Superlattice symmetry in magnetic multilayer systems

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The problem of superlattice symmetry, i.e., the question of periodicity along the growth direction (surface normal) in magnetic multilayer systems, is discussed using discrete Fourier transformations for the anisotropy energy, as well as, for the antiparallel and perpendicular interface exchange coupling. We analyze the system $Cu(100)/(Cu_3Ni_3)_n$, where n is the number of repetitions, for the case of free surfaces and surfaces capped semi-infinitely by Cu(100). It will be shown that for some magnetic properties, and only in certain situations, (almost) periodic behavior with respect to n applies, while for other properties an oscillatory behavior is characteristic. Also discussed are implications with respect to typical experimental situations and with respect to traditional supercell approaches. [S0163-1829(98)00313-0]

I. INTRODUCTION

Frequently when discussing physical properties of magnetic multilayer systems, periodicity along the surface normal is assumed in most theoretical approaches, but also in analyzing experimental data. Theoretically very often supercell calculations are performed, which of course, independent of the number of atoms per unit cell, use implicitly cyclic boundary conditions along the growth direction.[1–4] In the same manner, there is a tendency to interpret and explain results of experimental investigations in terms of superlattice effects.[5–9] Therefore, it seems that there is a definite need for investigating the applicability of such approaches. For this reason in the present paper magnetic properties of $(Cu_3Ni_3)_n$ on Cu(100), where n is the number of repetitions, are determined by considering free surfaces and surfaces capped semi-infinitely by Cu(100). Quite clearly one such unit (Cu_3Ni_3) serves as a building block and—by assuming periodicity along (100)—has to be viewed as the unit cell. By employing an approach that makes use only of two-dimensional translational symmetry, namely, within the planes of atoms, and that allows one to vary n, periodicity with respect to n can manifest itself (if it really exists) for various magnetic properties. The magnetic anisotropy energy and specific forms of multi-interface exchange coupling energies are chosen as characteristic examples.

II. THEORETICAL ASPECTS AND COMPUTATIONAL DETAILS

The fully relativistic spin-polarized version[10] of the screened Korringa-Kohn-Rostoker method[11] for layered systems[12] is applied to calculate selfconsistently the electronic structure and the magnetic properties of (a) free surfaces of $(Cu_3Ni_3)_n$ on Cu(100), denoted in the following as $Cu(100)/(Cu_3Ni_3)_n$/Vac, and (b) semi-infinitely capped surfaces, denoted by $Cu(100)/(Cu_3Ni_3)_n$/Cu(100), whereby all interlayer distances refer to a fcc parent lattice[13] corresponding to the experimental lattice spacing of Cu (no surface or interface relaxations). For each system, i.e., for each n, first the electronic and magnetic structure of the magnetic configuration corresponding to a *uniform* in-plane orientation of the magnetization in the Ni layers (magnetic reference configuration $\mathcal{C}_0$, see also Table I) is 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 obtained self-consistent layer-resolved effective potentials and layer-resolved effective magnetization fields in the spin-polarized Kohn-Sham-Dirac Hamiltonian (see, e.g., Ref. 15) are then used to evaluate the following differ-

TABLE I. Magnetic configurations.

Conf.	M_{Ni}	M_{Cu}	M_{Ni}	M_{Cu}	M_{Ni}	M_{Cu}	M_{Ni}	M_{Cu}	M_{Ni}	orientation of magnetization
$\mathcal{C}_0$:	↑	⋯	↑	⋯	↑	⋯	↑	⋯	↑	uniform in-plane
$\mathcal{C}_1$:	→	⋯	→	⋯	→	⋯	→	⋯	→	uniform perpendicular to plane
$\mathcal{C}_2$:	↑	⋯	↓	⋯	↑	⋯	↓	⋯	↑	antiparallel in-plane
$\mathcal{C}_3$:	↑	⋯	→	⋯	↑	⋯	→	⋯	↑	alternating in-plane and perpendicular to plane

ences in the band energies with respect to the magnetic configurations given in Table I:

$$\Delta E(\mathcal{C}_i)=E(\mathcal{C}_i)-E(\mathcal{C}_0). \tag{1}$$

It should be noted that in Table I configuration $\mathcal{C}_1$ refers to the case that uniformly in all Ni layers the orientation of the magnetization is perpendicular to the planes of atoms. Configuration $\mathcal{C}_2$ comprises again a case of in-plane orientations, arranged, however, alternatively antiparallel, while in configuration $\mathcal{C}_3$ in-plane and perpendicular-to-plane orientations alternate. $\Delta E(\mathcal{C}_1)$ refers to the band energy contribution to the magnetic anisotropy energy,[10,16] while $\Delta E(\mathcal{C}_2)$ and $\Delta E(\mathcal{C}_3)$ reflect multi-interface exchange coupling.

In principle the magnetic anisotropy energy and the multi-interface exchange coupling energy also contains a contribution arising from the magnetic dipole-dipole interaction,[10] which, however, only grows more or less linear with the number of magnetic layers.[10,17–19] In the case of the magnetic anisotropy energy, e.g., the magnetic dipole-dipole energy predominantly determines the so-called volume anisotropy.[20,19] In the present investigations the magnetic dipole-dipole interaction is not included.

If P denotes the total number of atomic layers in the intermediate regime,[12] i.e., the total number of atomic layers between the (nonmagnetic) semi-infinite systems, then $\Delta E(\mathcal{C}_i)$ can be partitioned into layerwise contributions $\Delta E_p(\mathcal{C}_i)$,

$$\Delta E(\mathcal{C}_i)=\sum_{p=1}^{P}\Delta E_p(\mathcal{C}_i)=\sum_{p=1}^{P}[E_p(\mathcal{C}_i)-E_p(\mathcal{C}_0)], \tag{2}$$

which in turn can be Fourier transformed using the following discrete Fourier transformation (FT)

$$F(q;\mathcal{C}_i)=\sum_{p=1}^{P}e^{iqp}\Delta E_p(\mathcal{C}_i) \tag{3}$$

or, in relation to their mean value $\Delta E(\mathcal{C}_i)/P$, as

$$\Delta F(q;\mathcal{C}_i)=\sum_{p=1}^{P}e^{iqp}\left[\Delta E_p(\mathcal{C}_i)-\frac{\Delta E(\mathcal{C}_i)}{P}\right], \tag{4}$$

where q is given in units of $2\pi/d$ with d being the interlayer distance.[21,19]

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 theoretical methods described in Ref. 10. By normalizing the absolute value of the Fourier transform in a suitable manner, e.g., to a unit area A,

$$A=\left[\int_0^{1/2}\left|\Delta F(q;\mathcal{C}_i)\right|dq\right]^{-1}, \tag{5}$$

comparison can made between different cases such as free and capped surfaces, and different numbers n of repetitions. Quite clearly any other layer-resolved quantity such as the magnetic moments or the Madelung potentials[12] can be transformed in the same manner.

If the physical property investigated is periodic with respect to the building block a period of six, i.e., a pronounced maximum in $|\Delta F(q;\mathcal{C}_i)|$ at $q=1/6$ has to show up, since one unit (Cu_3Ni_3) consists of six layers. A period of twelve ($q=1/12$) is characteristic if the quantity is periodic with respect to twice a building block. Of course the interesting and physically relevant question of using such discrete FT's is how large n has to grow in order to trace a periodic behavior. In the present paper the number of repetitions is restricted to $n\leqslant 11$, which in turn implies a maximum multilayer thickness of about 225 a.u.

By relating the band energy differences $\Delta E(\mathcal{C}_i)$ in Eq. (1) to the number of repetitions (band energy difference per unit cell), one further can examine whether for increasing n, $\Delta E(\mathcal{C}_i)/n$ approaches a constant or oscillates. The next section will show examples for both kinds of behavior.

It should be noted that both, discrete FT's and quantities per repetition (unit cell), are essential in describing what is sometimes called colloquially superlattice symmetry or colloquial lattice,[13] namely, in defining periodic behavior with respect to the surface normal.

III. RESULTS AND DISCUSSION

A. Layer-resolved band energies

In the following, in all figures showing layer-resolved quantities, the indexing of atomic layers starts at the Cu(100) substrate, i.e., the Cu substrate is to the left of the intermediate region and vacuum or the cap is to the right. For $n\leqslant 5$ the layer-resolved band energy contributions $\Delta E_p(\mathcal{C}_1)$ to the magnetic anisotropy energy are displayed in Fig. 1 for free and capped surfaces. For the free surface case one can easily see the strong perturbation caused by the surface, however, for $n\geqslant 4$ a period of six emerges since with increasing n the number of nearly identical peaks in the interior of the film is increasing. For the capped case the effect of the interfaces with the semi-infinite substrate on both sides is fairly marginal: for each n the corresponding entries are practically characterized by n identical peaks in $\Delta E_p(\mathcal{C}_1)$.

Completely different in shape are the layer-resolved band energy contributions $\Delta E_p(\mathcal{C}_2)$ to the (antiparallel) interface coupling energy shown in Fig. 2(a) in the case of capped

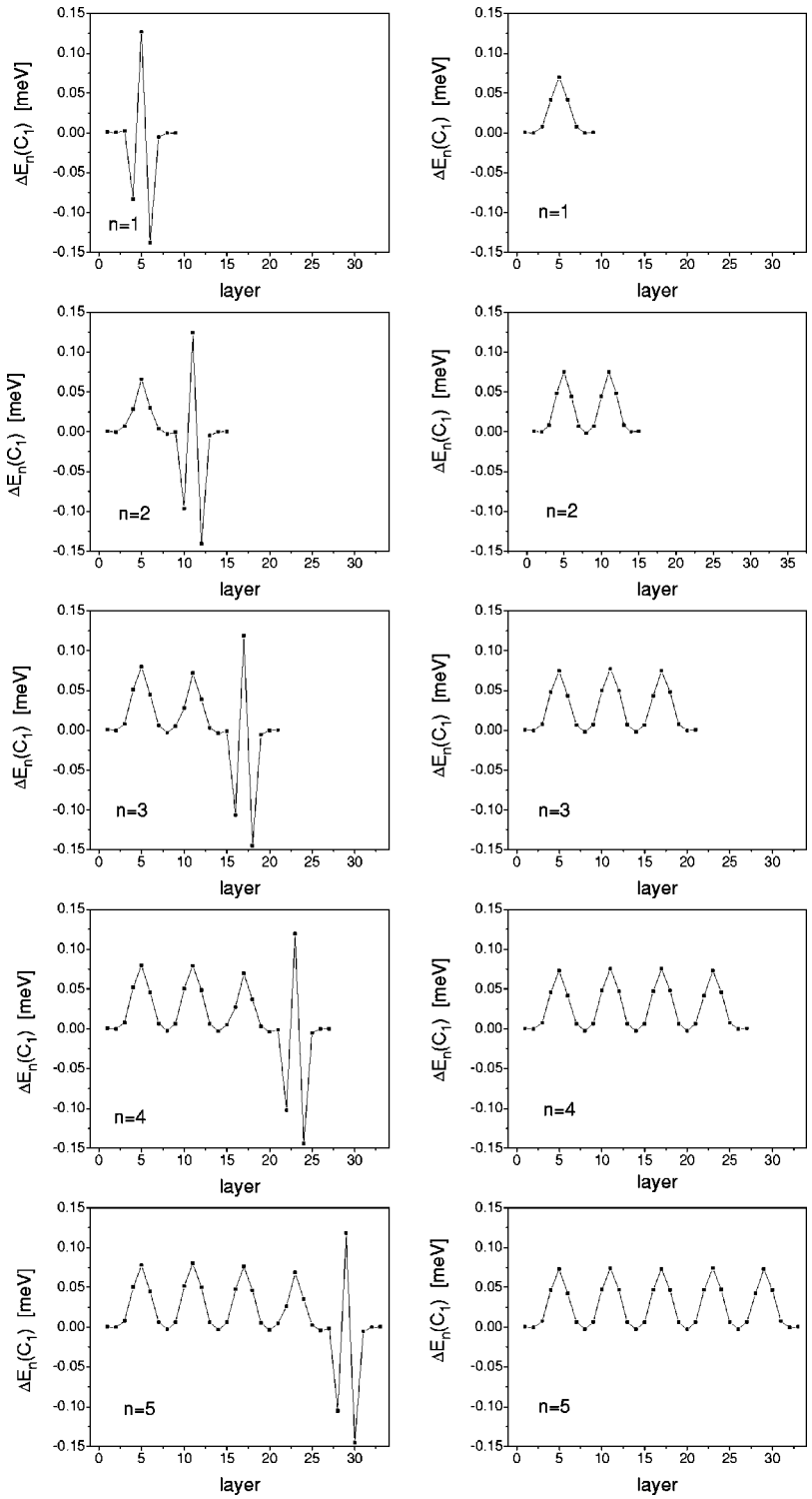

FIG. 1. Layer-resolved band energy contribution to the magnetic anisotropy energy $\Delta E_p(\mathcal{C}_1)$ in $(Cu_3Ni_3)_n$ multilayers on Cu(100). Left: free surfaces Cu(100)/$(Cu_3Ni_3)_n$/Vac, right: semi-infinitely capped surfaces Cu(100)/$(Cu_3Ni_3)_n$/Cu(100). The number of repetitions n is marked explicitly.

systems. Obviously, odd and even number of repetitions display a different kind of boundary conditions: for odd n periods of 12 are terminated symmetrically due to an inversion with respect to the geometrical center of the multilayer, whereas for even n this is not possible. Therefore, in Fig. 2(a) the entries corresponding to odd n's have a symmetric shape, while those corresponding to an even number of repetitions are asymmetric with a peak of positive sign at the right-hand-side boundary. Note that for even n's the shapes of $\Delta E_p(\mathcal{C}_2)$ in Fig. 2(a) will be reversed with respect to the labeling of layers if the orientation of magnetic moments is reversed simultaneously in each layer. It is easy to guess that for $n \geqslant 9$ the pattern to be seen follows the one shown in the right column of Fig. 2(a).

As can be seen from Fig. 2(b), for free surfaces a similar pattern as illustrated in Fig. 2(a) applies: for odd n the con-

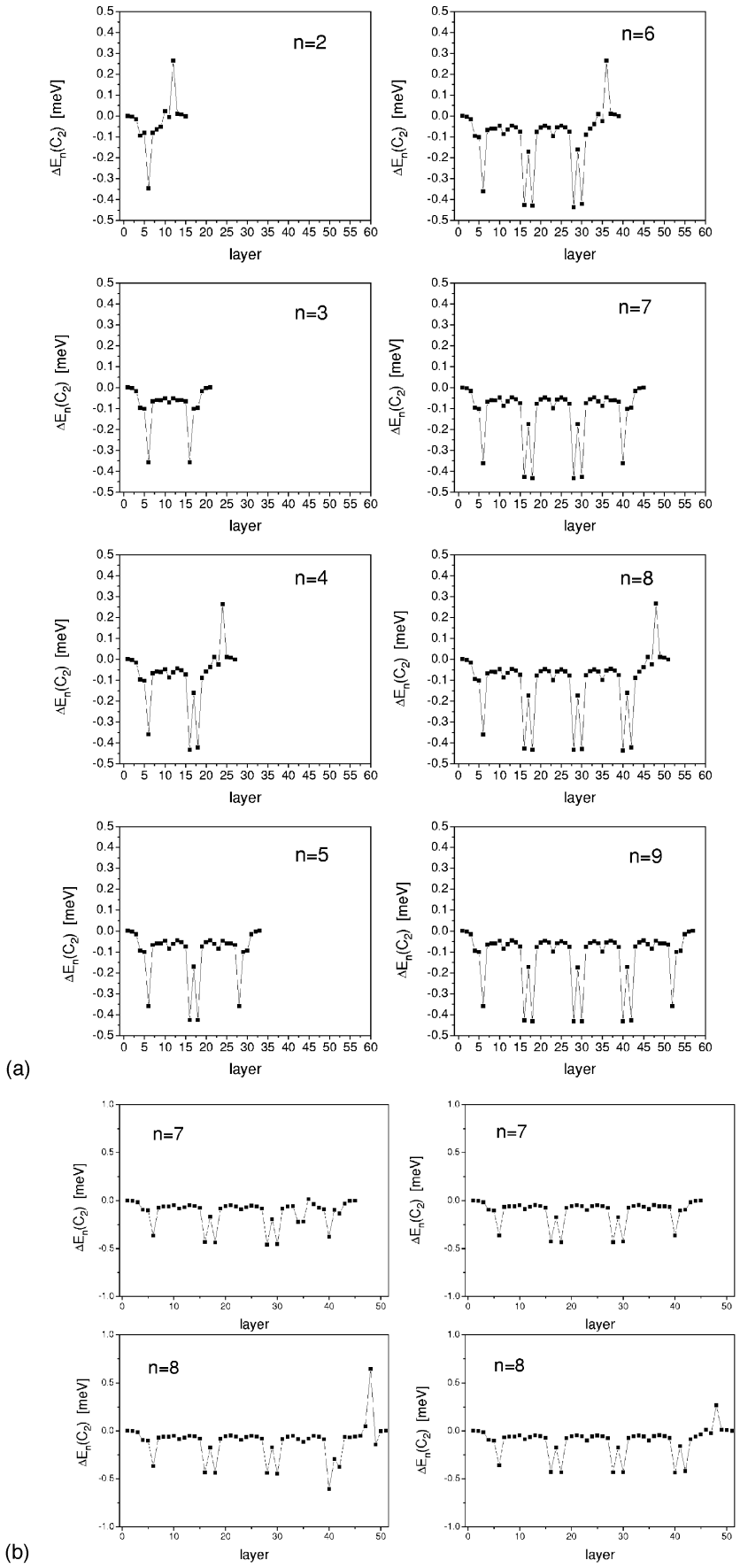

FIG. 2. Layer-resolved band energy differences for antiparallel interface exchange coupling $\Delta E_p(\mathcal{C}_2)$ in the case of (a) Cu(100)/$(Cu_3Ni_3)_n$/Cu(100) and (b) for $n=7,8$ for free surfaces Cu(100)/$(Cu_3Ni_3)_n$/Vac (left side) and for semi-infinitely capped surfaces Cu(100)/$(Cu_3Ni_3)_n$/Cu(100) (right side). The number of repetitions n is marked explicitly.

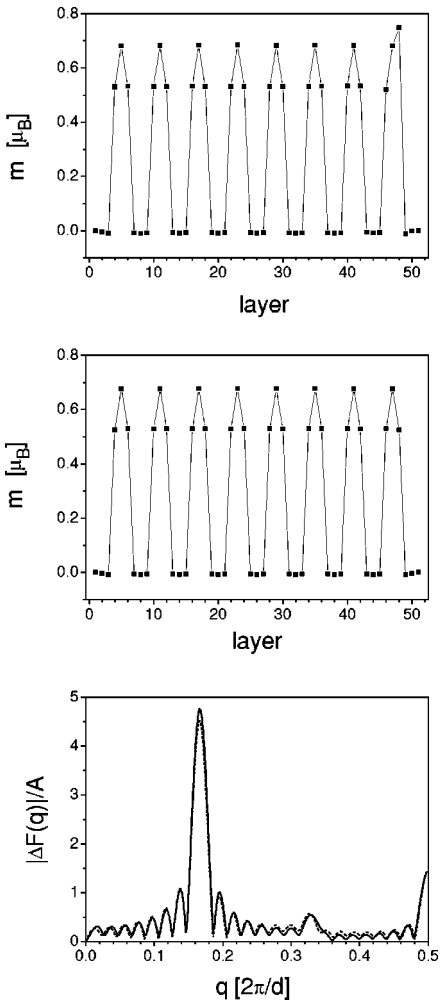

FIG. 3. Magnetic moments in $(Cu_3Ni_3)_8$ multilayers on Cu(100). Top: free surface, middle: capped surface, bottom: absolute value of the discrete Fourier transformation $A^{-1}|\Delta F(q;\mathcal{C}_1)|$ of the magnetic moments for the free surface (dashed line) and the capped surface (solid curve).

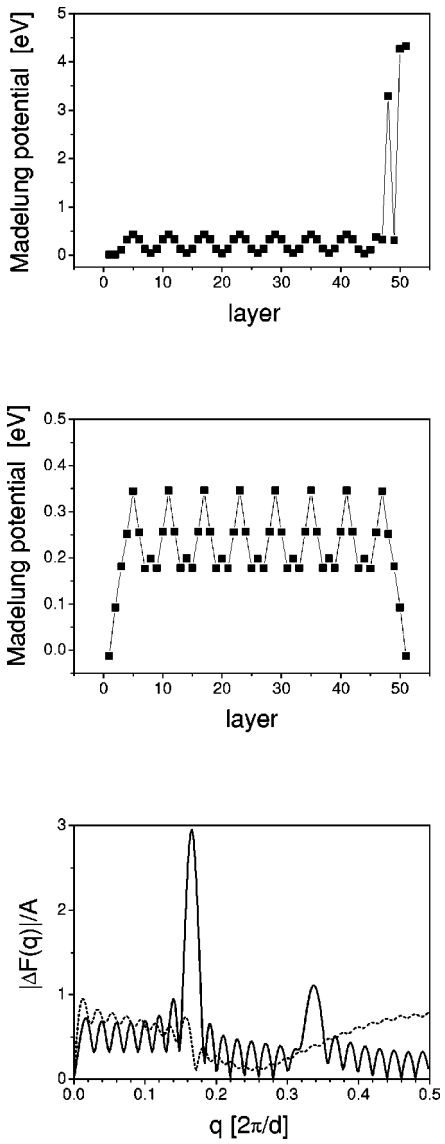

FIG. 4. Layer-dependent Madelung constants in $(Cu_3Ni_3)_8$ multilayers on Cu(100). Top: free surface, middle: capped surface, bottom: absolute value of the discrete Fourier transformation $A^{-1}|\Delta F(q;\mathcal{C}_1)|$ of the layer-dependent Madelung constants for the free surface (dashed line) and the capped surface (solid curve).

tributions from the two boundaries of the multilayer remain approximately equal in size and identical in sign, whereas for even n the surface induces a much bigger perturbation than for an odd n.

The above features of multi-interface exchange coupling are also characteristic for the pattern of $\Delta E_p(\mathcal{C}_3)$ (not shown), i.e., for the case of layer-resolved band energy contributions to the perpendicular interface coupling, whereby the peaks are about half as big as those in Figs. 2(a) and 2(b).

B. Magnetic moments and Madelung potentials

In Figs. 3 and 4 one particular case, namely, $n=8$, is examined in some detail. Figure 3 shows the distribution of magnetic moments for free and capped surfaces corresponding to the reference configuration $\mathcal{C}_0$ and their discrete FT's. As to be expected near the surface the Ni moment is slightly enhanced, however, in terms of the distribution of magnetic moments in the multilayer system, the free surface case differs only very little from that of the capped surface. This is directly mapped in the corresponding discrete FT's: in both cases a strong peak at $q=1/6$ is seen, the difference in peak heights being only marginal. As to be expected with increasing n the width of this peak shrinks and its height increases, while simultaneously—due to the increasing number of terms summed over—the background reduces.

A completely different pattern arises when considering the distribution of Madelung potentials corresponding to the reference configuration $\mathcal{C}_0$ (Fig. 4). Clearly enough in terms of electrostatics a remarkable perturbation at a surface has to be encountered, however, it is somewhat surprising to see that for the free surface in the discrete FT of the layer-resolved Madelung potentials the peak at $q=1/6$, which characterizes the capped system, is completely whipped out. It should be noted that in the latter case also a kind of ''aliasing'' at $q=1/3$, i.e., a period of 3 can be seen. In particular Fig. 4 illustrates and explains quite convincingly the different behavior of free and capped surfaces in Fig. 1 and Fig. 2(b).

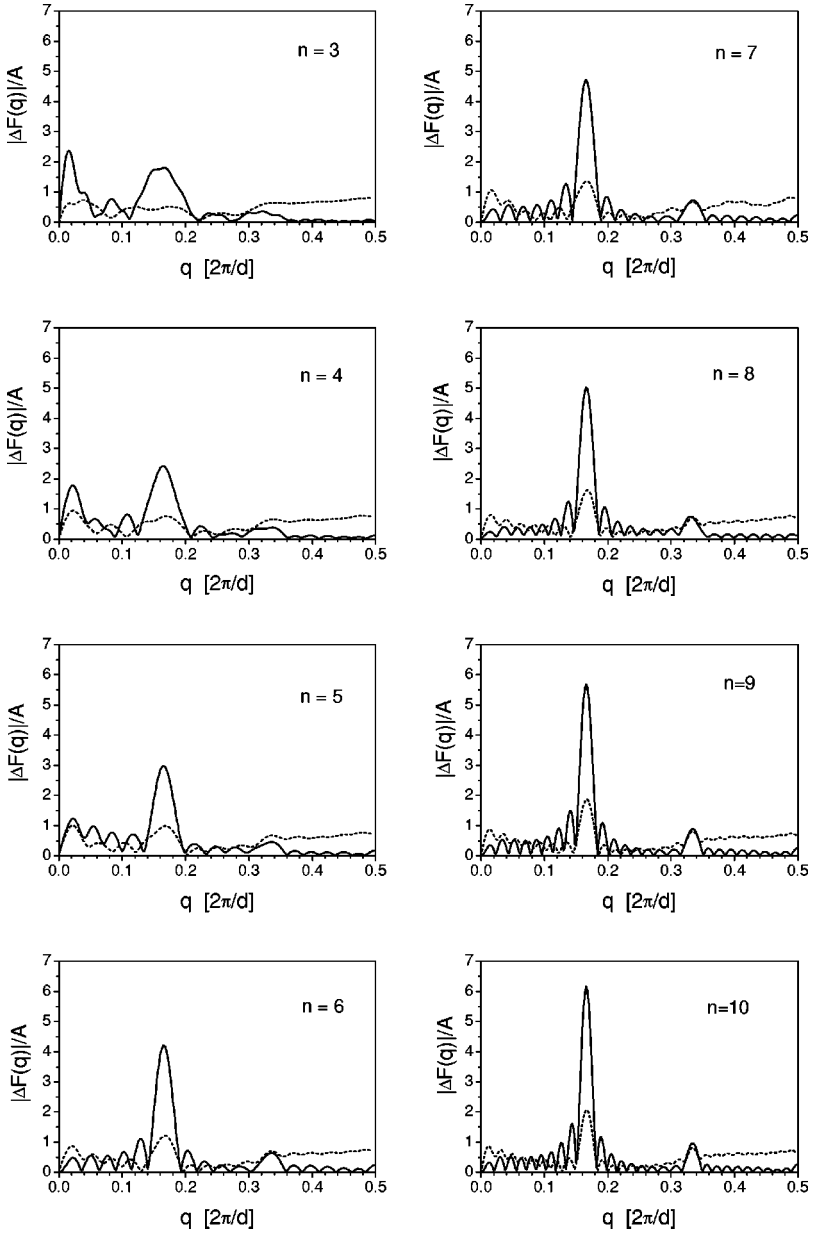

FIG. 5. Absolute value of the discrete Fourier transformation $A^{-1}|\Delta F(q;\mathcal{C}_1)|$ of the band energy contribution to the magnetic anisotropy energy for free surfaces (dashed lines) and capped surfaces (solid curves). The number of repetitions n is marked explicitly.

C. Discrete Fourier transformations of layer-resolved band energy differences

For $n \leqslant 10$ the discrete FT's of $\Delta E_p(\mathcal{C}_1)$ are displayed in Fig. 5 for free and capped surfaces. In this figure one can see that for capped surfaces with increasing n the peak at $q=1/6$ gets substantially sharper, while in the case of free surfaces—even after 10 repetitions—this peak is still rather weak and quite some intensity remains for $q>0.3$. For reasonably large n the capped surfaces obviously show a well-defined period of 6, whereas for free surfaces the presence of the interface to the vacuum almost prevents such a periodicity (see also Figs. 1 and 4).

In the discrete FT's of $\Delta E_p(\mathcal{C}_2)$ (Fig. 6) several rather well-developed peaks emerge with increasing n, namely, at $q=1/12$, 1/6, 1/3, 0.41, and 1/2. The main periods of 6 and 12 obviously reflect the number of atomic layers per building block and the geometrical arrangement of the orientations of the magnetization, since in every second building block the same orientation of the magnetic field applies. Somewhat surprising is that also a period of about 2.5 ($q=0.41$) can be seen, which quite likely refers to the so-called short period recorded in magnetic systems with a Cu spacer,[22,23] and which in the asymptotic limit frequently is related to a particular vector of the Fermi surface of fcc Cu.[22,24] At first glance for $n \geqslant 8$ the difference between free and capped surfaces seems to become unimportant. However, a closer inspection of the peak at $q=1/2$ shows that (a) for odd numbers of repetitions the peak height is considerably larger than for even numbers and (b) for odd n there is almost no difference between free and capped surfaces, while for even n a clear difference exists. Going back to Figs. 2(a) and 2(b) one can correlate this particular peak to the peaks in the layer-resolved quantities near the interfaces, which with alternating n alternate in sign. In particular from Fig. 2(b) it is clear

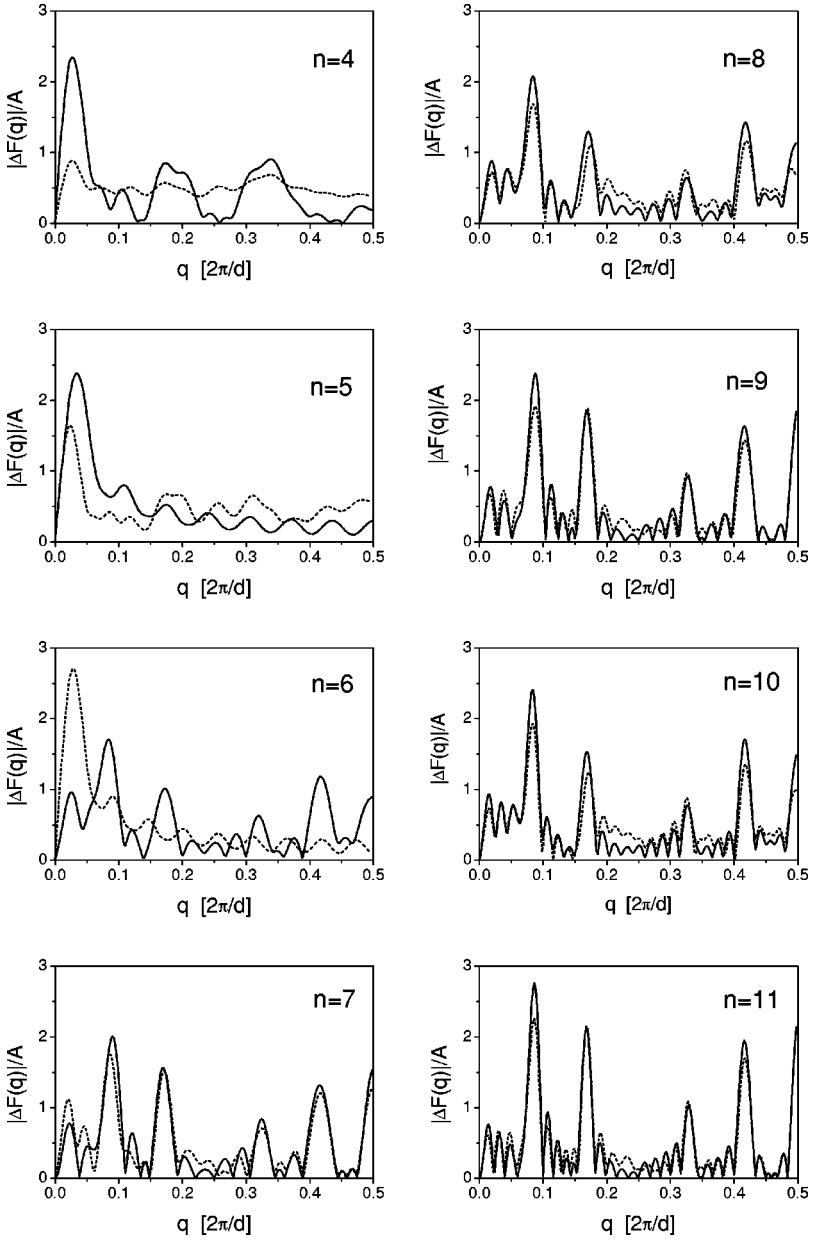

FIG. 6. Absolute value of the discrete Fourier transformation $A^{-1}|\Delta F(q;\mathcal{C}_2)|$ of the band energy contribution to the antiparallel interface exchange coupling energy for free surfaces (dashed lines) and capped surfaces (solid curves). The number of repetitions n is marked explicitly.

that for odd n the difference between free and capped surfaces is much smaller than for an even number of repetitions.

In Fig. 7 the results for the discrete FT's of the layer-resolved band energy differences due to perpendicular multi-interface exchange interactions are compiled. As one can see there is one prominent peak at $q=1/12$ evolving with increasing n. As compared to Fig. 6 the peaks at $q=1/6$ and 0.41 are less pronounced, while those at $q=1/3$ and 1/2 are of about the same peak heights. Unlike in the case of antiparallel interface exchange coupling the height of the peak at $q=1/2$ does not oscillate with respect to even and odd numbers of repetitions.

In comparing Figs. 5–7 the discrete FT's reveal periods of 6 (building block) in the case of the anisotropy energy, and of 12 (arrangement of the orientations of the magnetization) for the interface coupling situation. Quite obviously, if a period of 12 occurs (aliasing) signals corresponding to periods of 6 and 3 show up.

D. Energetic contributions per repetition

In Fig. 8 the total band energy contribution to the anisotropy energy, and to the two types of multi-interface exchange coupling are shown together with the corresponding quantity per repetition. In the case of capped surfaces $\Delta E(\mathcal{C}_1)/n$ is already a constant for $n \geqslant 8$, while for free surfaces the values for $\Delta E(\mathcal{C}_1)/n$ still go slightly up with increasing n. Since for an increasing number of repetitions $\Delta E(\mathcal{C}_1)/n$ asymptotically becomes a constant, this particular quantity, namely, $\Delta E(\mathcal{C}_1)/n$, then has to be called periodic in n. Stated differently, this implies that even for capped

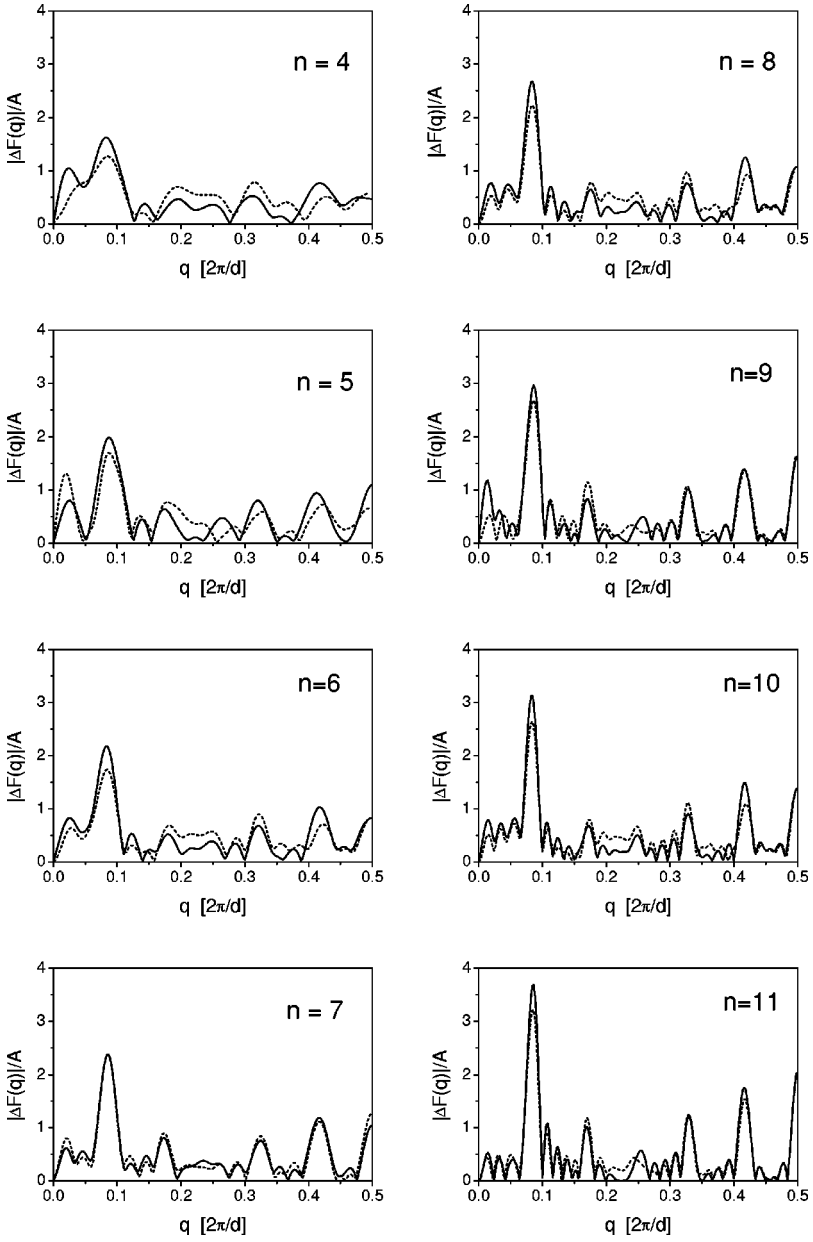

FIG. 7. Absolute value of the discrete Fourier transformation $A^{-1}|\Delta F(q;C_3)|$ of the band energy contribution to the perpendicular interface exchange coupling energy for free surfaces (dashed lines) and capped surfaces (solid curves). The number of repetitions n is marked explicitly.

surfaces such repeated multilayer systems have to be at least as thick as about 150 a.u. in order to justify a ''periodic'' approach.

For antiparallel and perpendicular multi-interface exchange coupling the total band energy per repetition shows oscillatory behavior with respect to n. In both cases a period of two can be read off from the corresponding entries in Fig. 8. Quite clearly $\Delta E(\mathcal{C}_2)/n$ and $\Delta E(\mathcal{C}_3)/n$ are not periodic in n, since their values oscillates with n. These oscillations seem to fit very well the theoretical predictions made by Aristov[25] in discussing indirect Ruderman–Kittel–Kasua–Yosida (RKKY) interactions.

In view of the period of 12 occurring in the FT's in Figs. 6 and 7, it is intriguing to consider multilayers of the type $(Cu_3Ni_3)_{2n}$, i.e., to double the building block (unit cell) and then relate the total band energy to n. Clearly enough such a representation no longer results in an oscillating quantity. However, as shown in Fig. 9 the convergence of $\Delta E(\mathcal{C}_2)/n$ and $\Delta E(\mathcal{C}_3)/n$ with respect to n is far from convincing. Even for a multilayer thickness of about 200 a.u., these two quantities have not reached a constant value.

E. Comparison to experiment

Experimentally mostly free surfaces of Ni on Cu(100) were investigated,[26–29] including in some cases surfaces capped by Cu.[27] For less than 7 monolayers (ML) of Ni the orientation of the magnetization is in-plane,[29] above 8 ML a reorientation transition to a perpendicular orientation occurs. For thin films a tetragonal distortion of the parent substrate fcc lattice was suggested,[1] while for thick Ni films the magnetic moments vary with film thickness, having a maximum

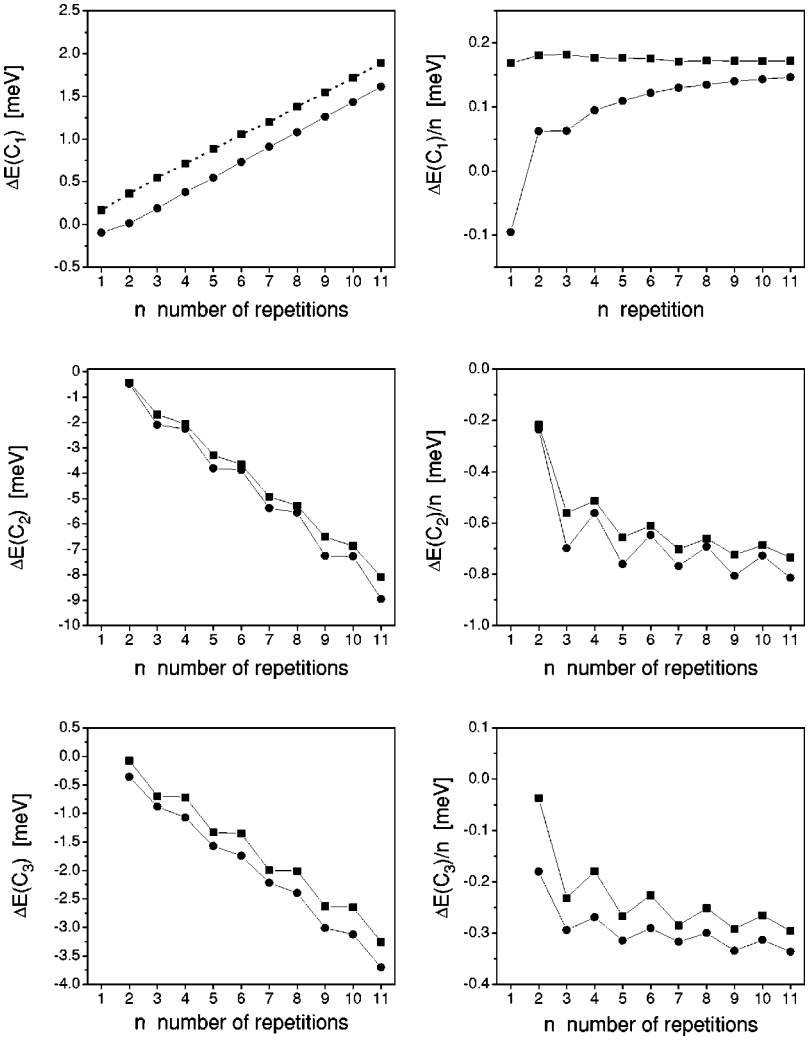

FIG. 8. Band energy contribution to the magnetic anisotropy energy (top), the antiparallel interface exchange coupling energy and the perpendicular interface exchange coupling energy for free surfaces (circles), and capped surfaces (squares) for $(Cu_3Ni_3)_n$ multilayers on Cu(100). The right column shows the corresponding quantity per repetition.

at a nominal thickness of about 100 Å.[30] There seem to be no experimental results for repeated multilayer systems like the one investigated in this paper.

IV. CONCLUSION

In the present paper we tried to address two important questions connected with physical properties of multilayer systems, namely, (1) is there a characteristic volume (unit cell) such that when repeated a particular quantity stays constant and (2) are there pronounced peaks in the discrete FT of the corresponding layer-resolved quantity with respect to the interlayer distance that suggest an almost Bloch periodic behavior in the direction of the surface normal. Quite clearly in the presence of three-dimensional translational symmetry unit cells and (three-dimensional) Bloch periodicity are automatically provided. At least for the systems and properties chosen here, no straightforward answer can be given. Free surfaces differ considerably from surfaces capped semi-infinitely with Cu(100). As was shown recently[31] different cap materials can induce, e.g., large effects in the anisotropy energy, just as a variation of the cap thickness can cause oscillations of the interface exchange coupling energy.[32] In view of these facts it has to be stated that only two, very specific types of systems have been considered. For the band energy part of the anisotropy energy it was found that repeated multilayer systems have to be at least 150–200 a.u.

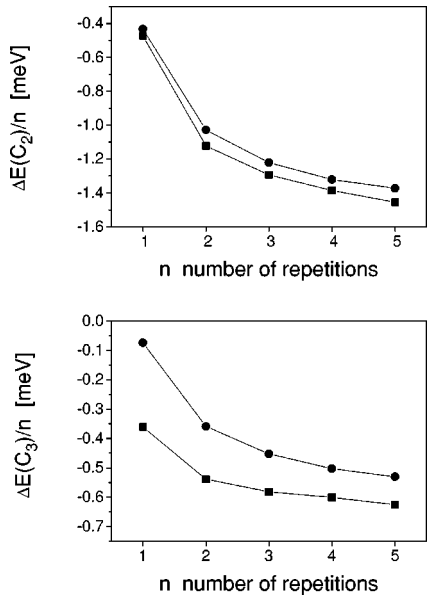

FIG. 9. Band energy contribution to the antiparallel (top) and perpendicular (bottom) interface exchange energy per repetition for $(Cu_3Ni_3)_{2n}$ multilayers on Cu(100). Free surfaces: circles; capped surfaces: squares.

thick to permit the use of a unit cell in practical terms. For multi-interface exchange interactions this thickness has to be almost twice as big.

The discrete FT's prove that with a few repetitions of (Cu_3Ni_3), namely, $n>6$, periods can be traced mapping the number of layers per repetition (6) or of the characteristic sequence of the orientation of the magnetization (12): the peak positions stay constant, whereas the peak heights and widths change when increasing n.

The present paper also shows that any interpretation of experimental results in terms of fitting models based on periodicity along the surface normal have to be used with extreme care. It might very well turn out that such models are only helpful for reasonably thick multilayers, namely those with a thickness of several hundred a.u. This in turn is exactly the regime where supercell calculations, i.e., computational schemes using three-dimensional translational symmetry, will be very useful. For thin multilayer systems, however, even a colloquial use of periodicity along the growth direction can obscure considerably the physics to be seen.

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