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Ab initio study of CPP transport in Fe/Cr/Fe trilayers: influence of transition metal impurities

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ABSTRACT

The transport properties of Fe(001)/Cr/Fe(001) trilayers are discussed with respect to the influence of transition metal impurities in form of layers. We are able to show that the periodicity of the giant magnetoresistance is directly influenced by the interlayer exchange coupling (IEC). Furthermore, it is observed that the behavior of the IEC strongly depends on whether an impurity overlayer of Mn or V is used. It turns out that the size of the GMR is only little effected by $3d$-transition metal impurities, which is in agreement with the experimental findings. The electronic and magnetic properties of the trilayers have been investigated within the fully relativistic, spin-polarized SKKR method and the LDA. The transport properties of the Fe/Cr/Fe systems have been derived from the fully relativistic spin-polarized Kubo-Greenwood equation.

INTRODUCTION

The discovery of the giant magnetoresistance (GMR) in Fe/Cr multilayers by Baibich *et al.* [1] and the observation of the oscillating interlayer exchange coupling (IEC) two years earlier by Grünberg and coworkers [2] was the starting point of many intense studies of the electronic transport in these systems [3–6]. Recently, some effort has been devoted to examine the IEC in Fe/Cr/Fe trilayers with Mn impurities in the Cr spacer [7]. This is interesting, because it is assumed that the third transition metal transforms the spin density wave of Cr into a commensurate AF state, which in turn should change size and/or phase of the IEC. However, the experiments of Heinrich *et al.* have only been carried out for transition metal overlayers. Due to the strong tendency of Mn to segregate to the surface it was impossible to examine diluted CrMn alloys. Furthermore, it has turned out that the GMR of Fe/Cr multilayers is not much affected by a thin overlayer [8].

Here, we have investigated the GMR in current perpendicular to the plane (CPP) geometry and the IEC of Fe/Cr/T_1/Fe trilayers in terms of *ab initio* methods, whereby T_1 stands for a single monolayer of Mn or V. The influence of the overlayer has been studied for varying thickness of the Cr layer. This goes beyond the experimental studies, which were only carried out for a Mn overlayer (one and two ML) and a fixed number of Cr layers [7]. In contrast to experiment we have been able to examine the case of homogeneously distributed impurity atoms in the Cr spacer,

see Ref. [9]. However, here we present results for perfect Mn or V monolayers on top of the Cr spacer.

CALCULATIONAL DETAILS

We have used systems consisting of two semi-infinite Fe leads, which cover the actual spacer plus a particular number of lead layers acting as a buffer. The selfconsistently calculated part is then of the form

$$\mathrm{Fe}_m/\mathrm{Cr}_n/\mathrm{T}_1/\mathrm{Fe}_m, \quad 9 \leq m \leq 11, \quad 2 \leq n \leq 42, \quad \mathrm{T} \in \{\mathrm{Mn}, \mathrm{V}\}.$$

The number of buffer layers varies, because of the special form of the two-dimensional structure constants [10]. All calculations have been performed on a bcc lattice with layer distance of 5.27 a.u. being the LDA value of bcc Fe. Relaxation effects have not been taken into account.

The electronic and magnetic properties of the above mentioned trilayers have been calculated within the fully relativistic spin-polarized version of the screened Korringa-Kohn-Rostoker (SKKR) method for layered systems developed by Szunyogh *et al.* [10, 11]. The calculations have been performed within the atomic sphere approximation (ASA) and the local density approximation (LDA). We have used two different magnetic configurations: parallel alignment of the magnetic moments of the two leads (FM) and antiparallel alignment (AF). In terms of total energies the interlayer exchange coupling can be defined by

$$\Delta E = E(\mathrm{AF}) - E(\mathrm{FM}). \tag{1}$$

In here, only the FM state has been calculated selfconsistently and the IEC has been investigated by using the magnetic force theorem [10]. The IEC is then given by the band energy difference of the two magnetic configurations

$$\Delta E_b = \int_{\epsilon_b}^{\epsilon_\mathrm{F}} \left[n_p(\epsilon, \mathrm{AF}) \, - \, n_p(\epsilon, \mathrm{FM}) \right] (\epsilon \, - \, \epsilon_\mathrm{F}) \, d\epsilon, \tag{2}$$

where n_p is the layer-resolved density of states for a given magnetic configuration.

The electric transport properties have been obtained from the fully relativistic spin-polarized Kubo-Greenwood equation [13], which is sufficient to describe the influence of the interface structure. Within this method the CPP GMR the resistance of the multilayers have been calculated depending on the magnetic configuration, spacer type, and thickness. For a given sandwich with thickness of the spacer l can be written as

$$r(\mathcal{C}, l, \delta) \, = \, \sum_{p,q}^{l} \rho_{pq}(\mathcal{C}, l, \delta), \quad l \, = \, n \, + \, 2m \, + \, 1. \tag{3}$$

Here, ρ_{pq} is the resistivity at layer p caused by a current at layer q. The imaginary part of the complex Fermi energy δ is chosen to be $2\,\mathrm{mRy}$, for details see Ref. [14]. It has been shown

elsewhere that the sheet resistance varies linearly with δ [14]. Therefore, the GMR for finite δ is rigidly shifted to lower values. Throughout this paper we have used the bounded definition of the GMR

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

where we have assumed that the resistance for the AF configuration corresponds to the zero field resistance.

RESULTS

First we have investigated the Fe/Cr/Fe multilayers without impurity layers. The results are plotted in Fig. 1. It should be mentioned that the IEC of similar systems has already been investigated in previous papers [6, 15]. Here, we mainly focus on the GMR and its relation to the IEC. Only some general features of the IEC will be discussed, for details we refer to Ref. [9]. We have found the typical short two monolayer (ML) oscillation period, which is known from, e.g., electron microscopy and Brillouin light scattering experiments [7, 16]. The longer (12 ML) period could not be directly observed. This oscillation is related to the RKKY interaction of the layers and could only be obtained from a fit procedure with some RKKY type energy terms [15]. However, besides the short period we have observed phase slips every 15 layers, which are caused by the spin density wave of Cr. In contrast to other calculations the phase slips can directly observed, Fig. 1 and have not to be calculated from the oscillation periods [15].

The GMR slowly decreases with growing number of spacer layers from 28 $\%$ at four layers to $\approx$5$\%$ at 42 ML of Cr (Fig. 1, top). The decrease is accompanied by a small oscillation of the GMR with the number of Cr layers. It can be suggested that these oscillations are related to the two ML period of the IEC. In order to verify this, we have plotted the oscillation depending on the number of Cr layers (Fig. 1, bottom). We have checked, whether the GMR(n) $<$ GMR(n+1) or vice versa. In the first case the value of the oscillation for the (n+1)-layer system is set to one, whereas in the second case it is chosen to be zero. A similar procedure has been used for the IEC choosing zero for AF coupling and -1 for FM coupling, respectively. The results are displayed in Fig. 1 (bottom panel). This viewgraph clearly reflects the two ML period of the IEC and the phase slips can clearly be seen. Furthermore, it is obvious that the GMR shows the same short ML period as the IEC, whereby the maxima in the GMR are connected to AF coupling and the minima to FM coupling. The phase slips also occur in the GMR depending on the number of Cr layers, but they are slightly shifted and smeared out. Experimentally only the long periods have been observed in the GMR [4]. The short period can usually not been observed.

How the IEC and GMR change when an impurity overlayer is added to the system is shown in Fig. 2. The short period survives if the Cr spacer is covered with a single monolayer of Mn. In agreement with the experimental findings [7] no phase shift occurs due to the impurity layer, i.e., even numbers of Cr layers are still AF coupled. It should be mentioned that this is only true for systems with $n \leq 15$, because at this point the first phase slip occurs in the original Fe/Cr/Fe trilayer and the two systems are out of phase. This was not found by Heinrich *et al.*, because they focussed only on very thin Cr layers. In addition, no phase slips have been observed in the IEC of

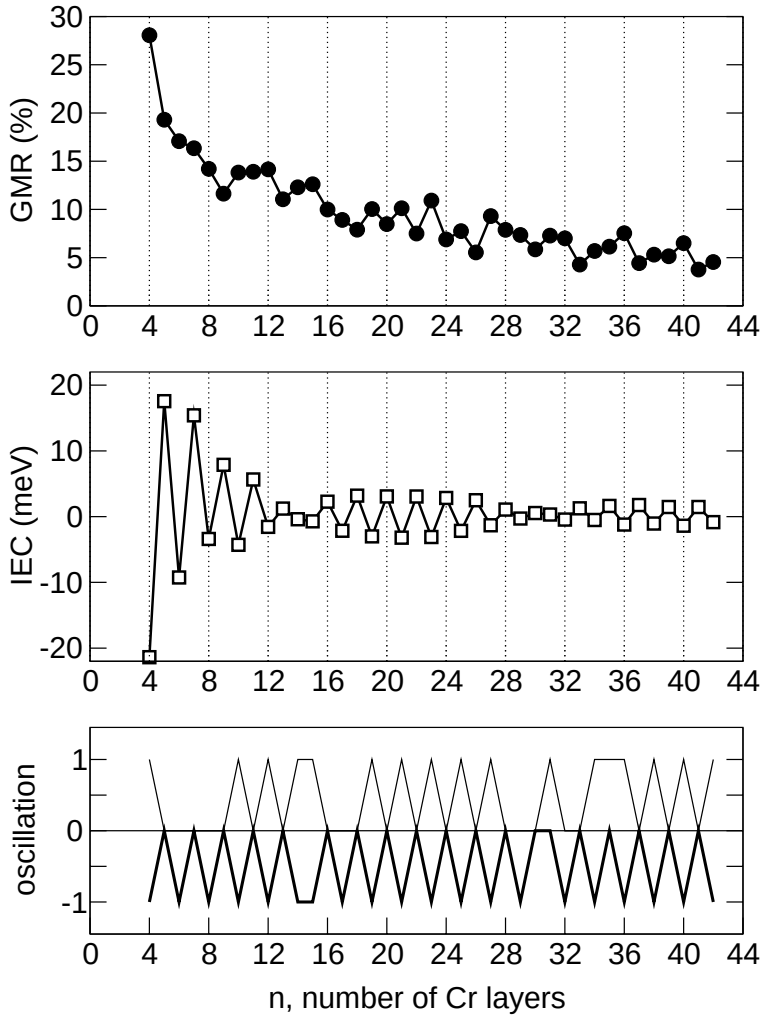

Figure 1. Top panel: The GMR of Fe/Cr/Fe trilayers depending on the thickness of the Cr Layer. Middle panel: The IEC for Fe/Cr/Fe as obtained from the band energy difference vs. the number of Cr layers. Bottom panel: Comparison of the oscillations of the GMR (thin lines) and the IEC (thick lines) of the above shown trilayers, for details see text.

Fe/Cr_n/Mn_1/Fe trilayers. This can be understood from the fact that the Mn monolayer transforms the Cr spin density wave in a commensurate AF state, for a detailed discussion see Ref. [9]. However, the IEC goes to zero at four and 18 ML, which may be still an indication of the spin density wave. In the regions far away from the phase slips of the original system the amplitude of the IEC does not change very much as compared to the Fe/Cr/Fe trilayer, see Figs. 1 and 2. Summarizing, the Mn overlayer leads only to small changes in the IEC. Similar observations have been made for the GMR (Fig. 2, bottom). The GMR of the two systems are comparable in size and phase, whereby the oscillations are more pronounced in the case of the Mn overlayer.

However, if a V overlayer is used instead of Mn the IEC and GMR behave different. In the case of V we have only examined systems with $6 \leq n \leq 12$ layers of Cr. Nevertheless, this results show already some trends. The GMR of the Fe/Cr_n/V_1/Fe systems is of the same size as the GMR of the

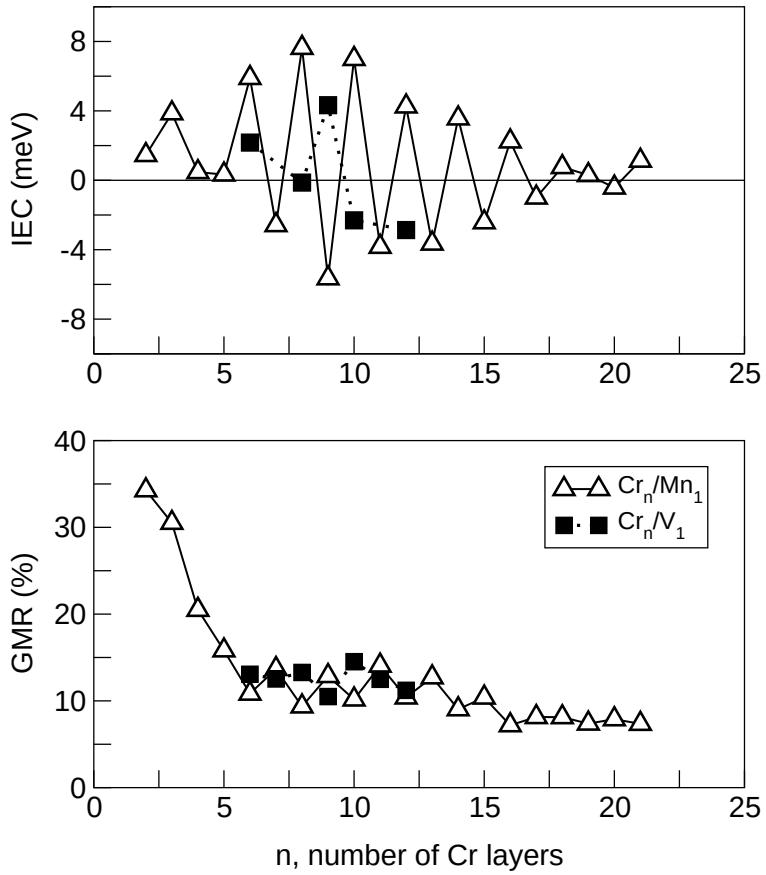

Figure 2. Top panel: The IEC of Fe/Cr$_n$/T$_1$/Fe multilayers vs. the number of Cr layers n. Two different types of impurity overlayers have been used: Mn (open triangles) and V (filled squares). Bottom panel: The GMR vs. the number of Cr layers for the above described systems.

two types of systems discussed above (Fig 2), which has been expected from the experiments of Baumgart, who studied the GMR of Fe(15 Å)/(Cr(12 Å)/T(t))$_{20}$ multilayers [8]. In the case of a V overlayer a similar period of the GMR can be observed as for the two previously discussed systems (Fig. 2, bottom). In contrast to the Mn impurities an overlayer of V leads to a shift in the GMR; now local maxima occur at even numbers of Cr. This suggests that the IEC has changed, which can be confirmed by the results shown in Fig. 2 (top). Though, there are very few data points, it can be suggested that AF coupling is related to even numbers of Cr layers. In addition, the amplitudes of the IEC are smaller as compared to the IEC of the system with Mn impurities. For a more detailed analysis of the influence of V impurities on the GMR and the IEC of Fe/Cr/Fe trilayers more data points have to be taken into account.

SUMMARY AND CONCLUSIONS

In this paper we have presented results for the GMR and IEC of Fe/Cr/Fe trilayers in particular focusing on systems with a Mn or V overlayer on top of the Cr spacer. We have demonstrated that the periods of the GMR are directly related to the oscillations of the IEC. In agreement with the

experimental findings we have observed that a Mn overlayer does not change the phase of the GMR or IEC. It has been shown that the phase slips are vanishing due to the Mn impurities. Furthermore, we have been able to predict that a V overlayer would cause a phase shift and the IEC would be smaller than in the original Fe/Cr/Fe trilayer.

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