Oscillatory behavior of the magnetic anisotropy energy in Cu(100)/Co$_n$ multilayer systems

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(Received 5 June 1997)

The oscillatory behavior of the magnetic-anisotropy energy in different types of Co$_n$ multilayers on a Cu(100) substrate, including free surfaces, capped surfaces, and Co/Cu spacer systems, is shown in terms of *ab initio*–like calculations using the self-consistent fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method. Deduced from direct representations and discrete (linear) Fourier transformations with respect to the number of Co layers, a period of two monolayers seems to be characteristic for these oscillations, whereas for a given number of Co layers and viewed with respect to the number of Cu-spacer layers they rapidly approach the value of the magnetic anisotropy energy for the corresponding Co$_n$ multilayer on Cu(100) with a semi-infinite Cu cap, the so-called biased value. By excluding the so-called preasymptotic regime a short and a long period of 2.5 and 5.5 monolayers, respectively, can be traced for the oscillations with respect to the number of Cu-spacer layers. All types of oscillations, namely, either with respect to the number of Co layers or with respect to the number of Cu-spacer layers, are analyzed in terms of layer-resolved band-energy contributions to the magnetic-anisotropy energy. Such a layerwise distribution of the magnetic-anisotropy energy allows one not only to characterize different regimes of thicknesses, but also to discuss the effect of the actual interface on the absolute values of the magnetic-anisotropy energy, shown in particular by considering a system with Co/Au interfaces. [S0163-1829(97)07845-4]

I. INTRODUCTION

The oscillatory behavior of interface exchange coupling has been responsible for some experiments but also for a (at the beginning rather contradictory) discussion of the asymptotic limit of these oscillations.[1,2] The magnetic-anisotropy energy, namely, the energy difference between an in-plane and a perpendicular orientation of the magnetization in magnetic multilayer systems, however, seemed to be primarily only of theoretical interest in the discussion of the reorientation transition of free surfaces[3] and its anomalous behavior in the case of capped surfaces.[4] Although it is fairly obvious to expect that also physical quantities other than interface exchange coupling, related in general to two different orientations of the magnetization in a multilayer system, show an oscillatory behavior, only very recently Cinal and Edwards[5] discussed oscillations of the magneto-crystalline anisotropy in Co/Pd structures using a (parametrized) Slater-Koster tight-binding formalism[6,7] and a corresponding perturbative treatment for the spin-orbit coupling.[8] By expressing the magnetic-anisotropy energy ϵ_a in terms of the anisotropy constants K_1 and K_2, $\epsilon_a = K_1\cos^2\delta + K_2\sin^2\delta\cos^2\varphi$, where δ and φ are the polar and the azimuthal angle of the direction of the magnetic moment with respect to the surface normal, respectively, they find oscillations with respect to the layer thickness. According to their theory for a fcc (100) surface, the second coefficient should vanish exactly. Their results for K_1 are indications of an oscillatory behavior of the magnetic-anisotropy energy with respect to the number of layers in a magnetic multilayer system on a (100) substrate. Very recently Družinić and Hübner[9] investigated the properties of the magnetic-anisotropy energy for free-standing chains of Fe adatoms in terms of a parametric model and found oscillations with re-

TABLE I. Investigated multilayer systems.

System	Case	n, number of Co layers	m, number of spacer layers
$Cu(100)/Co_n$	free surfaces	$1 \leqslant n \leqslant 15$	0
$Cu(100)/Co_n/Cu(100)$	capped surfaces	$1 \leqslant n \leqslant 15$	0
$Cu(100)/AuCo_nAu/Cu(100)$		$1 \leqslant n \leqslant 15$	0
$Cu(100)/Co_nCu_mCo_n/Cu(100)$	spacer systems	$1 \leqslant n \leqslant 15$	3
		1,4,6	$1 \leqslant m \leqslant 15$

spect to an even or odd number of Fe atoms. Almost simultaneously with these two papers a generalization of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction was presented,[10] predicting spatial oscillations of indirect RKKY exchange in the direction perpendicular to layers with a periodicity of the oscillations of exactly the double-interlayer spacing.

In the present paper the oscillatory behavior of the magnetic-anisotropy energy with respect to the number of Co layers is shown for free surfaces of Co_n on Cu(100) and for Co_n multilayers sandwiched by Cu(100). In order to investigate the influence of the Co/Cu interface on this behavior, a special case is considered in which the actual Co/Cu interface is replaced by a Co/Au interface, sandwiched, however, again by Cu(100). In particular, also oscillations of the magnetic-anisotropy energy with respect to the number of spacer layers in Co_n multilayer systems with a Cu spacer, namely, in systems of the type $Cu(100)/Co_nCu_mCo_n/Cu(100)$, are presented.

The paper is organized as follows. In Sec. II a short summary of the theoretical aspects and computational details is given. In Sec. III the results of the present investigations are presented and discussed. A conclusion finally summarizes the main results in Sec. IV.

II. THEORETICAL ASPECTS AND COMPUTATIONAL DETAILS

The fully relativistic spin-polarized version[3] of the screened Korringa-Kohn-Rostoker method[11] for layered systems[12] is applied to calculate self-consistently the electronic structure and the magnetic properties of (a) free surfaces of Co_n on Cu(100), (b) semi-infinitely capped surfaces, and (c) systems with a Cu spacer, whereby all interlayer distances refer to a fcc ''parent lattice''[13] corresponding to the experimental lattice spacing of Cu (no surface or interface relaxations).

In particular, the cases investigated are summarized in Table I. For each system in Table I, first the electronic and magnetic structures of the magnetic configuration corresponding to an in-plane orientation of the magnetization are calculated self-consistently using 45 $k_\parallel$ points in the irreducible part of the surface Brillouin zone (ISBZ) and the local density functional form of Ref. 14. The self-consistent layer-resolved effective potentials $V_p^{eff}(r)$ and effective magnetization fields $B_p^{eff}(r)$ obtained in the spin-polarized Kohn-Sham-Dirac Hamiltonian (see, e.g., Ref. 15),

$$H(r) = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V_p^{eff}(r) + \beta\Sigma_z B_p^{eff}(r), \qquad (1)$$

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

$$\Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad (2)$$

where the σ_i are the Pauli (spin) matrices and the index p refers to a particular layer, are then used to evaluate the magnetic-anisotropy energy $\epsilon_a(n,m)$,

$$\epsilon_a(n,m) = E_a(n,m) + E_{dd}(n,m), \qquad (3)$$

$$E_a(n,m) = E_a^{\parallel}(n,m) - E_a^{\perp}(n,m),$$

$$E_{dd}(n,m) = E_{dd}^{\parallel}(n,m) - E_{dd}^{\perp}(n,m). \qquad (4)$$

Here $E_a(n,m)$ is the difference in the band energies, $E_{dd}(n,m)$ is the difference in the magnetic dipole-dipole interaction energies with respect to a *uniform* in-plane and a perpendicular to the plane orientation of the magnetization in all planes of atoms, respectively, and n and m, as indicated in Table I refer to the number of Co and Cu-spacer layers, respectively. All band-energy differences presented in this paper were evaluated within the force theorem approximation (see in particular Ref. 16) by using 990 $k_\parallel$ points in the ISBZ and by applying the group-theoretic methods described in Ref. 3. In all cases considered, the convergence of $E_a(n,m)$ with respect to the applied $k_\parallel$ mesh in the ISBZ was checked by using in turn 325, 465, 630, and 990 $k_\parallel$ points. It was found that already 325 $k_\parallel$ points would be sufficient to give an essentially correct description of the oscillatory behavior of the magnetic-anisotropy energy.

In previous studies[17,18] of the magnetic-anisotropy energy of magnetic multilayer systems, layer-resolved band-energy differences $E_a^p(n,m)$,

$$E_a(n,m) = \sum_{p=1}^{P} E_a^p(n,m), \qquad (5)$$

where p is the layer index and P the total number of layers in the intermediate region,[12] i.e., the total number of layers between the perfect (nonmagnetic) semiinfinite regions, proved to be extremely illustrative for a discussion of the effects occurring. In the present study the intermediate region for the multilayer systems listed in Table I comprises at least two layers of Cu as a buffer to the semi-infinite Cu(100) substrate and, in the case of free surfaces, two vacuum layers as a buffer to the semi-infinite vacuum. For example, in a multilayer system of the type $Cu(100)/AuCo_nAu/Cu(100)$

the intermediate region is characterized by a layer sequence $Cu_qAuCo_nAuCu_q$ with $q \geq 2$.

In order to show the range of the oscillations with respect to the number of spacer layers, it is useful to relate $E_a(n,m)$ to the so-called biased value $E_a(n,\infty)$,

$$\Delta E_a(n,m) = E_a(n,m) - E_a(n,\infty), \tag{6}$$

$$E_a(n,\infty) = 2E_a(n,0), \tag{7}$$

where $E_a(n,0)$ corresponds to the respective Co_n multilayer on Cu(100) with a semi-infinite Cu cap.

In principle, the oscillatory behavior of $E_a(n,m)$ with respect to either the number of Co layers n or the number of Cu-spacer layers m can be analyzed in terms of a discrete (linear) Fourier transform. By keeping, for example, the number of Cu-spacer layers m constant such a Fourier transformation with respect to the number of Co layers n is defined by

$$F(q;m) = \frac{1}{N}\sum_{n=1}^{N} \omega(n) e^{iqn} E_a(n,m), \tag{8}$$

where, in analogy to the form used in order to describe the oscillatory behavior of interface exchange coupling,[19,20] a prefactor $\omega(n) = n^2$ is applied. The positions q_i of pronounced maxima of $|F(q;m)|$ then describe the periods of the oscillations. Furthermore, a discrete Fourier transform of $E_a(n,m)$ with respect to a reference level can be defined,

$$\Delta F(q;m) = \frac{1}{N}\sum_{n=1}^{N} \omega(n) e^{iqn} [E_a(n,m) - \langle E_a(m) \rangle], \tag{9}$$

where $\langle E_a(m) \rangle$, e.g., is given by the mean value

$$\langle E_a(m) \rangle = \frac{1}{N}\sum_{n=1}^{N} E_a(n,m). \tag{10}$$

Inspecting again Table I, one can see that for matters of consistency and comparison for all systems either n or m is restricted to 15. For the spacer systems $Cu(100)/Co_nCu_mCo_n/Cu(100)$ the set of $E_a(n,m)$ was augmented by calculations for $m > 15$ using the so-called frozen potential approximation,[16] namely, by using for a given value of n the (self-consistent) layer-resolved potentials and effective fields in Eq. (1) of the corresponding $m = 15$ case and repeating the central Cu-spacer layer. For $Cu(100)/Co_n/Cu(100)$ an equivalent procedure was applied by repeating the central Co layer.

In checking the validity of the frozen potential approximation for one particular case, namely for $n = 4$ and $m = 18$, it was found that a determination of the band part of the anisotropy energy based on self-consistent layer-resolved potentials and effective magnetization fields yielded a value of 0.242 meV as compared to a value of 0.249 meV when using the frozen potential approximation. At least for systems with a reasonably thick spacer the frozen potential approximation seems to yield quite reliable results.

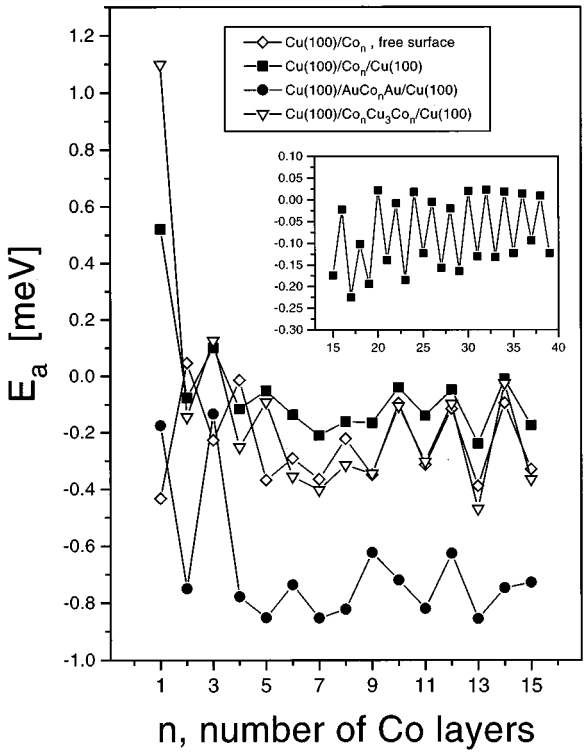

FIG. 1. Band-energy contribution to the magnetic-anisotropy energy as a function of the number of Co layers in $Cu(100)/Co_n$, $Cu(100)/Co_n/Cu(100)$, $Cu(100)/AuCo_nAu/Cu(100)$, and $Cu(100)/Co_nCu_3Co_n/Cu(100)$. The inset shows the continuation for $n \geq 15$ for the $Cu(100)/Co_n$ /Cu(100) systems.

III. RESULTS AND DISCUSSION

A. Oscillations with respect to the number of Co layers

In Fig. 1 the oscillations of the band-energy contribution to the magnetic-anisotropy energy with respect to the number of Co layers are shown for free surfaces of Co_n on Cu(100), capped surfaces, and one particular spacer system. As one immediately can see from this figure, there seem to be three different regimes of oscillations, namely, for (I) very thin films ($n \leq 4$), (II) moderately thin films ($4 < n < 10$), and (III) medium thick to thick films ($n \geq 10$). Also obvious is that in regime III the oscillations for free surfaces of Co_n on Cu(100) and for the systems with three Cu-spacer layers are indeed very similar in shape and are closely related to the oscillations for the capped surfaces. Set off in scale and also less pronounced are the oscillations for the systems with Co/Au interfaces. It should be noted that as compared to theoretically calculated oscillations of the interface exchange energy (see, e.g., Refs. 19 and 20), the oscillations of $E_a(n,m)$ are at least one order of magnitude smaller.

In the inset of Fig. 1 the continuation of the oscillations in the $Cu(100)/Co_n/Cu(100)$ sandwich systems is shown. It should be recalled that for $n > 15$ the band-energy parts of the magnetic-anisotropy energy were obtained by using the frozen potential approximation. From this inset one can see that even for rather thick Co slabs the oscillations in $E_a(n,m)$ with respect to n occur as a consequence of an even or odd number of Co layers, i.e., with a periodicity of two monolayers.

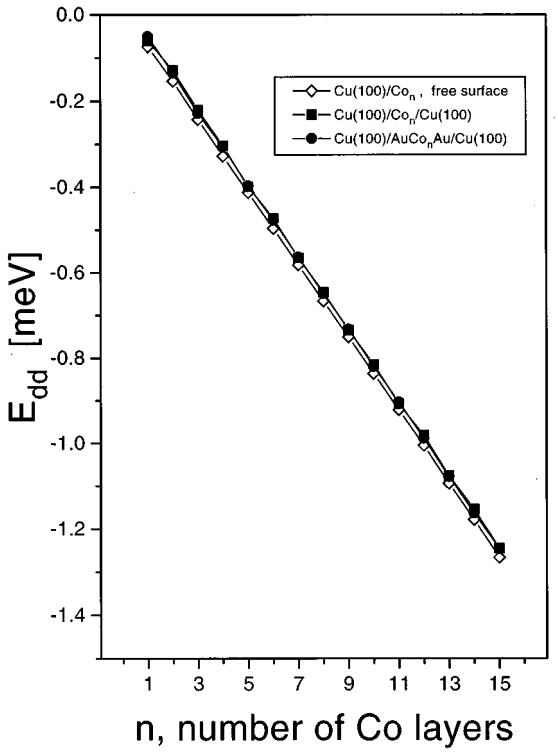

FIG. 2. Magnetic dipole-dipole energy contribution to the magnetic-anisotropy energy as a function of the number of Co layers in Cu(100)/Co$_n$, Cu(100)/Co$_n$/Cu(100), and Cu(100)/AuCo$_n$Au/Cu(100).

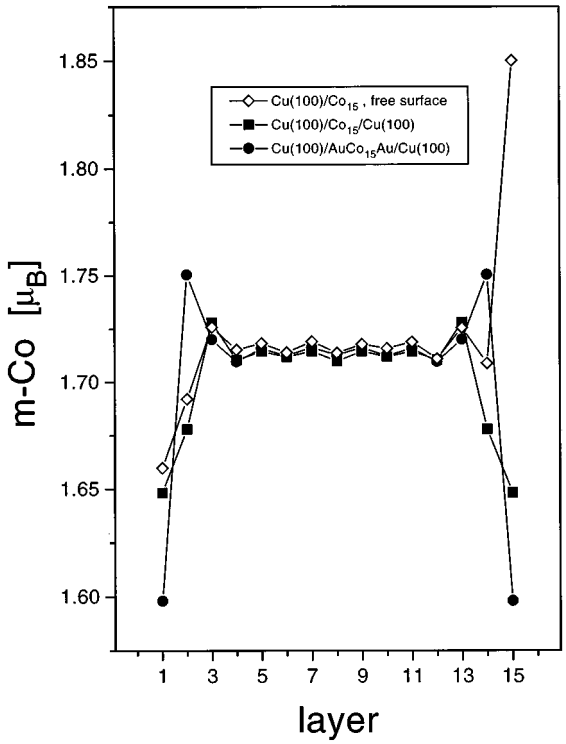

FIG. 3. Layer-resolved magnetic moments in Co$_{15}$ systems. Only the Co layers are shown.

In Fig. 2 the magnetic dipole-dipole contribution $E_{dd}(n,m)$ for free and capped surfaces of Co$_n$ on Cu(100) is displayed versus the number of Co layers. From this figure it is evident that very little variation with respect to the actual system, even in the case of Co/Au interfaces, pertains to this quantity: E_{dd} decreases nearly linearly with the number of Co layers. Keeping in mind that the anisotropy energy is the sum of $E_a(n,m)$ and $E_{dd}(n,m)$, it follows from Figs. 1 and 2 that only in the Cu(100)/Co$_n$/Cu(100) sandwich and in the Cu-spacer system (with three spacer layers) with $n=1$, i.e., for Co monolayers, the magnetization is perpendicular to the surface, while in all other cases ($n \geqslant 2$) the orientation of the magnetization is in plane. In light of the results shown in Fig. 2, in the following the discussion of the oscillatory behavior of the magnetic-anisotropy energy is confined to the band part $E_a(n,m)$.

The layer-resolved magnetic moments corresponding to an in-plane orientation of the magnetization are shown in Fig. 3 for the free and capped surfaces for $n=15$ including also the case with the Co/Au interfaces. Quite clearly the main changes with respect to the Co moment in the center layer occur at the interfaces. Figure 3 shows very nicely the effect of different interfaces on the variation of the Co moment: The interface Co moment is reduced, both at the Cu/Co and the Au/Co interface, whereas the moment of the second nearest Co layer depends on the kind of interface. In the case of the free surface the moment in the surface layer is substantially enhanced, while in the subsurface layers the moment varies almost like in the Cu(100)/Co$_{15}$/Cu(100) sandwich system. It should be noted, however, that in the

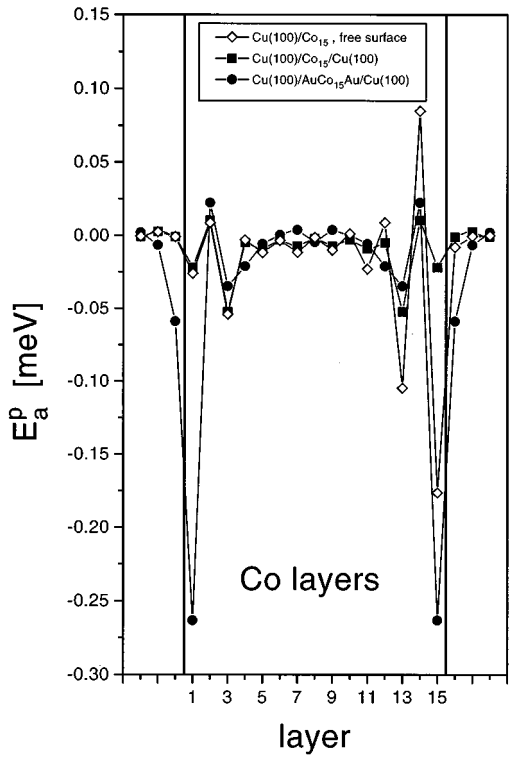

FIG. 4. Layer-resolved band-energy contributions to the magnetic-anisotropy energy in Co$_{15}$ systems. Only the Co layers are labeled.

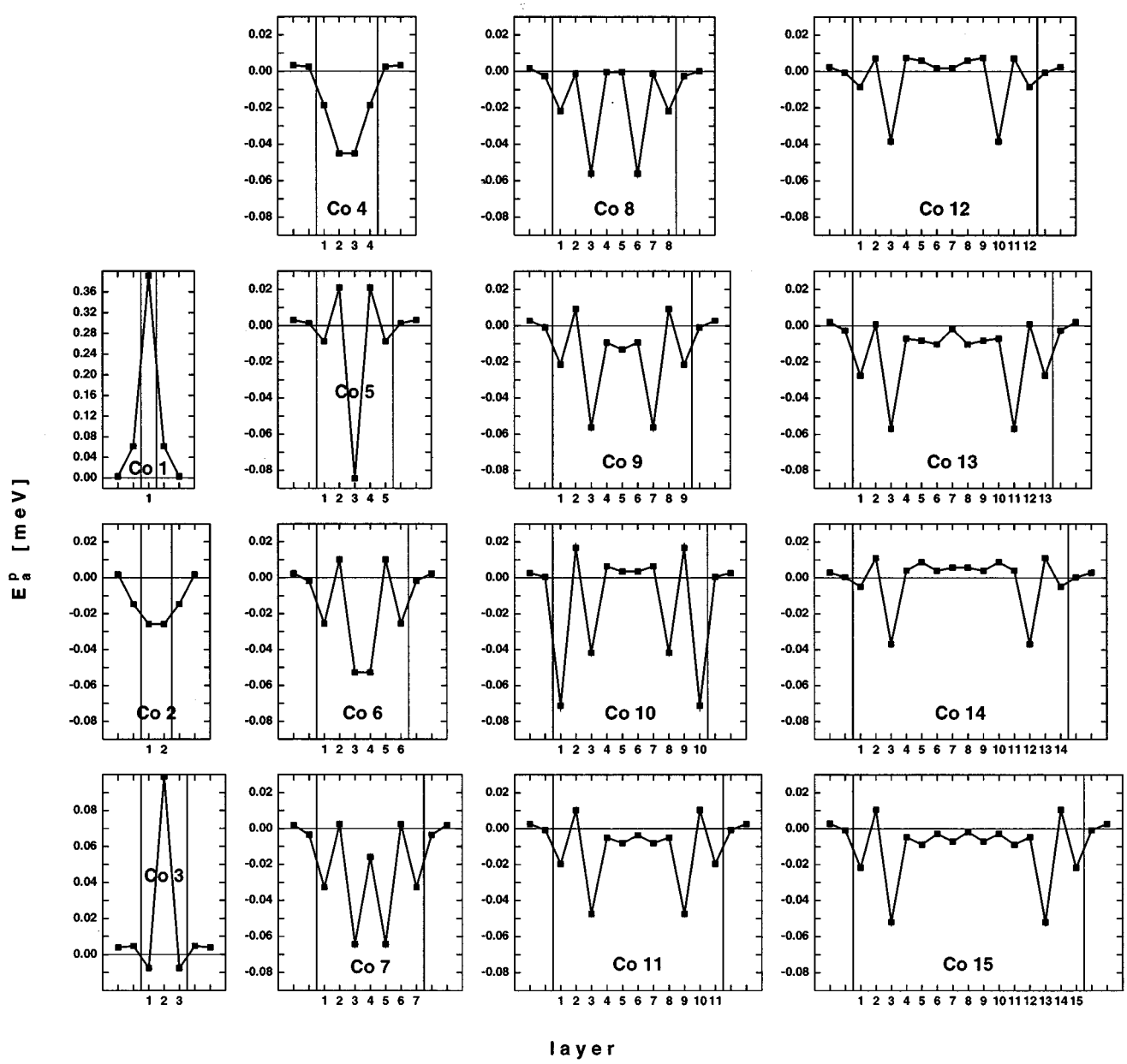

FIG. 5. Layer-resolved band-energy contributions to the magnetic-anisotropy energy for Cu(100)/Co_n/Cu(100), $n=1,2,\ldots,15$. Only the Co layers are labeled. Note the different scale for the Co_1 and Co_3 entries.

interior of the Co slab the magnetic moment shows weak oscillations with respect to the layer index.

In Fig. 4 for the same systems the layer-resolved band-energy parts of the magnetic-anisotropy energy $E_a^p(n,m)$ are displayed. As one can see in the case of the free surfaces, $E_a^p(n,m)$ oscillates considerably in the Co layers near the surface and then follows very closely the values for the Cu(100)/Co_{15}/Cu(100) sandwich system. In the system with the Co/Au interfaces the largest contributions to $E_a(n,m)$ result from the Co layers near the interfaces. For this system the variations in the interior of the Co slab are small compared to the contributions from the interfaces. Figure 4 illustrates convincingly the differences in the absolute values of $E_a(n,m)$ at $n=15$ for the systems shown in Fig. 1.

In order to interpret the oscillations of $E_a(n,m)$ with respect to the number of Co layers, the $E_a^p(n,m)$ in the Cu(100)/Co_n/Cu(100) sandwich systems are compiled in Fig. 5 for all Co thicknesses up to 15. Regime I ($n \leqslant 4$) and regime III ($n \geqslant 10$) can now be characterized as follows.

In regime I (very thin films) strong interface-interface interactions, visually similar to a bonding/antibonding situation, seem to govern the layerwise distribution of the band part of the magnetic-anisotropy energy. For an even number of Co layers, the contributions from the two layers in the center of the Co film are negative and biggest, while for an odd number of Co layers, the contribution from the center layer is substantially positive in value. An even number of Co layers favors an in-plane orientation of the magnetization, while for an odd number of Co layers the center layer tends to reverse this trend.

In regime III the main contributions to $E_a(n,m)$ arise from the first three Co layers next to the interface, whereby

obviously the (respective) third-nearest Co layer carries the biggest weight. Although it seems at a first glance that for $n>10$ the shape of the layer-resolved band-energy contributions with respect to the layer index is about the same, it is important to note that the variations of $E_a^p(n,m)$ in the interior of the Co slab actually determine the contribution from the Co layer third nearest the interface. If the number of Co layers is odd, then the contribution from the Co layer third nearest the interface is substantially bigger than when n is even. Quite obviously, in regime III the oscillations of $E_a^p(n,m)$ with respect to the number of Co layers arise from alternating even or odd numbers of Co layers in the interior of the Co slab $(n-6)$. As already stated, this particular feature pertains also for thicker Co slabs (as shown, e.g., in the inset of Fig. 1).

By defining for $n\geqslant 6$ the following partials sums over Co-like $E_a^p(n,m)$, namely, an ''interface'' contribution $E_a^{if}(n,m)$,

$$E_a^{if}(n,m)=2\sum_{p=1}^{3} E_a^p(n,m), \tag{11}$$

and an ''interior'' contribution $E_a^{int}(n,m)$,

$$E_a^{int}(n,m)=\sum_{p=4}^{n-3} E_a^p(n,m), \tag{12}$$

where p now labels only the Co layers, it is found that for the systems shown in Fig. 5 $E_a^{int}(n,m)$ is always positive for an even number of Co layers and negative for an odd number of Co layers. This is shown in Fig. 6, where $E_a^{if}(n,m)$ and $E_a^{int}(n,m)$ are compared with twice the contribution from the Co layer third nearest the interface. As one can see, the most pronounced oscillations with respect to even and odd numbers of Co layers are found for $E_a^{int}(n,m)$. Their influence on the contribution from the Co layer third-nearest the interface, as discussed above, is reflected by the same oscillation period. $E_a^{if}(n,m)$, in contrast, shows a different behavior. Thus Fig. 6 clearly shows the origin of the oscillations in $E_a(n,m)$ with respect to the number of Co layers, namely, alternating even and odd numbers of Co layers in the interior of the Co slab, and the destructive influence of $E_a^{if}(n,m)$ for $n\leqslant 10$.

Regime II appears to be an intermediate regime between very thin films and medium thick films. Cases with $n\geqslant 8$ show a precursor behavior towards regime III, while for $4\leqslant n<8$ a successive dying out of interface-interface interactions with increasing n seems to be characteristic.

The other systems displayed in Fig. 1, in particular the spacer systems, follow closely the pattern shown in Fig. 5. For the free surfaces, however, the asymmetry of band-energy contributions to the magnetic-anisotropy energy next to the Co/vacuum interface (see also Fig. 4) has to be accounted for as an additional feature. The interface sensitivity of $E_a(n,m)$, shown in Fig. 1, seems to be in rough agreement with the results obtained by Cinal and Edwards[5] for fcc(100) Co_n multilayers with Co/Pd interfaces, although their K_1 values do not oscillate characteristically with a period of two monolayers.

The magnetic anisotropy K per unit volume recorded experimentally[21] as Kt versus the thickness t (5 Å$\leqslant t\leqslant$30 Å) shows for the Cu/Co systems an almost linear decrease with increasing Co thickness, mapping basically the contributions of the magnetic dipole-dipole interactions to the magnetic-anisotropy energy; see Fig. 2. The experimental data[22] for the out-of-plane surface anisotropy k_s determined for free surfaces of Co_n on Cu(100) for $n\leqslant 6$ and $n=10$ indicate, however, an onset of oscillations of k_s with the number of Co layers. Furthermore, a comparison with Co_n multilayers on Cu(100) capped by two layers of Cu exhibits that (just as in Fig. 1) for two to five layers of Co the $E_a(n,m)$ versus n curves seem to be reversed in shape. Although a direct comparison with the experimental data in Ref. 22 is probably not very useful since for very thin films surface relaxation and roughness effects matter, these data clearly show the same kind of pattern as displayed in Fig. 1.

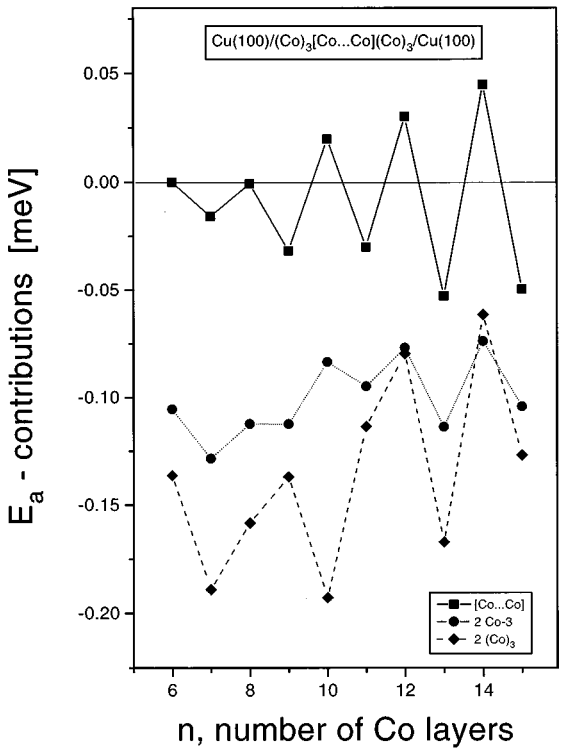

FIG. 6. ''Interior'' contribution $E_a^{int}(n,m)$ (squares), ''interface'' contribution $E_a^{if}(n,m)$ (bullets), and twice the contribution from the Co layer third nearest the interface (diamonds) as a function of the number of Co layers in Cu(100)/Co_n/Cu(100), $n\geqslant 6$. For definitions, see Eqs. (11) and (12).

B. Oscillations with respect to the number of Cu-spacer layers

In Fig. 7 the oscillations of $\Delta E_a(n,m)$ [Eq. (6)] with respect to the number of Cu-spacer layers are shown for three different values of n. It should be recalled that only parallel coupling between the two Co slabs applies and also that for $m>15$ the frozen potential approximation was used. As one can see from this figure, for thin spacers, i.e., $m\leqslant 10$, these oscillations are of about the same order of magnitude as the oscillations with respect to the number of Co layers. For $m>10$, however, they converge rather rapidly to the biased value. Unsurprisingly, the largest and longest outgoing oscillations are seen for monolayers of Co $(n=1)$, the smallest

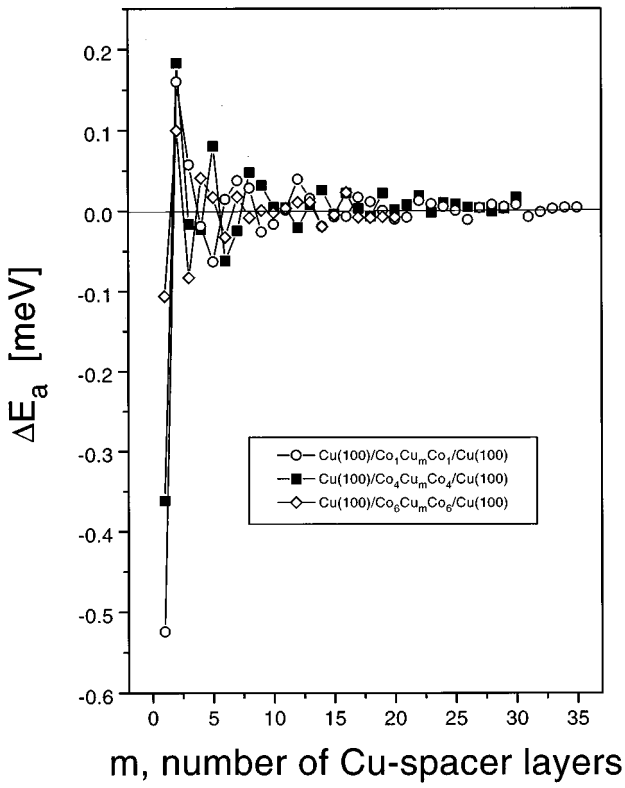

FIG. 7. Relative band-energy contribution to the magnetic-anisotropy energy $\Delta E_a(n)$ as a function of the number of Cu-spacer layers m in Cu(100)/$Co_n$$Cu_m$$Co_n$/Cu(100), $n=1,4,6$.

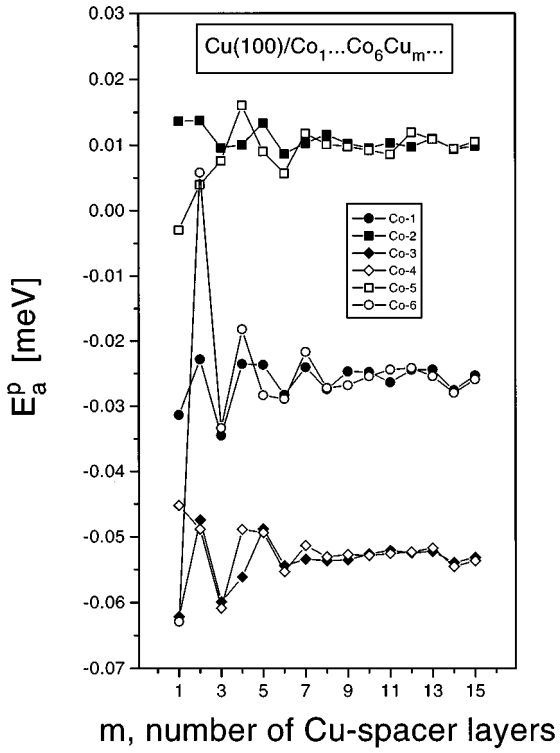

FIG. 8. Layer-resolved band-energy contributions to the magnetic-anisotropy energy as a function of the number of Cu-spacer layers m for the left Co slab in Cu(100)/$Co_6$$Cu_m$$Co_6$/Cu(100). Full symbols refer to the Co layers next to the substrate, open symbols to those neighboring the Cu spacer.

and most confined for $n=6$. Although similar to the case of the interface exchange coupling of Co slabs separated by a Cu spacer, for $m>10$ a period of about five monolayers seems to be present, its amplitude of less than 0.002 meV, however, is too small to be confirmed safely from a direct representation such as Fig. 7.

For one particular case, namely, for $n=6$, the layer-resolved $E_a^p(n,m)$ referring to the individual Co slabs are shown in Fig. 8 as a function of the number of Cu-spacer layers. As one can see from this figure, for $m\leqslant 7$ the oscillations in the magnetic-anisotropy energy are mainly caused by the Co layer neighboring the Cu spacer. For larger values of m even this particular contribution to the magnetic-anisotropy energy dies out very fast. By viewing at a particular value of m the $E_a^p(n,m)$ values in Fig. 8 arranged with respect to the number of Co layers, it is easy to see that such a presentation very closely resembles the Co_6 entry in Fig. 5.

C. Discrete (linear) Fourier transformations

Finally, in Fig. 9 examples of discrete (linear) Fourier transformations [see Eqs. (8)–(10)] are shown. In both panels a relative scale for the ordinate is used by displaying $f_1(q;i)=|F(q;i)|/|F(0;i)|$ and $f_2(q;i)=|\Delta F(q;i)|/|F(0;i)|$ versus q (in units of $2\pi/d$, with d being the interlayer spacing), where i refers to either n or m, i.e., referring to a discrete Fourier transformation keeping either the number of Cu-spacer layers m or the number of Co layers n constant. It should be noted that by displaying q in units of $2\pi/d$, eventual periods in units of d (monolayers) are simply given by q_0^{-1}, where q_0 denotes the position of a pronounced maximum in $|F(q;i)|$.

In the left panel of Fig. 9 these two functions are presented for the Cu(100)/Co_n/Cu(100) system, i.e., for $m=0$. Both functions $f_1(q;0)$ and $f_2(q;0)$ show a pronounced maximum of almost the same value at $q=1/2$. For $f_1(q;0)$ one can also see the trivial peaks at $q=0,1$, which are mostly removed in $f_2(q;0)$, i.e., by Fourier transforming the deviations of $E_a(n,0)$ from their mean value. Quite obviously in Cu(100)/Co_n/Cu(100) the band part of the magnetic-anisotropy energy oscillates with a period of two monolayers, a feature that was already seen in Fig. 1. The free surfaces of Co_n on Cu(100) and the capped surface with the Co/Au interfaces differ from the case shown in the left panel of Fig. 9 only by the amplitude of the peak at $q=1/2$. In all these cases a period of two monolayers can be deduced form the corresponding Fourier transformation with respect to the number of Co layers. The left panel of Fig. 9 confirms very nicely the predictions made using a generalized form of the RKKY interaction.[10] Stated oppositely, the asymptotic limit of the oscillations of the anisotropy energy with respect to the number of Co layers seems, as in the case of interface exchange coupling, to be governed by a RKKY-type behavior. It should be noted that by increasing N in Eq. (8) only the value of the maximum in $f_1(q,m)$ and $f_2(q,m)$ is increased; the peak position, however, remains located at $q=1/2$.

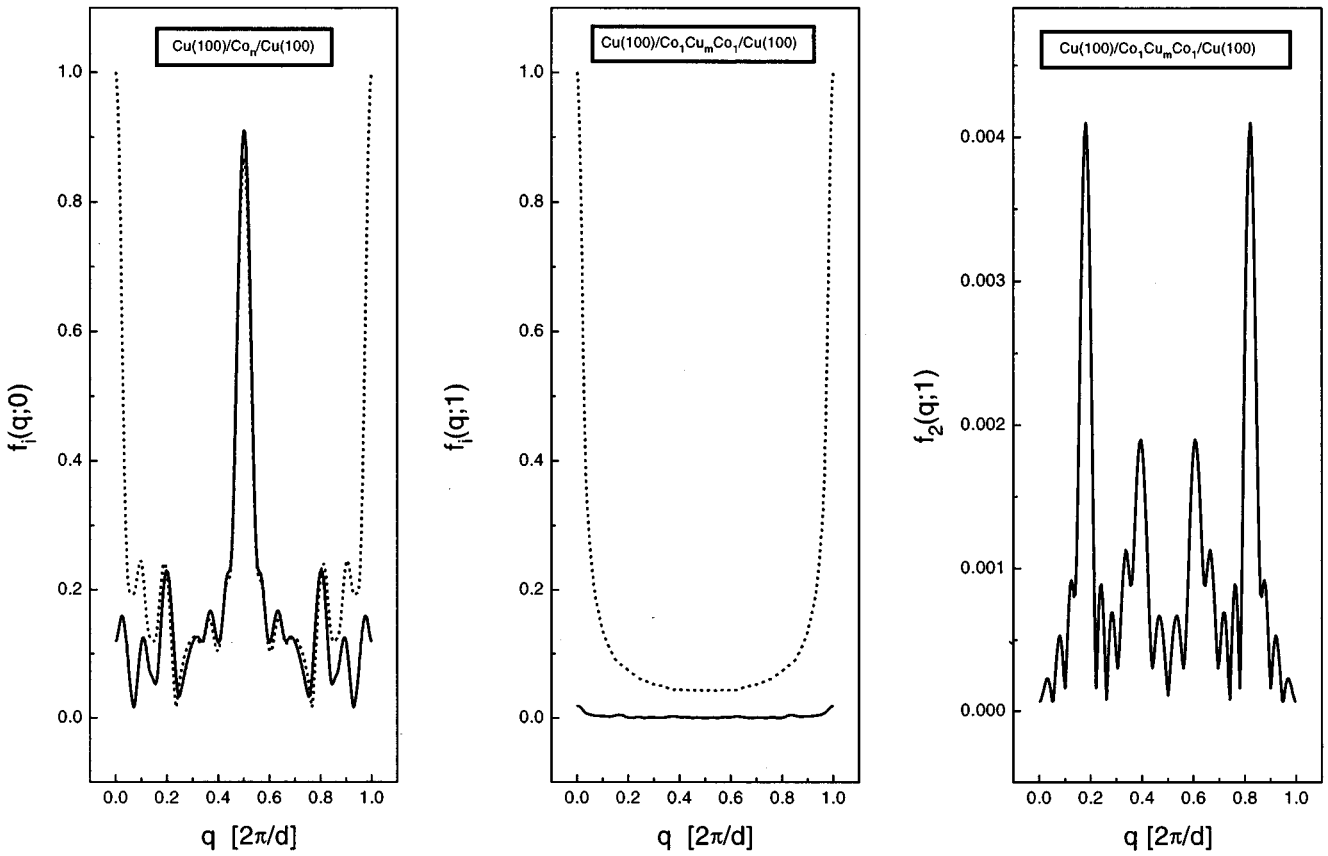

FIG. 9. Absolute values $f_1(q;i)$ (dashed line) and $f_2(q;i)$ (full line) of the Fourier transformations $F(q;i)$ and $\Delta F(q;i)$, respectively, $i=m,n$, both scaled by $|F(0;i)|$ and displayed as a function of q (in units of $2\pi/d$, where d is the interlayer distance): left panel, with respect to the number of Co layers n for Cu(100)/Co$_n$/Cu(100); middle panel, with respect to the number of Cu-spacer layers m for Cu(100)/Co$_1$Cu$_m$Co$_1$/Cu(100); and right panel, $f_2(q;1)$ with respect to the number of Cu-spacer layers m for Cu(100)/Co$_1$Cu$_m$Co$_1$/Cu(100) as obtained by excluding the preasymptotic regime.

For Cu(100)/CoCu$_m$Co/Cu(100), i.e., for $n=1$, the Fourier transformation with respect to m (Fig. 9, middle panel) yields no well-developed nontrivial periodicity. The fact that in the middle panel of Fig. 9 the function $f_2(q;1)$ is nearly zero in the whole range of q clearly demonstrates the rather rapid convergence of $E_a(1,m)$ with increasing m to the corresponding biased value $E_a(1,\infty)$.

By excluding explicitly the so-called preasymptotic regime, i.e., by using as a lower summation index in Eq. (9), for example, $m \geqslant 10$, and a similarly defined mean value $\langle E_a(m) \rangle$, peaks in $f_2(q;1)$ (Fig. 9, right panel) at $q=0.18$ and $q=0.40$ can be traced that correspond in turn to a long period of 5.56 monolayers and a short period of 2.5 monolayers. These periods are in surprisingly good agreement with those of Bruno and Chappert[25] (2.56 and 5.88 monolayers) and Kudrnovský *et al.*[19] (2.6 and 6.7 monolayers), found, however, for the interface exchange coupling of Co slabs separated by a Cu spacer and embedded in a Cu(100) host.

It should be noted that because of the previously mentioned smallness of the variations in $\Delta E_a(1,m)$, the values of $f_2(q;1)$ in the right panel of Fig. 9 are rather small. Nevertheless, this particular figure shows that the predictions made recently by Szunyogh and Gyorffy[23] concerning the oscillatory behavior of the anisotropy energy of an impurity near the surface of a metallic substrate also seem to apply to traditional spacer systems. As to be expected from Fig. 7, all the other spacer systems, discussed in Sec. III B, show a similar behavior.

IV. CONCLUSION

In the present paper it was shown that the magnetic-anisotropy energy of Co$_n$ multilayers on Cu(100), because of its oscillatory band-energy contribution, shows oscillations with respect to an increasing number of Co layers. For thin spacer systems additional variations of the magnetic-anisotropy energy with respect to the number of Cu-spacer layers occur. Considering a general multilayer system such as Cu(100)/Co$_{n_1}$Cu$_{m_1}$Co$_{n_2}$Cu$_{m_2}\cdots$, the magnetic-anisotropy energy $\epsilon_a(n_1,m_1,n_2,m_2,\ldots)$, which is a function of all slab thicknesses, can therefore show a rather complicated oscillatory behavior.

It was also clearly demonstrated that such oscillations are one order of magnitude smaller than those determined theoretically for the interface exchange coupling in the same kind of systems. In accordance with a recent RKKY generalization, the oscillations with respect to the number of Co layers on a Cu(100) substrate show a period of two monolayers, while in Cu-spacer systems viewing the oscillations as a function of the number of Cu-spacer layers, distinct periods are seen only if the preasymptotic regime is excluded. These

periods are similar to the short and long periods found for the interface exchange coupling in $Cu(100)/Co_nCu_mCo_n/Cu(100)$. In these kinds of systems the oscillations of the band part of the magnetic-anisotropy energy with respect to the number Cu-spacer layers rapidly approaches the corresponding biased value, i.e., the value of a Co_n multilayer on Cu(100) with a semi-infinite Cu cap. A similar effect was very recently discovered[24] for the interlayer exchange coupling in $Cu(100)/Co_1Cu_{m_1}Co_1/Cu_{m_2}$, when considering the interface exchange coupling energy as a function of the cap thickness m_2.

ACKNOWLEDGMENTS

This paper resulted from a collaboration partially funded by the TMR network on *ab initio* calculations of magnetic properties of surfaces, interfaces, and multilayers (Contract No. EMRX-CT96-0089). Financial support was provided also by the Center of Computational Materials Science (Grant No. GZ 308.941), the Austrian Science Foundation (Grant No. P11626), and the Hungarian National Science Foundation (Grant No. OTKA T22609). We also wish to thank the computing center IDRIS at Orsay as part of the calculations was performed on their Cray T3D machine.

[1] See, for example, P. Bruno and C. Chappert, Phys. Rev. B **46**, 261 (1992); J. Mathon, M. Villeret, and D. M. Edwards, J. Magn. Magn. Mater. **127**, L261 (1993).
[2] V. Drchal, J. Kudrnovský, I. Turek, and P. Weinberger, Phys. Rev. B **53**, 15 036 (1996).
[3] L. Szunyogh, B. Újfalussy, and P. Weinberger, Phys. Rev. B **51**, 9552 (1995).
[4] B. Újfalussy, L. Szunyogh, P. Bruno, and P. Weinberger, Phys. Rev. Lett. **77**, 1805 (1996).
[5] M. Cinal and D. M. Edwards, Phys. Rev. B **55**, 3636 (1997).
[6] M. Cinal, D. M. Edwards, and J. Mathon, Phys. Rev. B **50**, 3754 (1994).
[7] M. Cinal, D. M. Edwards, and J. Mathon, J. Magn. Magn. Mater. **140-144**, 681 (1995).
[8] P. Bruno, Phys. Rev. B **39**, 865 (1989).
[9] R. Družinić and W. Hübner, Phys. Rev. B **55**, 347 (1997).
[10] D. N. Aristov, Phys. Rev. B **55**, 8064 (1997).
[11] R. Zeller, P. H. Dederichs, B. Újfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B **52**, 8807 (1995).
[12] L. Szunyogh, B. Újfalussy, P. Weinberger, and J. Kollár, Phys. Rev. B **49**, 2721 (1994).
[13] P. Weinberger, Philos. Mag. B **77**, 509 (1997).
[14] S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).
[15] P. Weinberger, *Electron Scattering Theory for Ordered and Disordered Matter* (Clarendon, Oxford, 1990).
[16] L. Szunyogh, B. Újfalussy, P. Weinberger, and C. Sommers, Phys. Rev. B **54**, 6430 (1996).
[17] B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B **54**, 9883 (1996).
[18] L. Szunyogh, B. Újfalussy, and P. Weinberger, Phys. Rev. B **55**, 14 392 (1997).
[19] J. Kudrnovský, V. Drchal, I. Turek, and P. Weinberger, Phys. Rev. B **50**, 16 105 (1994).
[20] J. Kudrnovský, V. Drchal, I. Turek, M. Šob, and P. Weinberger, Phys. Rev. B **53**, 5125 (1996); V. Drchal, J. Kudrnovský, I. Turek, and P. Weinberger, *ibid.* **53**, 15 036 (1996); J. Kudrnovský, V. Drchal, P. Bruno, I. Turek, and P. Weinberger, *ibid.* **54**, R3738 (1996); J. Kudrnovský, V. Drchal, C. Blaas, I. Turek, and P. Weinberger, Phys. Rev. Lett. **76**, 3834 (1996); J. Kudrnovský, V. Drchal, R. Coehoorn, M. Šob, and P. Weinberger, *ibid.* **78**, 358 (1997).
[21] F. J. A. den Broeder, W. Hoving, and P. J. H. Bloemen, J. Magn. Magn. Mater. **93**, 562 (1991).
[22] P. Krams, F. Lauks, R. L. Stamps, B. Hillebrands, and G. Güntherodt, Phys. Rev. Lett. **69**, 3674 (1992).
[23] L. Szunyogh and B. L. Gyorffy, Phys. Rev. Lett. **78**, 3765 (1997).
[24] J. Kudrnovský, V. Drchal, P. Bruno, I. Turek, and P. Weinberger, Phys. Rev. B **56**, 8919 (1997).
[25] P. Bruno and C. Chappert, Phys. Rev. Lett. **67**, 1602 (1992).