Reorientation transition in Cu(100)/Ni/Co

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The magnetic anisotropy energy of Cu(100)/Ni/Co_m, $0 \leqslant m \leqslant 5$, is calculated using the spin-polarized fully relativistic screened Korringa-Kohn-Rostoker method for layered systems. The Ni film was divided into two regions, one consisting of Ni layers epitaxially grown on Cu(100) and tetragonally relaxed with a c/a ratio of 0.945 and, subsequently a transient region subject of strain relaxation, the other one consisting of Ni layers corresponding to a fcc Ni parent lattice. For both regions, separate calculations were performed and then combined with each other on the basis of an analysis of layer decomposed contributions to the anisotropy energy. By varying the thickness of both regions the critical (total) thickness for the reorientation transition of the magnetization from perpendicular to in-plane is determined. Capping the Ni film with Co is found to show an unexpected behavior: the number of Ni layers, at which the reorientation occurs, is first increased until 2 ML of Co are added and then decreases rapidly with the addition of more Co layers. This feature is mainly attributed to changes in the band part of the anisotropy energy induced by the Ni/Co interface as seen in terms of layer-resolved contributions.

It was shown both experimentally[1] and theoretically[2,3] that beyond 7 layers of Ni in the system Cu(100)/Ni the magnetization is perpendicularly oriented, whereby in comparison to the parent fcc lattice of the Cu substrate the Ni interlayer distance is compressed by -5.5%. By capping Ni films with Co measurements revealed that the orientation of the magnetization switches to in-plane with an increasing number of Co layers. Epitaxial Cu(100)/Ni(8 Å)/Co(2–10 Å)/Ni(17 Å)/Cu structures, e.g., did not show a perpendicular magnetic anisotropy, in fact, 2 Å Co turned out to be the critical thickness for a perpendicular magnetization. These findings were thought to result from the Co magneto-elastic volume anisotropy due to strain.[4] Furthermore, the system Si(100)/Cu(1000 Å)/Ni(60 Å)/Co(step-wedge)/Cu(30 Å) was studied[5] in an attempt to control the critical thickness for the perpendicular magnetization: it was found that the magnetization turns in-plane at a critical Co thickness of 6.15 ± 1.25 Å. As reported by O'Brien *et al.*[6] strain relaxations in the Ni layers set in beyond about 13 of the (-5.5%) uniformly relaxed Ni layers.

In the present paper the fully relativistic spin polarized screened Korringa-Kohn-Rostoker (SKKR) method[7,8] is applied to provide a theoretical description of the reorientation transitions in the ground state of the Cu(100)/Ni/Co system. In order to treat layer relaxation, the occurring screened structure constants[10,11] have been derived for a system of layers sharing only the same in-plane translational symmetry,[12] but otherwise can differ in the respective interlayer distance. Making use of two-dimensional lattice Fourier transformations[13] requires, however, that one and the same two-dimensional lattice has to apply for all layers under consideration. Different in-plane lattice spacings can therefore at present only be handled using a ''physically motivated'' model. For this reason we considered two independent subsystems with different in-plane lattice constants to be combined by demanding that in corresponding layers the characteristic quantities, namely the layer-resolved band energy contributions to the magnetic anisotropy energy (MAE) and the magnetic moments, coincide in value.

In Table I different model systems (A–D) are characterized together with *system E* which is supposed to reflect the experimental situation. In the present paper an attempt is made to describe the MAE of *system E* by combining *system A*, namely $Cu(100)/Ni_{15}(-5.5\%)/Ni_{12}(0\%)$, containing a $Cu(100)/Ni(-5.5\%)$ and a $Ni(-5.5\%)/Ni(0.0\%)$ interface with *system D*, i.e., with $Ni(100)/Ni_{12}(0\%)/Co_m$, $0 \leqslant m \leqslant 5$, containing a free Ni surface (for $m=0$) or a Ni/Co interface and a free Co surface ($m>0$). Note that for *system A* the percentages in the parentheses denote tetragonal relaxations relative to an fcc Cu parent lattice ($a_0 = 6.8309$ a.u.), while for *system D*, an fcc Ni(100) parent lattice ($a_0 = 6.6590$ a.u.) with no tetragonal relaxation was assumed. In reality, in Cu(100)/Ni/Co_m, see *system E* in Table I, the in-plane lattice constant of the Ni layers relaxes beyond a region of pseudomorphic growth in which all layers are uniformly relaxed by -5.5% (with respect to fcc Cu), to the in-plane lattice constant and interlayer distance of fcc Ni(100). Comparisons to *systems B* and *C* are made in order to confirm the validity of our approach and also visualize the spatial extend of the $Ni(-5.5\%)/Ni(0.0\%)$ interface.

The spin-polarized local density functional as parametrized by Vosko *et al.*[9] was used to perform selfconsistent

TABLE I. Systems under consideration. The substrate determines the in-plane lattice constant, the relaxation of the substrate interlayer distance is given in percent.

System A: [fcc Cu(100)]	System B: [fcc Cu(100)]	System C: [fcc Ni(100)]	System D: [fcc Ni(100)]	System E: [fcc Cu(100)]
$\begin{bmatrix} Cu_1 \\ \vdots \quad 0\% \\ Cu_3 \end{bmatrix}$	$\begin{bmatrix} Cu_1 \\ \vdots \quad 0\% \\ Cu_3 \end{bmatrix}$			$\begin{bmatrix} Cu_1 \\ \vdots \quad 0\% \\ Cu_3 \end{bmatrix}$
$\begin{bmatrix} Ni_1 \\ \vdots \quad -5.5\% \\ Ni_{15} \end{bmatrix}$	$\begin{bmatrix} Ni_1 \\ \vdots \quad -5.5\% \end{bmatrix}$	$\begin{bmatrix} Ni_1 \\ \vdots \quad 0\% \end{bmatrix}$	$\begin{bmatrix} Ni_1 \\ \vdots \quad 0\% \end{bmatrix}$	$\begin{bmatrix} Ni_1 \\ \vdots \quad -5.5\% \\ Ni_{n1} \end{bmatrix}$
$\begin{bmatrix} Ni_1 \\ \vdots \quad 0\% \\ Ni_{12} \end{bmatrix}$	$\begin{bmatrix} \vdots \quad -5.5\% \\ Ni_{21} \end{bmatrix}$	$\begin{bmatrix} \vdots \quad 0\% \\ Ni_{18} \end{bmatrix}$	$\begin{bmatrix} \vdots \quad 0\% \\ Ni_{12} \end{bmatrix}$	$\begin{bmatrix} Ni_1 \\ \vdots \quad 0\% \\ Ni_{n2} \end{bmatrix}$
			$\begin{bmatrix} Co_1 \\ \vdots \quad 0\% \\ Co_m \end{bmatrix}$	$\begin{bmatrix} Co_1 \\ \vdots \quad 0\% \\ Co_m \end{bmatrix}$
[vac]	[vac]	[vac]	[vac]	[vac]

calculations for the effective potentials and effective exchange fields with a uniform orientation of the magnetization perpendicular to the planes. Here a cutoff of $l_{max}=2$ in the angular momentum space is applied and we used typically 45 $k_{\|}$ points in the irreducible part of the surface Brillouin zone (ISBZ) to achieve self-consistency. In all cases 3 layers of Cu served as ''buffer'' at the Cu/Ni interface and at least two ''empty'' layers as ''buffer'' to the Co/Vacuum interface. It is important to note that the ideal semi-infinite Cu bulk and vacuum regions are properly taken into account within the SKKR method.

The magnetic anisotropy energy ΔE_a, defined as the energy difference between a uniform in-plane and a uniform perpendicular orientation of the magnetization of the system,

$$\Delta E_a = E(\|) - E(\perp), \tag{1}$$

was obtained[7,8] by making use of the force theorem, namely as a sum of the respective band energy difference ΔE_b and the magnetic dipole-dipole energy contribution ΔE_{dd},

$$\Delta E_a = \Delta E_b + \Delta E_{dd}. \tag{2}$$

The band energy difference ΔE_b can be split up into layer-resolved band energy differences ΔE_b^n,

$$\Delta E_b = \sum_{n=1}^{N} \Delta E_b^n, \tag{3}$$

where N denotes the total number of atomic layers considered. When evaluating ΔE_b, Eq. (3), again a cutoff of $l_{max}=2$ was used, however, 325 $k_{\|}$ points in the ISBZ was taken to ensure reliable convergency. Note that, following Eq. (1), positive or negative values of ΔE_a refer to perpendicular or in-plane magnetization of the system, respectively.

In Fig. 1 the layer-resolved band energy anisotropies are displayed for the uncapped systems. Following the observations made also in other systems, see, e.g., Ref. 14, the basic idea of our approach is to group ΔE_b^n into contributions from the surface, the interfaces and interior layers, in which the ΔE_b^n are approximately constant. On top of Fig. 1 *system A* and *B* are compared by viewing both systems from the Cu substrate (left-hand side). Evidently, the ΔE_b^n of the first 13 Ni layers from the left (Cu/Ni interface) in *system A* hardly differ from those of *system B*. At the bottom of Fig. 1 *system A* is compared to *system C* by viewing from the vacuum (right-hand) side. Apparently again, the first 12 ΔE_b^{Ni} from the right in *system A* are very close in value to those of *system C*. It is therefore obvious that in *system A* a transition region of about three layers can be identified (see thick vertical lines in Fig. 1) between a regime of layers corresponding to an in-plane lattice constant of fcc Cu and by a 5.5% contracted interlayer spacing (*regime 1*) and a regime of layers corresponding to a parent fcc Ni lattice (*regime 2*) as outside of this transition region the ΔE_b^{Ni} seem to be unaffected by the interface between *regime 1* and *regime 2* (labeled by boxes in Fig. 1). It should be noted that in the present study an abrupt change from the relaxed to unrelaxed Ni regions is assumed. From Fig. 1 follows also that this assumption causes an almost linear behavior of the ΔE_b^{Ni} in the crossover region from *regime 1* to *regime 2*. Therefore, for a continuous structural transition we expect this region of layers to be somewhat broader, but not to modify the MAE of the whole system drastically.

Figure 1 also shows that for layers in the interior of *regime 1* (layers further than 8 layers from the Cu/Ni interface) the corresponding ΔE_b^{Ni} are nearly constant (~ 0.09 meV). Addition of such a Ni layer to *system A* would increase ΔE_b of the corresponding system, i.e., $Cu(100)/Ni_{16}(-5.5\%)/Ni_{12}(0\%)$ by the same amount. Since furthermore the layer-resolved magnetic moments (not shown in here) for such layers remain practically constant, ΔE_{dd} and, consequently, also ΔE_a [see Eq. (2)] for these systems can easily be estimated as a function of n_1, that is the number of tetragonally relaxed Ni layers. Although some oscillations of ΔE_b^{Ni} can be observed for layers in the interior of *regime 2*

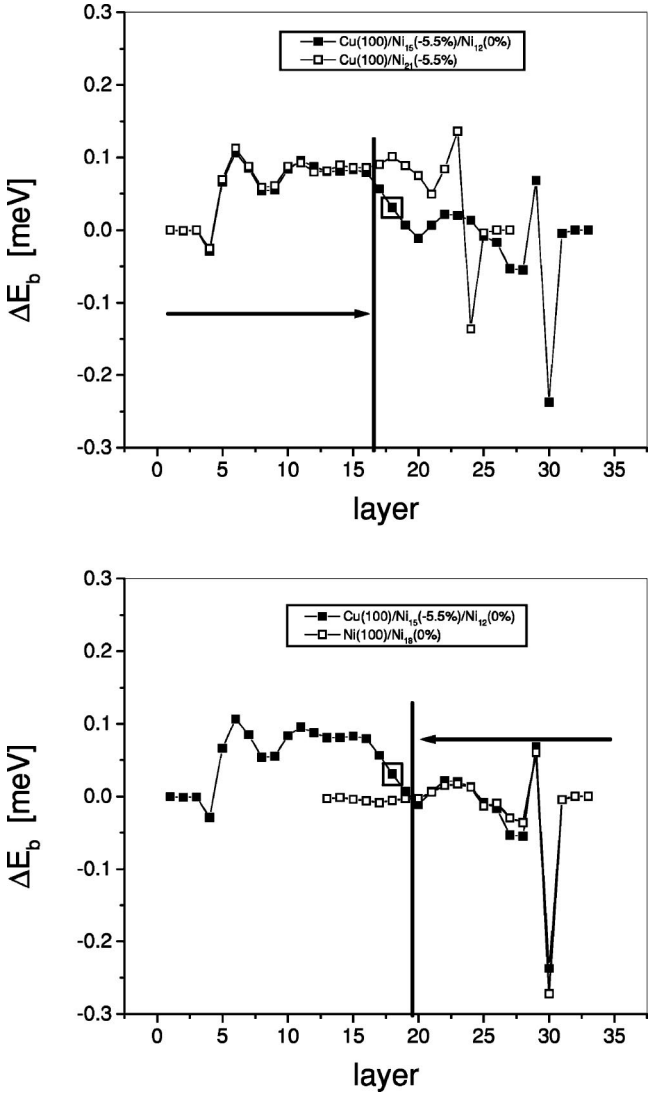

FIG. 1. Comparison of the layer-resolved band energy contributions ΔE_b^n of $Cu(100)/Ni_{15}(-5.5\%)/Ni_{12}(0.0\%)$ (*system A*, squares) with $Cu(100)/Ni_{21}(-5.5\%)$ (*system B*, open squares, top), and in $Ni(100)/Ni_{18}$ (*system C*, open squares, bottom). In all cases the first layers to the right denote vacuum layers. In the case of *system A* the first three layers to left refer to Cu layers. The view from the Cu/Ni and from the Ni/Vac interface is indicated by arrows. The small boxes denote the last relaxed Ni layer in *system A*.

(layers further than 10 layers from the surface in *system C*), on the average for those layers the corresponding $\Delta E_b^{Ni} \simeq 0$. Since for ΔE_{dd} similar arguments apply as above, at least for $n_2 > 10$, ΔE_a for *system C* can be approximated quite reasonably as a function of n_2 (number of Ni layers with geometry of a parent fcc Ni lattice). By combining then the contributions to the MAE of *systems A* and *C* we get an estimate of ΔE_a for *system E* ($m=0$) as a function of $n_1(>8)$ and $n_2(>10)$, which in turn is based on the observation that in the interior of *regime 1* and of *regime 2* the relevant physical quantities, namely the ΔE_b^{Ni} and the corresponding magnetic moments, are nearly constant.

Let us turn to the calculated magnetic anisotropy energies for the system with a Co cap. It is important to mention that for thicker Co caps ($m>3$) the Ni and Co moments at the Ni/Co interface are only slightly enhanced (0.69 μ_B and 1.7

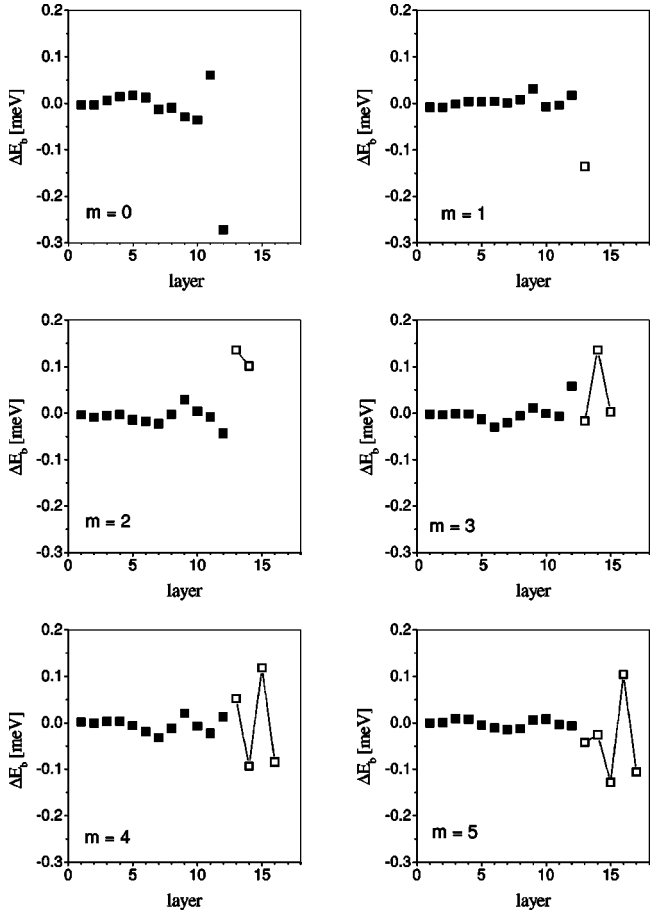

FIG. 2. Layer resolved band energy difference ΔE_b^n for free surfaces of 0 to 5 Co layers on $Ni(100)/Ni_{12}(0\%)$. Full and open squares denote Ni and Co layers, respectively.

μ_B) with respect to their corresponding bulk values (fcc Ni: 0.68 μ_B and fcc Co: 1.66 μ_B). This presumably implies that due to very similar (minority) *d*-bands of Co and Ni, the Ni/Co interface hardly modifies the electronic structure of the two constituents. Consequently, because of different boundary conditions, a free surface of Ni and a Ni slab capped by Co can be expected to show distinct differences for the MAE. In Fig. 2, which shows the layer resolved contributions to ΔE_b in *system D* ($0 \leqslant m \leqslant 5$), one can see that capping with Co drastically changes the contributions of Ni at the surface (for $m \geqslant 1$ at the Ni/Co interface): the large negative ΔE_b of the surface Ni layer becomes much less in magnitude and also changes sign when capped by additional Co layers. The contributions of the individual Co layers vary also rapidly: when increasing the number of Co layers this obviously results in a maximum of ΔE_b^{Co} for $m=2$. This kind of changes in the MAE have been seen in many cases in thin films when varying the thickness of the film or of the capping overlayer and were attributed to surface induced interfacial hybridizations in the electronic structure leading to anomalous perpendicular anisotropy.[15]

In addition, far from the Ni/Co interface, i.e., in the interior of *regime 2* as defined above, the small ΔE_b^{Ni} are hardly affected by the number of capping Co layers *m*. Therefore, ΔE_a of *system E* ($m>0$) can be obtained as a function of n_1 and n_2 as well as of *m* by combining *systems A* and *D* in a similar way as described before. For $n_1=13$ and $n_2=17$ the

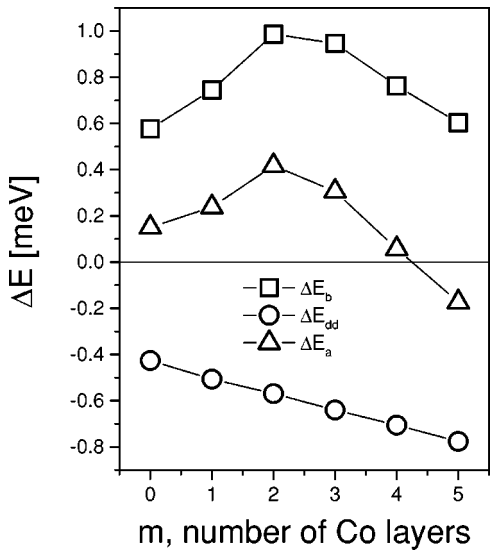

FIG. 3. Calculated band energy, ΔE_b and magnetic dipole-dipole energy contributions, ΔE_{dd} to the total magnetic anisotropy energy, ΔE_a in $\mathrm{Cu(100)/Ni}_{13}(-5.5\%)/\mathrm{Ni}_{17}(0\%)/\mathrm{Co}_m$.

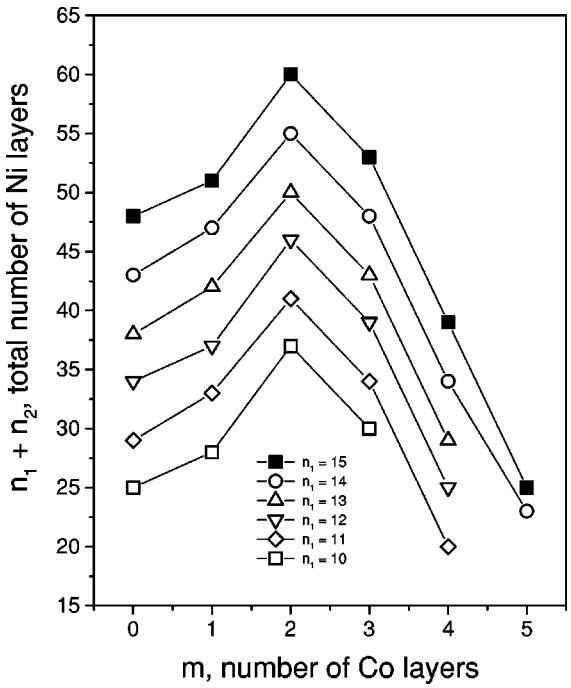

FIG. 4. Total number of Ni layers (n_1+n_2) at which the magnetic anisotropy energy, ΔE_a of $\mathrm{Cu(100)/Ni}_{n_1}(-5.5\%)/\mathrm{Ni}_{n_2}(0\%)/\mathrm{Co}_m$ changes sign, displayed as a function of the number of Co layers (m).

calculated results for ΔE_b, ΔE_{dd}, and ΔE_a are displayed in Fig. 3 as a function of the number of the capping Co layers, m. Although, as to be expected, ΔE_{dd} decays monotonously, the dependence of ΔE_a with respect to m is clearly overruled by ΔE_b leading to a maximum at $m=2$ just mentioned.

Clearly, as a result of such calculations the total number of Ni layers, n, at which ΔE_a changes sign, i.e., at which a reorientation transition of the magnetization from perpendicular to in-plane occurs can be determined. By varying n_1 from 10 to 15, i.e., in the vicinity of the estimated value of 13,[6] this is shown in Fig. 4 as a function of m. One can obviously conclude that irrespective of the number of the tetragonally relaxed Ni layers (n_1), a maximum is reached at a coverage of 2 layers of Co, while by increasing further the number of capping Co layers the critical thickness rapidly decreases.

There are only a few experimental studies discussing the reorientation transition of the magnetization from perpendicular to in-plane in the system Cu(100)/Ni. Farle *et al.*[1] reported that the magnetization is in-plane above 41 ML of Ni, while O'Brien *et al.*[6] noted that this transition starts at 37 Ni layers and is of second order. Quantitative LEED measurements[16] and STM studies[17] confirmed a structural homogeneity up to 11 ML of Ni and a nearly perfect pseudomorphic growth of the relaxed layers. Furthermore, O'Brien *et al.*[6] observed that the coercive field of Ni on Cu shows a rapid rise at 13 ML of Ni indicating the formation of dislocations. It seems therefore that 13 ML of Ni is the critical thickness for the pseudomorphic region. Using this value for our n_1, for free surfaces of Ni on Cu(100) the present model predicts the (second) reorientation transition to occur at 38 Ni layers which is in excellent agreement with the above quoted value of 37 ML.

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