical amplitude modulation of the magnetic moment (Fig. 3), which has already been reported by Vernes *et al*. Two nodes, i.e., phase slips, occur due to the SDW of Cr. The distance between the two nodes is about 17 ML, which is slightly smaller than the experimentally observed distance between two phase slips of 20 ML (Unguris *et al*., 1991). If Mn is added in or on the spacer the SDW is obviously strongly damped or even destroyed, see Fig. 4. From the left panel in Fig. 4 it can nicely be seen

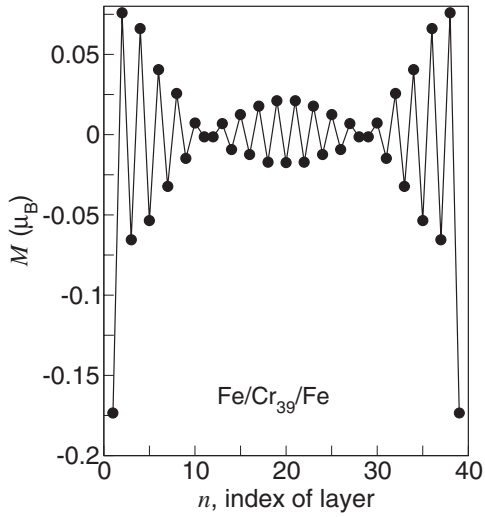

FIGURE 3 Magnetic moments M of the Cr layers in an $Fe/Cr_{39}/Fe$ trilayer.

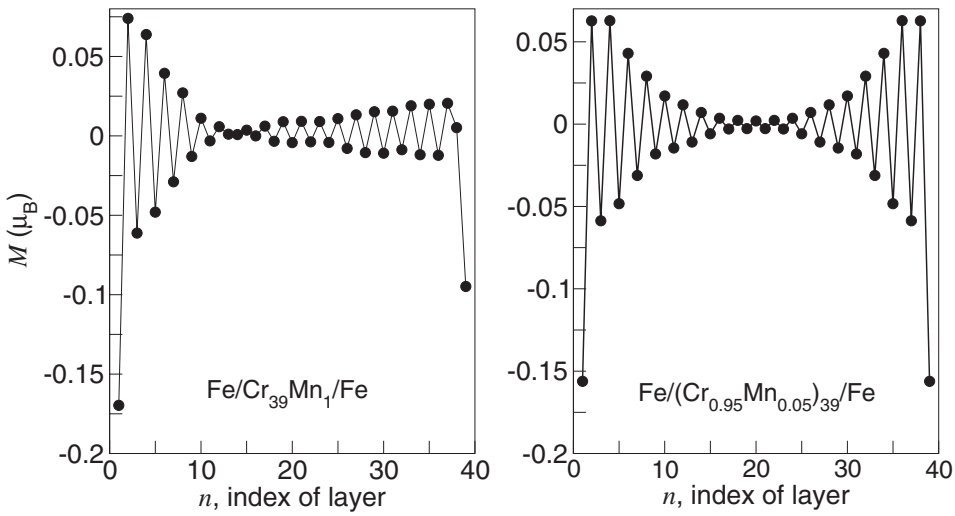

FIGURE 4 Magnetic moments M of the Cr layers in an $Fe/Cr_{39}/Mn_1/Fe$ (left panel) and in an $Fe/(Cr_{0.95}Mn_{0.05})_{39}/Fe$ (right panel) system.

that the phase slip vanishes on that side where Mn has been placed, whereas the node on the other side still exists. The SDW, however, completely vanishes if the Mn atoms are distributed randomly within the spacer (Fig. 4). Due to the homogeneous distribution of the Mn atoms the magnetic configuration is transformed into a commensurate AF structure, whereby the amplitude of the induced moments decreases with the distance from the leads. It should be mentioned that the relatively small moments of the Cr atoms arise from the fact that the LDA bcc Fe lattice constant is used in here, which is smaller than the Cr bulk lattice constant. In agreement with the experimental results it has been shown that only 5% of Mn is sufficient to destroy the SDW.

4. GIANT MAGNETORESISTANCE

The above discussion has shown that the magnetic configuration is significantly changed by Mn impurities. In order to gain information about which parts of the system contribute mostly to the GMR it is useful to consider normalized differences of the layer-resolved sheet resistances for AF and FM alignments of the leads,

$$\Delta r_p(n) = r_p(\mathrm{AF}) - r_p(\mathrm{FM}). \tag{8}$$

These differences have been calculated by using Eq. (6). The results for the particular cases of 20 and 21 spacer layers are displayed in Fig. 5. The systems are partitioned into five characteristic parts: left/right lead, left/right interface, and the spacer, see Fig. 5. In here, the interface region has been defined to consist of three lead layers and three layers of the spacer plus the Mn layer if applying. The distributions looks quite similar for all three cases (Fig. 5). The main contributions stem from the interface regions and the spacer itself. However, in contrast to former investigations for Fe/Si/Fe trilayers (Herper *et al.*, 2002) the sheet resistance difference Δr_p does not completely vanish for the leads. It should be noted that this contribution from the leads has to be correlated with the fact that the partitioning in these five regions is arbitrary. The contributions from the spacer are quite large and always negative. This can be understood from the fact that Cr favors AF magnetic configurations. Therefore, the sheet resistances of the Cr or Cr-dominated layers are increased due to FM coupling of the leads. This effect is heavily damped, if the Cr spacer is covered by a monolayer of Mn, see Fig. 5. In this case the main contribution of the GMR stems from the interfaces.

As can be guessed from the above discussion of Δr_p, the behavior of the GMR is similar in all three cases. Making use of Eq. (7) the GMR has been investigated for different spacer thicknesses (Fig. 6). The GMR decreases with the growing number of spacer layers, whereby the GMR ratios for Fe/Cr/Fe trilayers and for

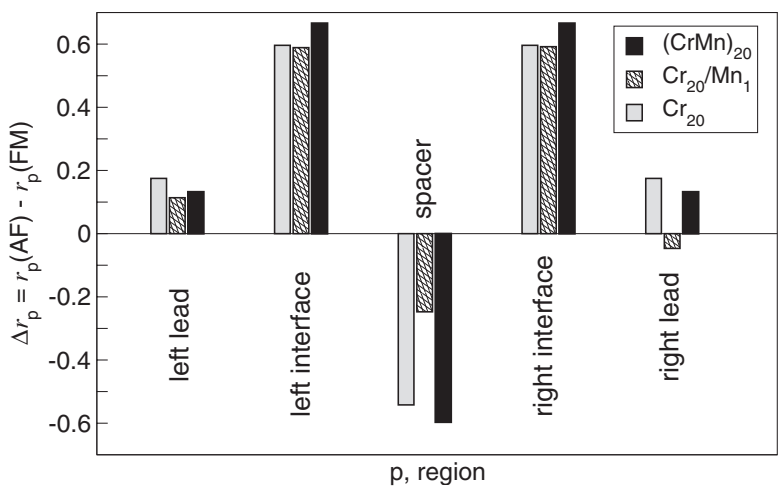

FIGURE 5 Differences of the sheet resistances Δr_p for the five characteristic regions of the trilayers (see text) for different types of pacers.

systems with Mn impurities are of the same size. This means that the GMR effect is hardly influenced by Mn 'overlayers' or by alloy formation in the spacer. However, the Mn impurities affect the oscillating behavior of the GMR. In a previous paper (Herper *et al.*, 2003b) it has already been shown for the ideal system that the oscillations of GMR can directly be related to the oscillations in the interlayer exchange coupling (IEC) (Herper *et al.*, 2003b). Experimentally for systems with more than 9 ML of Cr a short 2 ML period occurs in the IEC (Heinrich *et al.*, 1999). It has been shown in various calculations that this period can also be obtained from *ab initio* calculations (Mirbt *et al.*, 1996; Vernes *et al.*, 2002). Similar oscillations can be observed in the GMR, whereby the local maxima corresponds to the AF IEC and minima to FM coupling (Herper *et al.*, 2003c). Between 15 and 17 ML of Cr a phase slip occurs (Fig. 6), which is caused by the SDW of Cr. The 2 ML period and the local extrema become more distinct if a monolayer Mn is placed on top of the Cr spacer, see Fig. 6. Here, the maxima occur for even numbers of spacer layers (odd numbers of Cr layers).

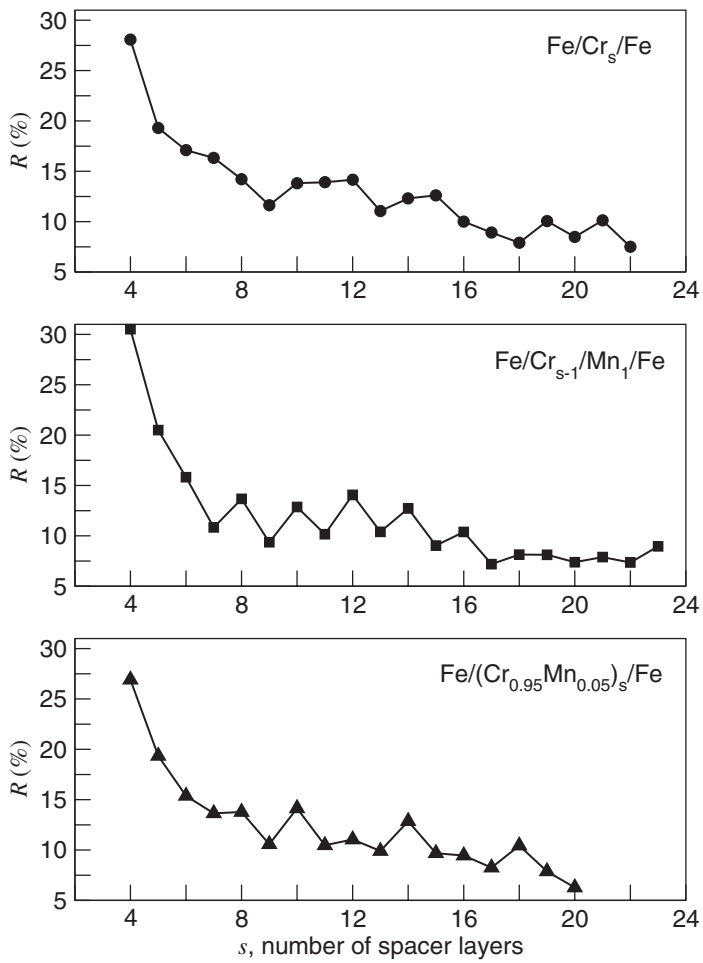

FIGURE 6 GMR ratio *R versus* the number of spacer layers *s* for different spacer structures: ideal Fe/Cr/Fe trilayers (top), systems with an Mn overlayer (middle), and trilayers with spacers consisting of disordered CrMn alloys (bottom).

This corresponds to the experimental results by Heinrich *et al*. (1999) for the IEC of an $Fe/Cr_{11}/Mn_1/Fe$ system. Between 18 and 19 spacer layers (17 and 18 ML of Cr) an indication of a phase slip can be observed and for thicker Cr layers the sequence of local maxima and minima is reversed. This phase slip completely vanishes if Mn atoms are distributed randomly in the spacer, i.e., if a $Cr_{0.95}Mn_{0.05}$ alloy is used. The local extrema due to the short period are now less pronounced. This may be correlated with the fact that the 2 ML period is overlaid by a second longer period, which is related to the disorder of the alloy, see Herper *et al*. (2003c). In general, the changes in the magnetic coupling due to the Mn impurities are also present in the GMR, although they apply only to the oscillations of the GMR, not to its size.

5. CONCLUDING REMARKS

The influence of Mn impurities on the magnetic configuration of the Cr spacer has been investigated using *ab initio* SKKR calculations. The present results confirm the experimental suggestions that Mn impurities transform the SDW of Cr in a commensurate AF structure, whereby the transformation is nearly perfect in the case of a CrMn spacer with 5% of Mn. Systems with Mn overlayers still show a typical amplitude modulation and the nodes induced by the SDW as in Fe/Cr/Fe (at least in a sufficient distance from the Cr–Mn interface). In agreement with the experimental results it is observed that the size of the GMR is not much affected by Mn impurities provided that the amount is sufficiently small. A distinct relationship between the oscillation periods and the structure of the spacer has been found. The 2 ML period can be observed just as well as the phase slips. The Kubo–Greenwood approach also allows a layer-resolved analysis of the sheet resistances, by which the assumption that the interfaces are mostly responsible for the GMR can be confirmed. In contrast to semiconducting spacers there are also reasonably large contributions from the spacer.

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