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Layer- and component-resolved magnetic moments and anisotropy energies in $(Fe_xCo_{1-x})_n$/Cu(100)

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ABSTRACT

The magnetic moments in the $(Fe_xCo_{1-x})_n$/Cu(100) system are calculated and shown for $2 \leq n \leq 7$ and $x = 0.9$ as resolved with respect to layers and components. While, as reported previously, in the ground state antiferromagnetic interlayer coupling between buried Fe layers occurs, surprisingly, also antiferromagnetic Co–Co and Fe–Co interlayer coupling is found. However, by assuming only ferromagnetic nearest-neighbour Fe–Co and Co–Co interactions on top of the dominating antiferromagnetic Fe–Fe nearest-neighbour interactions, it is revealed that a simple Ising model is consistent with the results of the selfconsistent calculations. When analysing also the layer- and component-like band energy contributions to the magnetic anisotropy energy, remarkably different behaviour for the Fe and Co contributions can be seen.

§1. INTRODUCTION

A recent experimental study by Dittschar *et al.* (1998) of epitaxially grown thin Fe_xCo_{1-x} films on a Cu(100) substrate revealed the presence of a spin-reorientation transition at film thicknesses of two to four monolayers and above Fe concentrations of approximately 75–80%. These results have been supported in a recent paper by the present authors (Zabloudil *et al.* 1998) in which perpendicular magnetization for high Fe concentrations and for more than two monolayers of Fe_xCo_{1-x} has been predicted theoretically. In that study which relied on the force theorem (Weinert *et al.* 1985, Dalderoop *et al.* 1990, Szunyogh *et al.* 1995) the transition from a parallel ($\parallel$) to a perpendicular ($\perp$) orientation of the magnetization was attributed to the presence of antiferromagnetic coupling in the ground state, leading in consequence to an enhanced band-energy contribution, $\Delta E_b = E_b(\parallel) - E_b(\perp)$, to the magnetic anisotropy energy (MAE).

All calculations have been performed by using the (relativistic) spin-polarized, screened KKR method (Szunyogh *et al.* 1994) as combined with the coherent potential approximation (CPA) to treat disorder in layered systems (Weinberger *et al.* 1996). Within this approach the magnetic moments and band energies can conveniently be resolved into layer- ($p = 1, \ldots, n$) and component-like ($\alpha = A, B$) contributions,

$$M = \sum_{p=1}^{n} m_p = \sum_{p=1}^{n} \sum_{\alpha=A,B} c_\alpha m_{p\alpha}, \tag{1}$$

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$$\Delta E_b = \sum_{p=1}^{n} \Delta E_b^p = \sum_{p=1}^{n} \sum_{\alpha=A,B} c_\alpha \Delta E_b^{p\alpha}, \tag{2}$$

respectively. In order to shed somewhat more light to the origin of the reorientation, it is useful to investigate also the $m_{p\alpha}$ and the $\Delta E_b^{p\alpha}$ for various film thicknesses for a typical concentration with an antiferromagnetic ground state.

§2. Results and discussion

2.1. *Magnetic moments*

Figure 1 shows the magnetic moments of the Fe and Co atoms in each layer for film thicknesses of two to seven layers for the magnetic ground state configuration at a Fe concentration of $x = 0.9$. Note that for $n > 2$ and roughly above $x > 0.8$ the ground state also comprises antiferromagnetic interlayer coupling. As confirmed also in terms of 'spin-flip' energies (Szunyogh *et al.* 1998b), for a given film thickness n the ground state configuration of the averaged moments m_p for any concentration

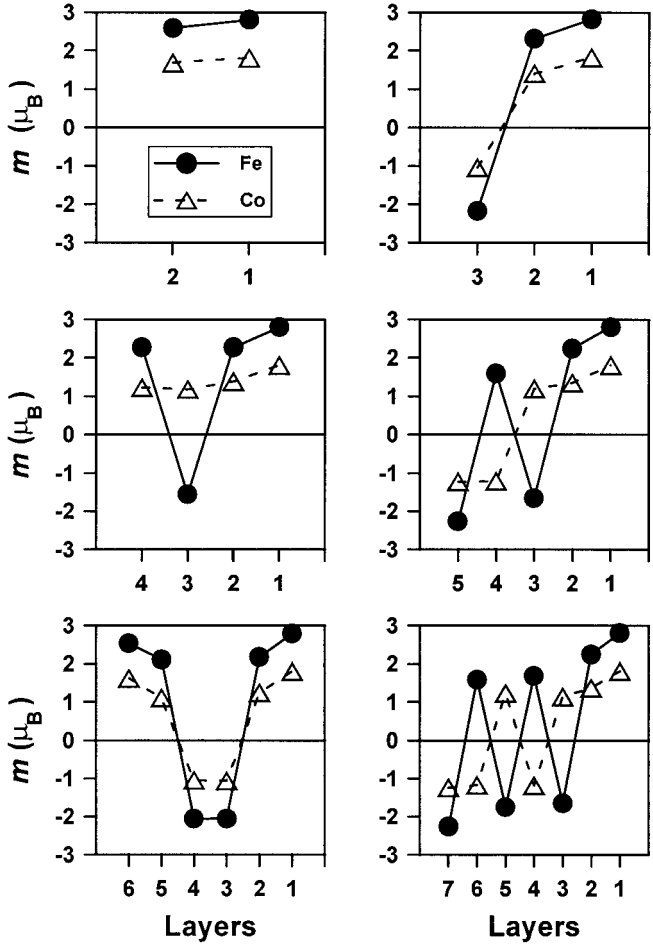

Figure 1. Calculated magnetic moments for $(Fe_{0.9}Co_{0.1})_n$/Cu(100), $n = 2,3,\ldots,7$. The results refer to the corresponding ground states, the numbering of the layers starts at the surface.

$x > 0.8$ was the same as in the pure Fe case (Szunyogh *et al.* 1997). In the Fe-rich regime, it is thus not surprising that this kind of coupling refers basically to the coupling between Fe moments. This is quite obvious if one compares the Fe moments displayed in figure 1 to the corresponding values in table 1 of Szunyogh *et al.* (1997).

In figure 1, the configuration of the Co moments shows only partial correlation with that of the Fe moments: for $n = 2$, 3 and 6 it follows the configuration of the Fe moments, however, for $n = 4$, 5 and 7 it is remarkably different from that. Although one automatically assumes ferromagnetic exchange interactions for nearest-neighbour Co–Co and Fe–Co pairs, interestingly, also antiferromagnetic Co–Co interlayer coupling does occur. In what follows, we employ a simple Ising-like model in order to explain qualitatively these differences.

Restricting ourselves to ferromagnetic ordering within each plane in an unrelaxed fcc(100) layered geometry, a nearest-neighbour Ising Hamiltonian of our compositionally disordered system can be written as

$$H = x^2 H_{\mathrm{FeFe}} + 2x(1-x)H_{\mathrm{FeCo}} + (1-x)^2 H_{\mathrm{CoCo}}, \tag{3}$$

$$H_{AB} = \sum_{p=1}^{n} H_{AB}^{p}, \quad H_{AB}^{p} = -2\left(J_{AB}^{p-1,p}\, S_A^{p-1} + J_{AB}^{p,p}\, S_A^{p} + J_{AB}^{p+1,p}\, S_A^{p+1}\right) S_B^{p}, \tag{4}$$

$$(A, B = \mathrm{Fe\ or\ Co},\ S_A^p = \pm 1,\ J_{AB}^{0,1} = J_{AB}^{n+1,n} = 0).$$

Quite clearly, for x close to 1 the ground state is governed by H_{FeFe}, that is, as stated above, for $n > 2$ the antiferromagnetic configuration of the Fe moments has to be ruled out. On top of this dominating effect, the Co moments have to be oriented (S_{Co}^p) in order to minimize H. In leading order we may consider only H_{FeCo}, stressing thus that in the dilute Co regime the orientation of the Co moments is determined by the orientation of the neighbouring Fe moments. Supposing for brevity $J_{\mathrm{FeCo}}^{p-1,p} = J_{\mathrm{FeCo}}^{p,p} = J_{\mathrm{FeCo}}^{p+1,p} = J_{\mathrm{FeCo}} > 0$ for all p, tables 1 and 2 list the values of S_{Co}^p which minimize H_{FeCo}^p for different orientations of the Fe moments.

Obviously, for $p = 1$ a similar table as for $p = n$ applies. As one can easily check, the above tables explain the orientations of all the Co moments in figure 1, except the ones closest to the substrate in the case when the two Fe layers closest to the substrate couple antiferromagnetically, i.e. for film thicknesses $n = 3$, 4, 5 and 7. As can be read off from figure 1, in these cases $S_{\mathrm{Co}}^n = S_{\mathrm{Fe}}^n$, while our simple model does not distinguish energetically between $S_{\mathrm{Co}}^n = +1$ or -1. However, first-principles calculations of the exchange coupling constants (Szunyogh and Udvardi 1998) show that

Table 1.

S_{Fe}^{p-1}	S_{Fe}^{p}	S_{Fe}^{p+1}	S_{Co}^{p}	H_{FeCo}^{p}
+1	+1	+1	+1	$-6J_{\mathrm{FeCo}}$
−1	+1	+1	+1	$-2J_{\mathrm{FeCo}}$
+1	−1	+1	+1	$-2J_{\mathrm{FeCo}}$
+1	+1	−1	+1	$-2J_{\mathrm{FeCo}}$
−1	−1	+1	−1	$-2J_{\mathrm{FeCo}}$
−1	+1	−1	−1	$-2J_{\mathrm{FeCo}}$
+1	−1	−1	−1	$-2J_{\mathrm{FeCo}}$
−1	−1	−1	−1	$-6J_{\mathrm{FeCo}}$

Table 2.

S_{Fe}^{n-1}	S_{Fe}^{n}	S_{Co}^{n}	H_{FeCo}^{n}
+1	+1	+1	$-4J_{FeCo}$
-1	+1	±1	0
+1	-1	±1	0
-1	-1	-1	$-4J_{FeCo}$

the $J^{p,p}$ at surface or interface layers are significantly larger in magnitude than those for buried layers. This in turn clarifies the above anomaly between the orientations of the calculated moments and those obtained from the above qualitative model.

Increasing the concentration of Co, i.e. decreasing x, the third term in equation (3), which comprises the strong ferromagnetic Co–Co exchange coupling, becomes more and more important. Calculations for the J's in the Co_n/Cu(100) and Fe_n/Cu(100) systems (Szunyogh and Udvardi 1998) reveal that J_{CoCo} is in general 5–10 times larger in magnitude than J_{FeFe}. A rough estimate based on equation (3) thus indicates that for about $x < 0.7$ the term H_{CoCo} indeed plays a dominant role, which is in excellent agreement with the results of the self-consistent total energy calculations by Zabloudil *et al.* (1998), as in this concentration range a ferromagnetic ground state was found.

2.2. *Magnetic anisotropy energies*

In figure 2 the ΔE_b as resolved with respect to layers and components are shown for two to seven monolayers of $Fe_{0.9}Co_{0.1}$. It should be noted that from the Cu layers included as 'buffer' in the calculations only the one at the substrate-overlayer interface yields a non-negligible contribution to ΔE_b. In comparing the contributions related to the Fe layers to the corresponding entries in figure 4 of Szunyogh *et al.* (1997), an overall similarity can be found. Since there these contributions were discussed in quite some detail, we now can focus mainly on the differences of the ΔE_b between Co and Fe layers.

As is well known and understood, a Co monolayer on Cu(100) substrate exhibits an in-plane magnetization with a $\Delta E_b \simeq -0.38$ meV (Wang *et al.* 1994, Szunyogh *et al.* 1998a, b). Although smaller in magnitude, the negative ΔE_b of the Co layer at the surface for $2 \leq n \leq 7$ can be related to this fact. Except in the case of $n = 6$, the contribution of Co to the MAE is nearly zero for buried layers. Most likely, due to hybridization effects with Cu, Co in the layer at the interface to the substrate tends to have a positive ΔE_b (see the cases $n = 4, 5$ and 7 in figure 2). Therefore, the total contribution of Co to the MAE becomes in general very small. As can be seen in figure 1, and as was pointed out already by Szunyogh *et al.* (1997), the magnetic configuration for $n = 6$ is very special, showing up also in a very different distribution of the ΔE_b of Co as for other film thicknesses. In conclusion, however, we can state that the reorientation from a perpendicular to an in-plane magnetization with increasing Co content does not arise from an increasing (negative) contribution of Co to the MAE, but from an abrupt decrease of the ΔE_b of Fe due to the subsequent antiferromagnetic–ferromagnetic transition (Szunyogh *et al.* 1997, Zabloudil *et al.* 1998).

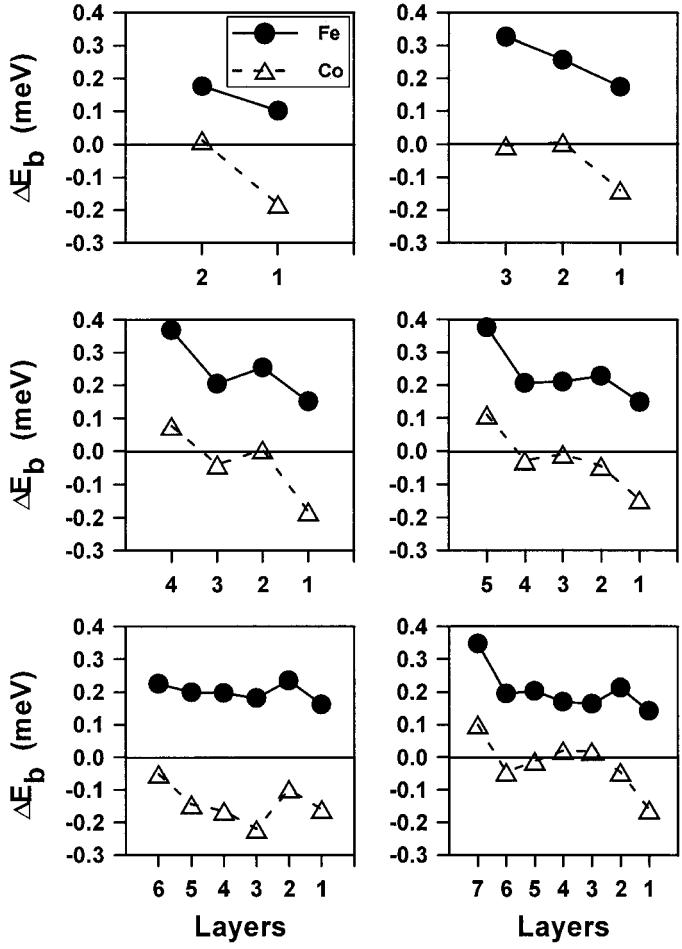

Figure 2. Layer– and component–resolved band energy contributions to the magnetic anisotropy energy in $(Fe_{0.9}Co_{0.1})_n/Cu(100)$, $n = 2,3,\ldots,7$. The numbering of the layers starts at the surface.

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