Concentration dependent spin-flip energies for alloyed surface magnets

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Abstract
Single and double spin-flip energies are calculated for n layers of
homogeneously disordered Fe_cCo_{1-c} on Cu(100) with n varying between three
and six. It is found that these spin-flip energies describe quite accurately the type
of most favourable magnetic coupling between the magnetic layers and also give a
rather detailed picture for the occurrence of certain magnetic configurations. A
phase diagram of ferromagnetic versus antiferromagnetic coupling with respect to
the number of layers and Fe concentration turns out to be closely related to the
phase diagram of the reorientation transition in this system.

§1. Introduction

Suppose that in a magnetic multilayer system of N layers the magnetic reference
configuration C_0 is given by a system of ferromagnetically coupled layers of ferro-
magnetically ordered planes of atoms,

$$\mathbf{c}_0 = \{\mathbf{n}_1, \mathbf{n}_2, \ldots, \mathbf{n}_N\} = \{\mathbf{n}_i | \mathbf{n}_i = \mathbf{n}_0; i = 1, N\}, \tag{1}$$

where $\mathbf{n}_i$ is the orientation of the magnetization in layer i and $\mathbf{n}_0$ is a given direction
such as, for example, in-plane or perpendicular-to-plane. Suppose further that the
(total) energy of this reference configuration is denoted by $E(\mathbf{c}_0)$. By 'flipping' the
orientation of the magnetization in one particular layer, say i, i.e. by considering the
following configuration,

$$\mathbf{c}_i = \{\mathbf{n}_k | \mathbf{n}_k = \mathbf{n}_0; \quad \forall k \neq i; \quad \mathbf{n}_i = -\mathbf{n}_0\}, \tag{2}$$

and the corresponding (total) energy $E(\mathbf{c}_i)$, the single spin-flip energy H_{ii} for layer i is
then defined by

$$H_{ii} = E(\mathbf{c}_i) - E(\mathbf{c}_0). \tag{3}$$

In a similar manner double spin-flip energies H_{ij} can be defined by the energy
difference

$$H_{ij} = E(\mathbf{c}_{ij}) - E(\mathbf{c}_0), \tag{4}$$
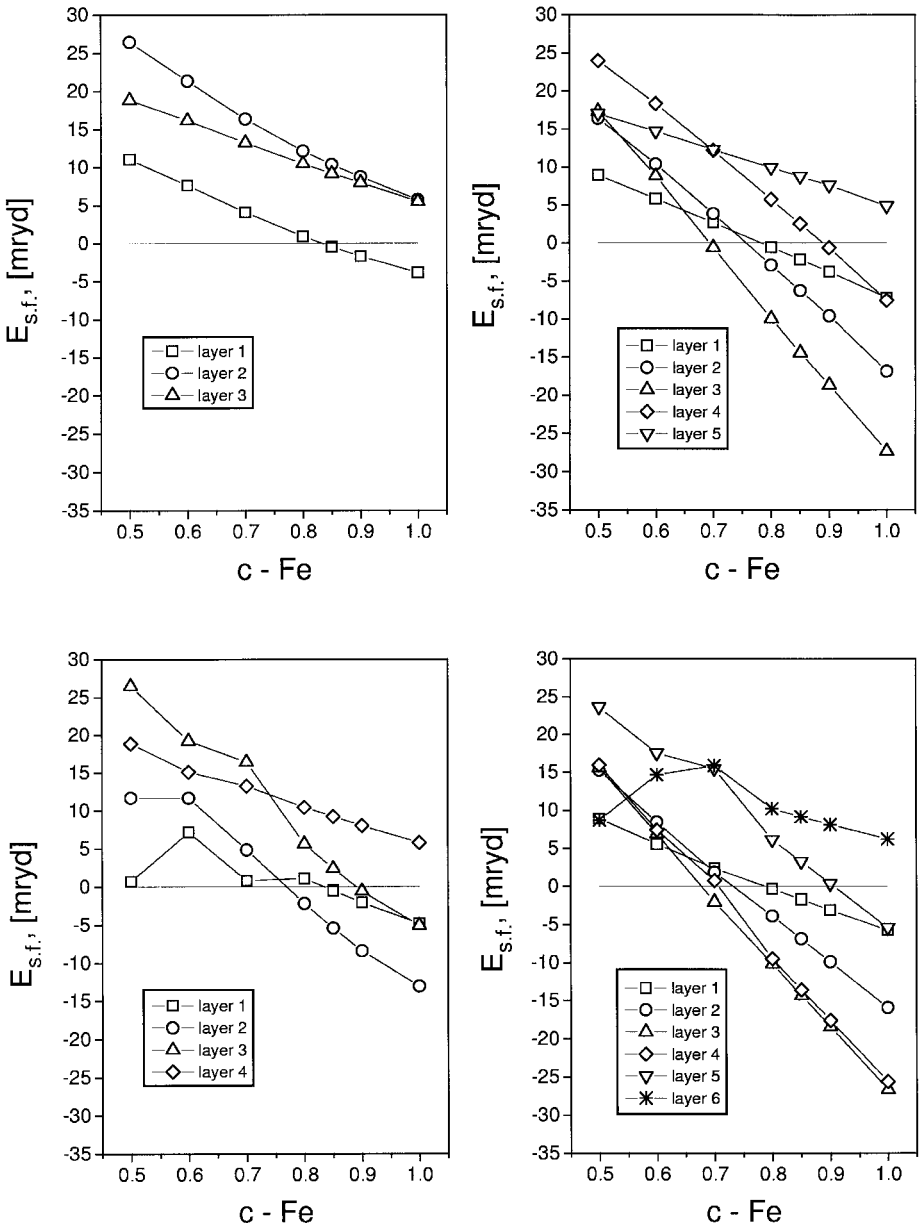
Figure 1. Concentration-dependent single spin-flip energies in $Cu(100)/(Fe_cCo_{1-c})_n$. The numbering of layers starts at the substrate side.

where the (total) energy $E(\mathbf{c}_{ij})$ corresponds to a magnetic configuration in which simultanously in two (different) layers the orientation of the magnetization is 'flipped',

$$\mathbf{c}_{ij} = \left\{ \mathbf{n}_k \mid \mathbf{n}_k = \mathbf{n}_0; \quad \forall k \neq i,j; \quad \mathbf{n}_i = \mathbf{n}_j = -\mathbf{n}_0 \right\}. \tag{5}$$

It should be noted that—speaking in general terms—single and double spin-flip energies are nothing but anisotropy energies less the magnetic dipole–dipole contri-

bution as they refer to (total) energy differences between two magnetic configurations. Quite clearly they can be viewed as single and double interface exchange energies.

The double spin-flip energies can also be written as

$$H_{ij} = H_{ii} + H_{jj} + V_{ij}, \tag{6}$$

with V_{ij} being a kind of vertex correction that decays rapidly with the distance between layers i and j. The single and double spin-flip energies form a symmetric matrix of order N, $\mathcal{H} = \{H_{ij}\}$, from which the (total) energy part of the anisotropy energy $\Delta E(\mathbf{c})$ for any magnetic configuration $\mathbf{c}$ with $\leq N/2$ spin-flips can be obtained very easily (Weinberger 1998):

$$\Delta E(\mathbf{c}) = \mathbf{c}^{\dagger} \mathcal{H} \mathbf{c}. \tag{7}$$

By using the so-called Force Theorem, i.e. by expressing the occurring energy differences as differences in the band energy, the above formulation can readily be extended to disordered magnetic multilayer systems provided that use is made of the (in general inhomogeneous) coherent potential approximation (CPA) for semi-infinite systems (Weinberger *et al.* 1996).

§2. RESULTS AND DISCUSSION

All calculations of spin-flip energies are based on the Force Theorem and were performed in terms of the spin-polarized relativistic screened KKR method (see Szunyogh *et al.* (1995, 1996, 1997) and Újfalussy *et al.* (1996)), by using the self-consistent potentials of $(Fe_cCo_{1-c})_n$ on Cu(100) (Zabloudil *et al.* 1998) correspond-
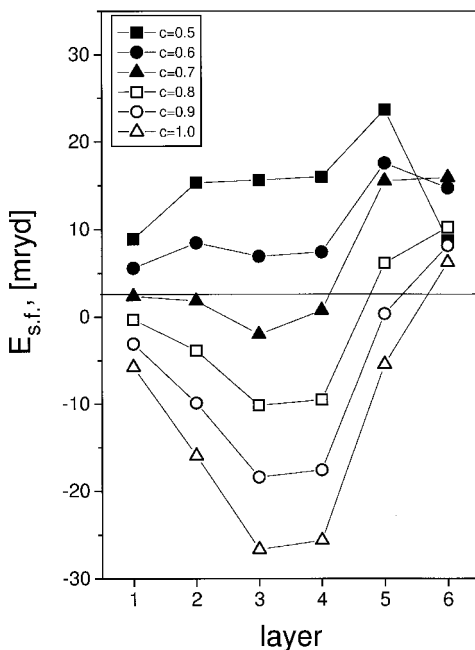

Figure 2.   Layer-dependent single spin-flip energies in Cu(100)/$(Fe_cCo_{1-c})_6$. The numbering of layers starts at the substrate side.

ing to the ferromagnetic configuration with the magnetization pointing along the surface normal.

In figure 1 the concentration-dependent single spin-flip energies for Cu(100)/$(Fe_cCo_{1-c})_n$ are shown for $n \leq 6$. As can be seen from this figure, in all cases the least tendency for the occurrance of a single spin-flip is in the surface layer. One also can see that if a change of sign occurs, this happens in a regime of Fe concentrations between 65 to 80%. Figure 2 illustrates the layer-wise variation of the single spin-flip energies in Cu(100)/$(Fe_cCo_{1-c})_6$ for various concentrations. It is worthwhile to note that the single spin-flip energies for the third and fourth layer are by far the biggest and similar in magnitude. For $c > 0.7$ it is essentially these two single spin-flip energies that determine the energetically most favourable state.

Figures 3 and 4 illustrate the behaviour of double spin-flip energies. For $c_{Fe} \leq 0.7$ the layer-wise display of these quantities in figure 3 shows a clear separa-
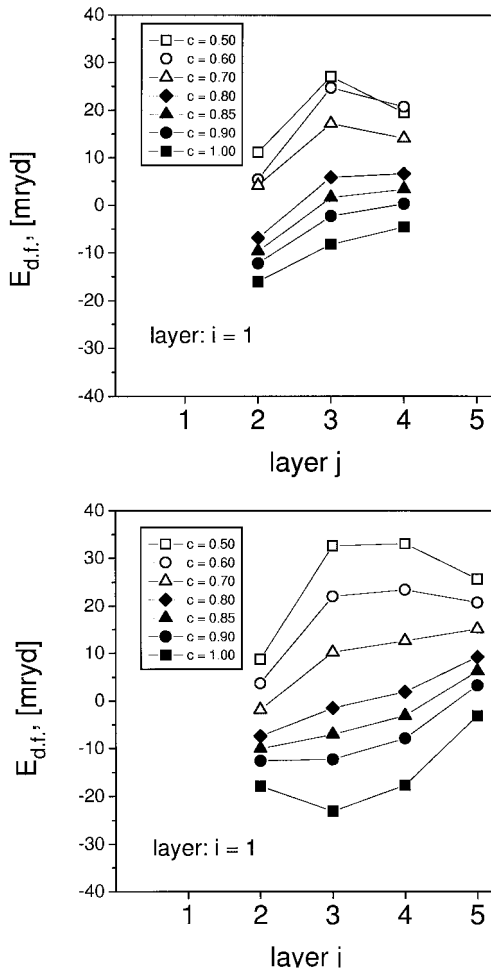

Figure 3.   Layer-dependent double spin-flip energies in Cu(100)/$(Fe_cCo_{1-c})_n$ for $n = 4$ (top) and $n = 5$ (bottom). The first layer is kept constant, the numbering of layers starts at the substrate side.
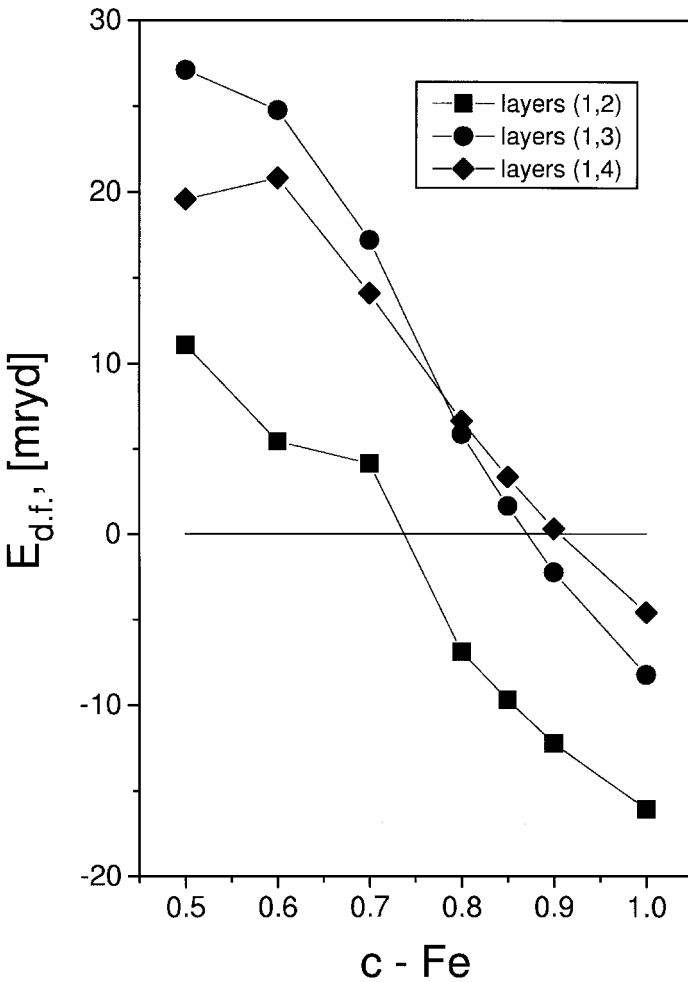
Figure 4. Concentration-dependent double spin-flip energies in $Cu(100)/(Fe_cCo_{1-c})_4$.

tion in shape from those with higher Fe concentrations. Like the single spin-flip energies in figure 1, the concentration-wise representation of double spin-flip energies in $Cu(100)/(Fe_cCo_{1-c})_4$ is characterized by a change of sign around $c_{Fe} \leq 0.7$.

Figure 5 deals with the correction terms defined in equation (6). As one can see for all concentrations investigated these correction terms tend to zero as the distance between two chosen layers increases. For reasonably thick magnetic layers therefore the double spin-flip energies corresponding to distant layers can simply be approximated by the sum of the corresponding single spin-flip energies. Furthermore, since with increasing film thickness the single spin-flip energies in the middle of the film tend to a constant, a very restricted set of spin-flip energies seems to be sufficient to describe the energetics of very thick magnetic films, even if the films show statistical disorder.

In figure 6, for $n = 6$, the energy differences, equation (7), for particular magnetic configurations are shown as a function of the Fe concentration. As one can see, in accordance with figure 2, one and the same most stable arrangement of antiferro-
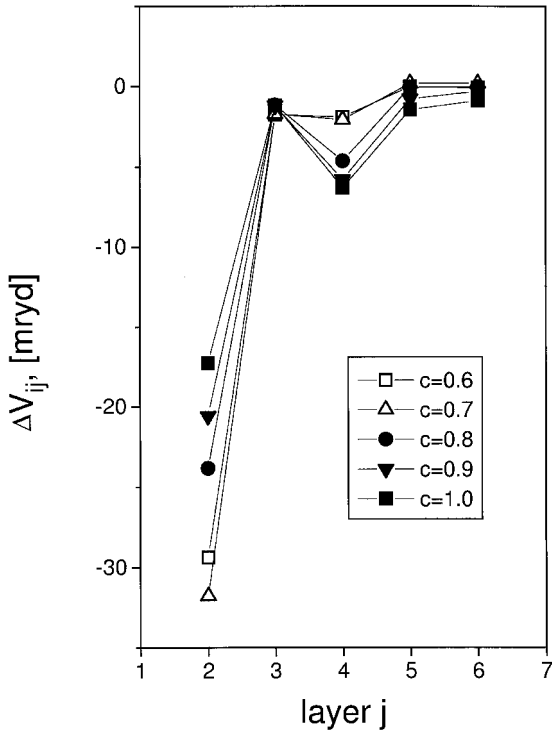
Figure 5. Layer-dependent correction terms V_{ij} (see text) in Cu(100)/(Fe$_c$Co$_{1-c}$)$_6$. The first layer index is kept constant, the numbering of layers starts at the substrate side.
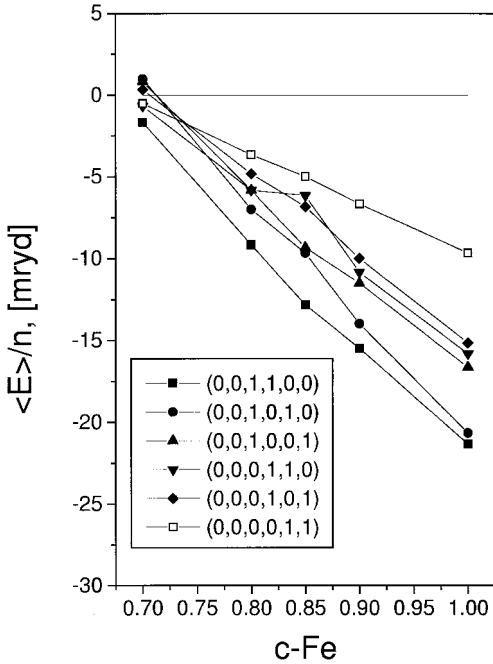

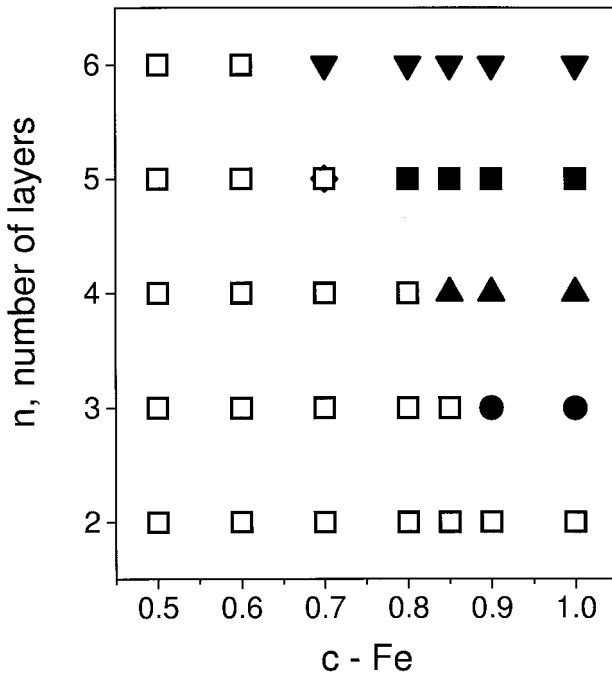Figure 6. Concentration and configuration dependent energy $\langle E \rangle$ in Cu(100)/(Fe$_c$Co$_{1-c}$)$_6$.

Figure 7. Ferromagnetic/antiferromagnetic phase diagram for $Cu(100)/(Fe_cCo_{1-c})_n$. Open squares: ferromagnetic, full symbols: antiferromagnetic. $n = 3$: circles: $(1,0,0)$; $n = 4$: up triangles: $(0,1,0,0)$; $n = 5$: squares: $(0,1,1,0,0)$: diamond: $(0,0,1,0,0)$; $n = 6$: down triangles: $(0,0,1,1,0,0)$. A ferromagnetic configuration would refer to $(0,0,\ldots,0)$.

magetically coupled layers pertains throughout $c_{Fe} > 0.7$. In figure 7 finally, a kind of 'phase-diagram' for the occurrence of antiferromagnetic coupling is displayed. In this figure open symbols refer to the case that the ferromagnetic coupling between the layers is the more stable one. All other symbols correspond to the most stable antiferromagnetic coupling.

It was noted by Zabloudil *et al.* (1998) that the reorientation transition of the magnetization as observed experimentally by Dittschar *et al.* (1998), in homogeneously alloyed Fe_cCo_{1-c} on $Cu(100)$ is most likely caused by a change of a ferromagnetic to an antiferromagnetic coupling between the magnetic layers. The 'phase-diagram' shown by Zabloudil *et al.* (1998), is very similar to the one in figure 7, however, as the anisotropy energy calculated by these authors refers to a self-consistent calculation for the so-called ground state magnetic configuration, the concentration at which this change in magnetic coupling occurs is 5–10% higher in Fe concentration as in the present case of using only spin-flip energies. With the exception of $n = 5$, for which already for pure layers of Fe on $Cu(100)$ a calculation (Weinberger 1998) in terms of spin-flip energies of the most probable antiferromagnetic coupling predicted a configuration $(0,1,1,0,0)$ rather than the next higher in energy, namely $(1,0,1,0,0)$, which was identified by *ab-initio*-like calculations by Szunyogh *et al.* (1997), as the so-called ground state configuration for Fe_n on $Cu(100)$, the present states of lowest energy are exactly those used by Zabloudil *et al.* (1998). Since they assumed that the type of antiferromagnetic coupling would not change when alloying Fe with Co, the present calculations are an *a posteri* proof of their assumptions.

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