Anisotropy effects in switching the direction of the magnetization in a spin-valve system with exchange-bias pinning

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The electronic, magnetic, and electric transport properties of spin valves of the type Cu(111)/CoO/Co/Cu/Co/Cu(111) are investigated in terms of the local density functional theory by means of the fully relativistic screened Korringa-Kohn-Rostoker and the Kubo-Greenwood equation. This investigation concentrates on anisotropy effects for twisting energies and electric transport perpendicular to the planes of atoms. It is found that by rotating uniformly the orientation of the magnetization in the free layer with respect to the one in the pinned layer, for most of the spacer thicknesses considered (14–48 monolayers) the twisting energy shows strong deviations from a $(1-\cos\Theta)$ behavior, while the corresponding sheet resistances and the magnetoresistance do follow this simple law. Furthermore, it is shown that interdiffusion in the two atomic layers forming the Co/Cu interfaces is only of maginal importance for anisotropy effects in the twisting energies; however, it reduces—as to be expected—the magnetoresistance.

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I. INTRODUCTION

Twenty years after the introduction of digital versatile discs (DVD's) and about 15 years after the discovery of the giant magnetoresistance (GMR) effect[1,2] materials for optical and magnetic data storage still seem to be of topical interest.[3,4] For both types of recording magnetic anisotropy effects proved to be very important. In essence a typical GMR device consists of an antiferromagnetic (AF) part used to pin a rather thick magnetic layer that in turn is separated by a metallic spacer such as Cu [nonmetal in the case of the so-called tunneling magnetoresistance (TMR)] from a thin magnetic layer usually called a free layer. This stack of layers very often is covered by a cap. Of course an important detail is also the type of electric transport considered—namely, whether the electric current flows parallel to the planes of atoms [current in plane (CIP)] or perpendicular (CPP). The leads, which serve as electron reservoirs, are usually made from Cu. In principle the AF part can be any suitable material that combined with a metallic system produces a reasonably large exchange bias. The critical thickness of the AF part varies from about 400 Å in the case of NiO to only 80 Å for IrMn. The magnetic layers very often consist of Co/Fe alloys (hard magnets) and Ni/Fe alloys (soft magnets); the spacer material is usually Cu. In principle, in metallic spin valves the current can flow either CIP or CPP. In the case of TMR devices the spacer is a Al_2O_3 or MgO "barrier"; the geometry for electric transport is always CPP.

In the present paper a spin-valve-type system with a CoO AF part, which is known to show one of the largest exchange-bias effects,[5] is investigated in terms of the local density functional theory by means of a fully relativistic approach for the electronic, magnetic, and electric transport properties. This investigation concentrates on anisotropy effects and electric transport. Since CPP transport is assumed, the results obtained are applicable to changes of the orientation of the magnetization in the free layer caused by an external field or by applying a current perpendicular to the planes of atoms.

II. COMPUTATIONAL DETAILS

For all cases of the system $Cu(111)/Cu_6/(CoO)_{12}/Co_{24}/Cu_n/Co_6/Cu_{6+m}/Cu(111)$, $14 \leqslant n \leqslant 48$ (see Fig. 1), the parallel magnetic configuration was calculated self-consistently by means of the fully relativistic screened Korringa-Kohn-Rostoker method[6] making use of

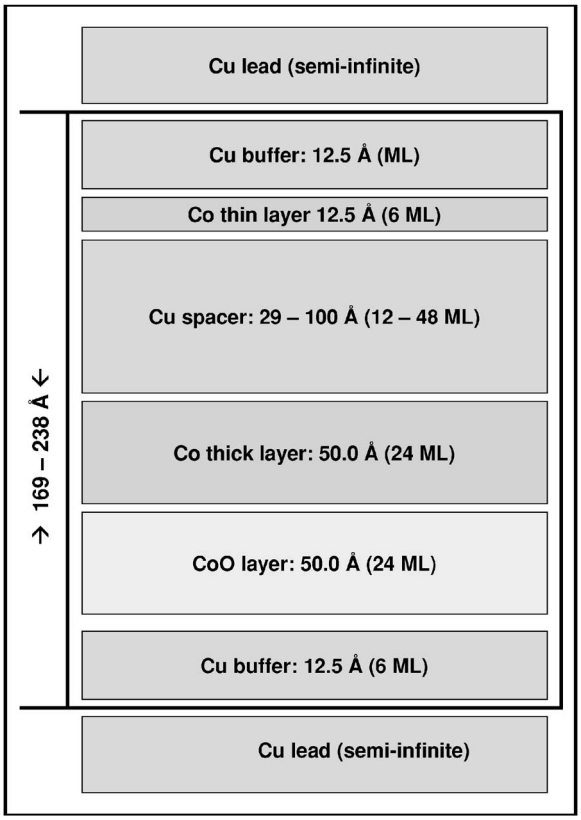

FIG. 1. The system investigated: a Co/Cu/Co spin valve with semi-infinite Cu leads and a "thick" Co layer pinned by an antiferromagnetic CoO slab.

two-dimensional translational invariance and the density functional parametrization of Vosko *et al.*[7] In these spin-valve-type systems 6 Cu layers on the left and $(6+m)$, $m \leqslant 2$, Cu layers to the right served as buffers to the semi-infinite Cu leads.[9] The antiferromagnetic part consists of alternating Co and O layers and a thick (pinned) magnetic slab of 24 Co layers, and the so-called free layer is formed by 6 Co layers. It should be noted that since semi-infinite Cu leads are used, the Fermi energy is that of bulk fcc Cu. The thickness of the structures evaluated self-consistently varies therefore between 169 Å and 238 Å.

Suppose now that the orientation of the magnetization in the free layer is rotated uniformly by an angle Θ with respect to the one in the pinned layer. The energy needed (or gained) to perform this rotation, the so-called twisting energy, is then given by

$$\Delta E(\Theta;n) = E(\Theta;n) - E(\Theta=0;n), \quad 0 \leqslant \Theta \leqslant \pi, \tag{1}$$

implying that for a given spacer thickness n [monolayer (ML)] the actual magnetic ground-state configuration is defined by

$$E(\Theta_{GS};n) = \min_{\{\Theta\}}[E(\Theta;n)]. \tag{2}$$

The twisting energies were obtained via the magnetic force theorem[8] by calculating the grand potentials[6,11] $E(\Theta;n)$ in Eq. (1) using a sufficient number of **k** points in the surface Brillouin zone in order to guarantee stable convergence,

$$E(\Theta;n) = \sum_{k=1}^{N} E_k(\Theta;n), \tag{3}$$

$$E_k(\Theta;n) = \int_{\epsilon_0}^{\epsilon_F} n_k(\Theta;\epsilon)(\epsilon-\epsilon_F)d\epsilon, \tag{4}$$

where $n_k(\Theta;\epsilon)$ is the density of states (per unit cell) of the k-atomic layer at a given value of Θ, ϵ_0 is the valence band bottom, ϵ_F the Fermi energy, and N refers to the total number of layers included (Cu buffer layers, CoO and Co layers, and n spacer layers).[6] The "characteristic volume" for $\Delta E(\Theta;n)$ corresponds therefore to N unit cells. The magnetoresistance for in general noncollinear configurations is defined by

$$MR(\Theta;n) = \frac{r(\Theta;n) - r(\Theta=0;n)}{r(\Theta;n)}. \tag{5}$$

The sheet resistances $r(\Theta;n)$ in Eq. (5) were evaluated in terms of the fully relativistic Kubo-Greenwood equation[10,11] using again a sufficiently large enough **k** set (1830 **k** vectors in the irreducible part of the surface Brillouin zone). In all cases the effect of interdiffusion at the Co/Cu interfaces is discussed by treating chemical disorder in terms of the (inhomogeneous) coherent potential approximation.[6]

Before presenting the results of the present study a few general remarks have to be made. First of all, without using a relativistic approach no magnetic anisotropy effects can be described; i.e., at least the inclusion of spin-orbit coupling is required. Second, clearly enough in experimental or technological samples interface roughness and layer mismatch occur. Dealing theoretically with surface or interface roughness implies that two-dimensional translational symmetry within the atomic layers no longer applies—i.e., requires the use of real space methods. These in turn are restricted by the number of atoms that can be included and can suffer from artificial boundary conditions when used self-consistently. Layer relaxation, on the other hand, can in principle be described theoretically rather well, provided that there is some experimental guidance about the size of the effects to be expected. An *ab initio* description of layer relaxation requires so-called full potential schemes and is presently possible only for thin films (a few atomic layers) on top of a suitable substrate.

In the system considered in here there are five interfaces, three of which are of different kinds (Cu/CoO, CoO/Co, Co/Cu); the total number of atomic layers varies between 80 and 114. Because of the large number of atomic layers that has to be taken into account, no layer relaxations are considered; i.e., the interlayer spacing is that of the leads (2.087 Å). The results presented in the next section refer therefore to an fcc lattice with the lattice spacing of Cu, decorated by two semi-infinite Cu leads and by Co, O, and Cu layers.

III. RESULTS

The magnetic (spin-only) moments in the antiferromagnetic part of the systems investigated are typically $2.05\mu_B$ and $-0.05\mu_B$ for Co and O, respectively. In the pinned Co layer they amount to about $1.71\mu_B$. The magnetic moment of the Co layers adjacent to the Cu spacer is reduced to $1.65\mu_B$; that of the penultimate plane of Co atoms in the free layer is slightly enhanced $(1.72\mu_B)$ as compared to the moment of Co planes farther off the Cu/Co interface. Within the spacer the Cu atoms are very weakly polarized; the magnitude of the moments oscillates approximately with a period of two monolayers.

A. Noninterdiffused (pure) systems

In Figs. 2 and 3 the twisting energies as defined in Eq. (1) are displayed versus the rotation angle Θ. As can be seen in nearly all cases the twisting energies are not of the form $\Delta E(\Theta;n)=a(n)(1-\cos\Theta)$, where $a(n)$ is half of the interlayer exchange coupling energy. For quite a few spacer thicknesses $\Delta E(\Theta;n)$ shows a maximum at $\Theta \neq 0, \pi$. It also can be seen that the value of Θ that corresponds to a particular maximum is not necessarily at $\pi/2$ (perpendicular coupling). The most interesting spacer thicknesses, however, are those for which $E(0;n)$ and $E(\pi;n)$ are of about the same magnitude. This is the case for $n=23$, 31, and 41 (see also Figs. 2 and 3), since then switching the orientation of the magnetization in the free layer by either an external magnetic field or a current applied perpendicularly to the planes of atoms drives the system to a metastable state (see in particular the case for $n=23$ in Fig. 2), separated by an energy barrier from the magnetic ground state. As can be seen from Figs. 2 and 3 magnetic anisotropy effects show up for most spacer thicknesses considered. There are only very few cases in which these effects are of minor importance (see, e.g., the

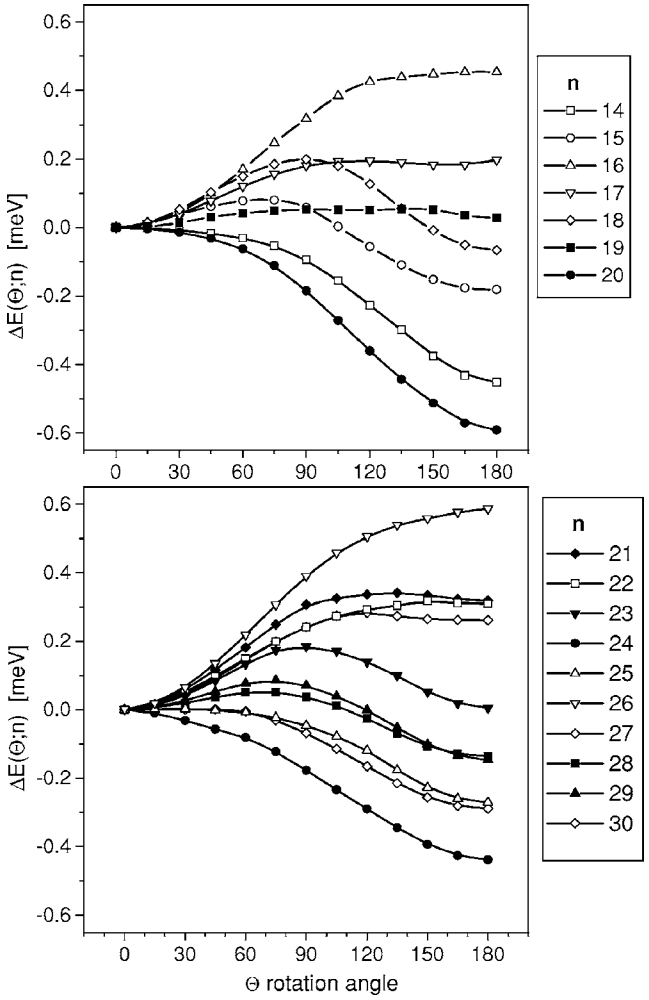

FIG. 2. Twisting energies $\Delta E(\Theta;n)$ for spacer thicknesses between 14 and 30 ML.

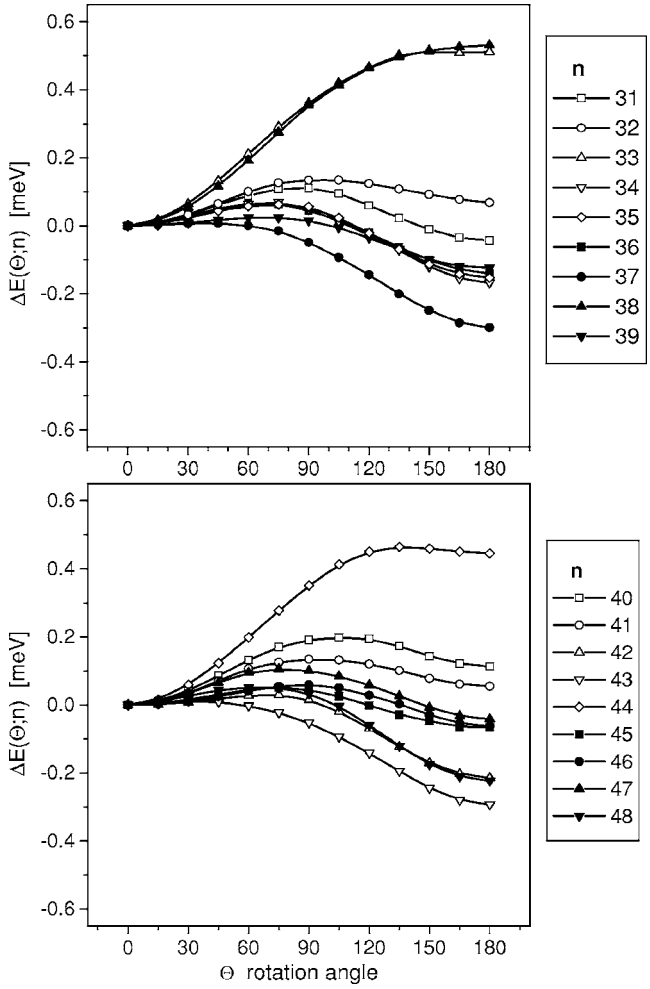

FIG. 3. Twisting energies $\Delta E(\Theta;n)$ for spacer thicknesses between 31 and 48 ML.

entry for $n=20$ in Fig. 2). It also can be seen from Figs. 2 and 3 that—like in many other material-specific properties—there are no obvious systematic changes in the twisting energy with respect to the number of spacer layers.

The layer-resolved twisting energies in Fig. 4 [see also Eq. (4)] prove that the positive anisotropy causing the maximum in the twisting energies, for $\Theta \neq 0, \pi$, is essentially an interface property. It is the second closest Co layer to the Cu/Co interfaces of the free layer that contributes the most, while the contributions from all other interfaces and atomic layers are only minute. The sheet resistances and consequently also the magnetoresistance show almost no anisotropy effects with respect to Θ. As can be seen from Fig. 5 for the example of three spacer thicknesses, the sheet resistances vary very closely to

$$r(\Theta;n) = b(1-\cos\Theta), \quad b = [r(\pi;n) - r(0;n)]/2, \tag{6}$$

and similarly the magnetoresistance like

$$\mathrm{MR}(\Theta,n) = \mathrm{MR}(\pi;n)(1-\cos\Theta)/2. \tag{7}$$

At $\Theta=0,\pi$, e.g., the sheet resistances can easily be fitted to a linear form

$$nr(\Theta;n) = a(\Theta) + b(\Theta)n. \tag{8}$$

In Fig. 6 the calculated values of $nr(\Theta;n)$ are shown for the parallel and antiparallel alignments with respect to the number of spacer layers together with the respective linear fit (upper part) and the corresponding magnetoresistance (lower part),

$$\mathrm{MR}(\Theta;n) = \frac{b_{AP}(\Theta) - b_P(\Theta)}{b_{AP}(\Theta)} - \frac{a_P(\Theta)}{b_{AP}(\Theta)n}. \tag{9}$$

B. Effects of interdiffusion

From Fig. 5 it is evident that for the twisting energies the Co/Cu interfaces of the free layer matter, while the Co/Cu interface of the pinned Co layer is of little importance. For the sheet resistance of course all interdiffusion effects are important, since it is well known that the contributions from the interfaces to the sheet resistance are the largest. In order to illustrate the significance of interdiffusion effects in the following as an example the very special case of 23 Cu spacer layers (see Fig. 2) is considered. Restricting interdiffusion at all Co/Cu interfaces to two layers implies that in-

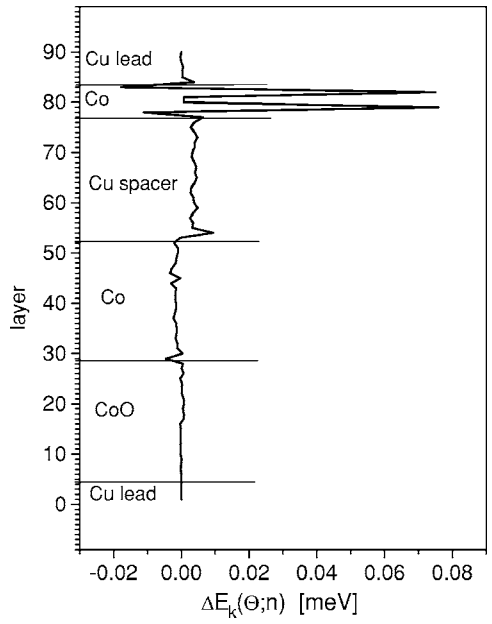

FIG. 4. Layer-resolved band energies $\Delta E_k(\Theta;n)$ [see Eq. (4)] for the case of 23 Cu spacer layers and perpendicular coupling ($\Theta=90°$) (see also Fig. 3).

stead of the two adjacent Co and Cu layers forming an interface, two layers Co_cCu_{1-c} and $Co_{1-c}Cu_c$, where c is the interdiffusion concentration, are considered. Assuming that in each of these two layers statistical disorder applies, the coherent potential approximation (CPA) can be used to describe the alloyed layers. Since the Co concentration in each of these two layers is different, the so-called inhomogeneous CPA, discussed at length in Ref. 6, has to be applied.

In the upper part of Fig. 7 the twisting energy for $n=23$ is displayed versus the rotation angle Θ. The lower part of this figure shows the twisting energy at $\Theta=90°$ and 180° with respect to the interdiffusion concentration. It is interesting to note that the near degeneracy in energy of the parallel and antiparallel configurations for $n=23$ is gradually lifted as the interdiffusion concentrations grows (see the lower part of Fig. 7) and that concomitantly the position of the maximum moves to values of Θ larger than 90°.

In Fig. 8 the layer-resolved twisting energies in the vicinity of the free layer are shown for the interdiffusion concentrations 0% (no interdiffusion) and 1%. As one might have guessed from Fig. 4 the influence of a two-layer interdiffusion on the size of the (positive) anisotropy contribution to the twisting energy is rather very small since its main contributions arise from the penultimate Co layers on each side of the free layer. Unfortunately very little is known about the actual interdiffusion profiles at the interfaces, about how many layers are effected by what concentration gradients (see also the following section). Finally, in Fig. 9 the magnetoresistance in the case of interdiffused interfaces is depicted and essentially confirms the well-known fact that in the presence of interdiffusion at the interfaces the magnetoresistance is decreased.

IV. DISCUSSION AND CONCLUSIONS

In viewing the magnetoresistance as a function of the relative angle between the orientations of the magnetization

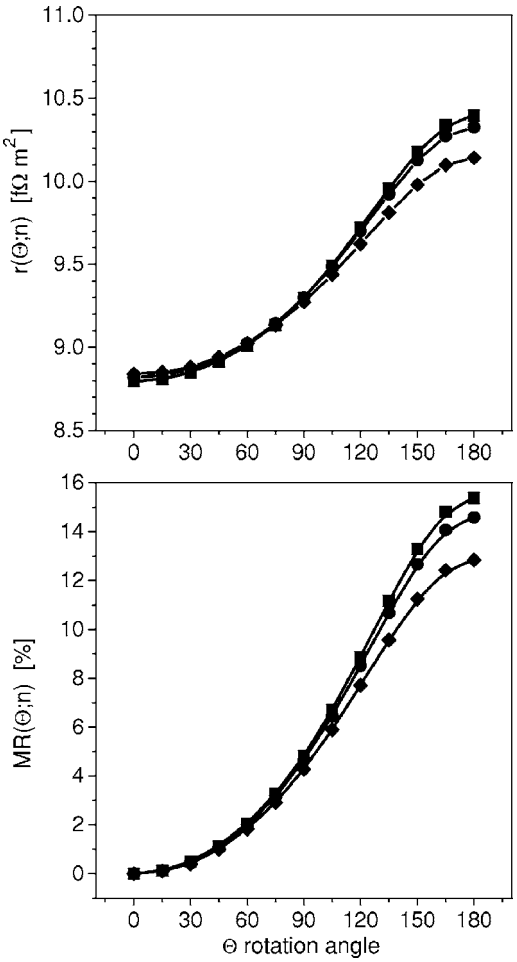

FIG. 5. Variation of the sheet resistance (upper part) and the magnetoresistance (lower part) [see Eq. (5)] with respect to the rotation angle for $n=21$ (squares), $n=24$ (circles), and $n=30$ (diamonds).

in the pinned and in the free layer usually a $(1-\cos\Theta)$ dependence is found[12] with the proportionality constant being half of the magnetoresistance with respect to the two collinear configurations. This seems to be the case for all systems for which up to now such an angular dependence was investigated.[13–15]

Much more involved are the questions of (a) what energetic path prevails when changing this relative angle, since anisotropy effects—i.e., relativistic effects—are of crucial importance, and (b) what is the magnetic ground state of a particular system? While for $Cu(100)/Py/Cu_n/Py/Cu(100)$, $18\leqslant n\leqslant 30$,[14] the magnetic ground-state configuration was found to be always a noncollinear configuration (the preferred coupling is perpendicular), for $Co(100)/Cu_n/Co(100)$,[13] as well as for the present systems, it is (nearly) always a collinear configuration. In the $Py/Cu_n/Py$ system the magnetic anisotropy contribution to the twisting energy was negative in the whole range of spacer thicknesses considered; in the $Co/Cu_n/Co$ systems it is positive. In the latter system at $n=25$ the parallel and antiparallel configurations were energetically nearly degenerated.

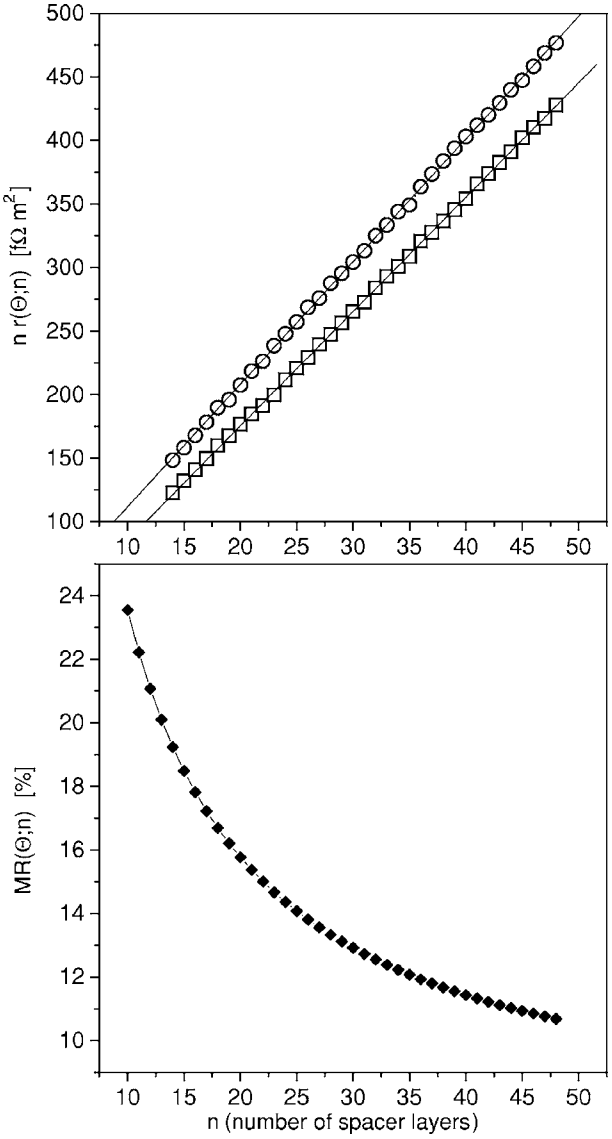

FIG. 6. Upper part: variation of $nr(\Theta;n)$ for $\Theta=0°$ (parallel, diamonds) and $\Theta=180°$ (antiparallel, circles) and of the respective fits (solid lines) with respect to the spacer thickness (ML). Lower part: the magnetoresistance $\mathrm{MR}(\Theta;n)$ at $\Theta=180°$ [see Eqs. (8) and (9)] for spacer thicknesses between 14 and 48 ML.

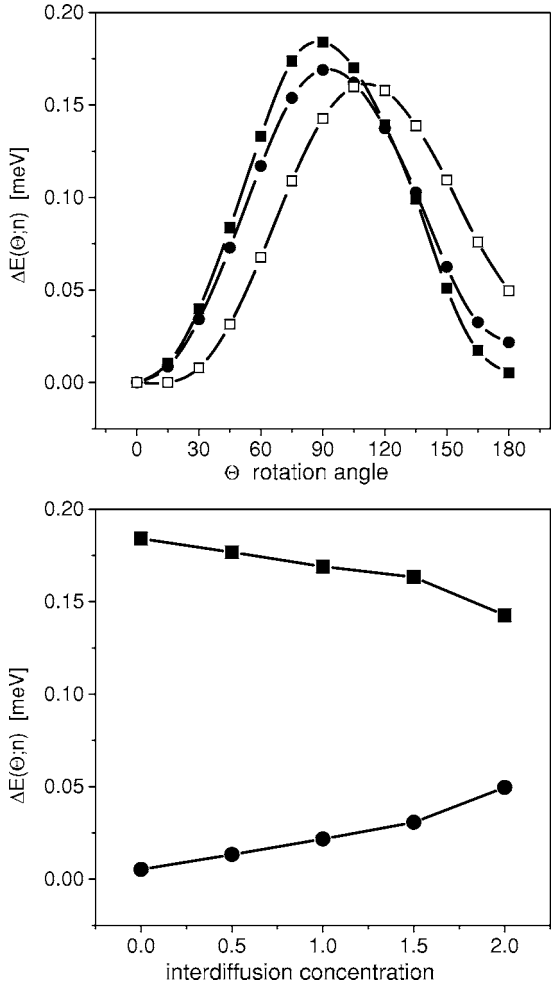

FIG. 7. Upper part: twisting energy $\Delta E(\Theta;n)$, $n=23$, for the interdiffusion concentrations 0% (solid squares), 1% (circles), and 2% (open squares) as a function of the rotation angle Θ. Lower part: twisting energy $\Delta E(\Theta;n)$ for $n=23$ at $\Theta=90°$ (squares) and 180° (circles) versus the interdiffusion concentration.

Considering two-atomic layer interdiffusion effects at the interfaces in $(100)\mathrm{Co}/\mathrm{Cu}_n/\mathrm{Co}(100)$,[15] even at rather very small interdiffusion concentrations, the anisotropy contribution to the twisting energy changed sign, causing thus a noncollinear ground-state configuration to be formed. Comparing these findings with the present results it is obvious that (a) the stacking sequence and (b) the type of leads (Co versus Cu) are important, since the leads (theoretically) govern the interlayer distance and serve as electron reservoirs (they supply the Fermi energy for the total system).

It should be noted that similar to the present results for the layer-resolved twisting energies, it was found that, for thin films of Co on Cu(111),[16] the main contribution to the magnetic anisotropy energy can be attributed to the penultimate Co layer. It therefore seems that a practical approach to judge whether or not interdiffusion effects are important is to evaluate layer-resolved twisting energies for the perpendicular and antiparallel configurations of the pure systems and find out which of the atomic layers near an interface contributes the most.

In principle—as already said—switching the orientation in the free layer can be achieved by applying an external magnetic field or by running a current perpendicular to the planes of atoms. While in the first case the external field can directly be correlated to the twisting energies, in the case of current-induced switching—i.e., in the case of an interaction with an external electromagnetic field—the situation is much more complicated, since so far all formulations of so-called "spin torques" as additional terms in a phenomenological Landau-Lifshitz equation are either based on semiclassical models or on nonrelativistic descriptions in which the electronic "spin" is included more or less heuristically.[17,18] The practical use of a proper fully relativistic formulation of the time evolution of polarization densities[19]—i.e., a theoretical description of all torques caused by the interaction with an external electromagnetic field treating the spin relativistically—is only at the very beginning since, most

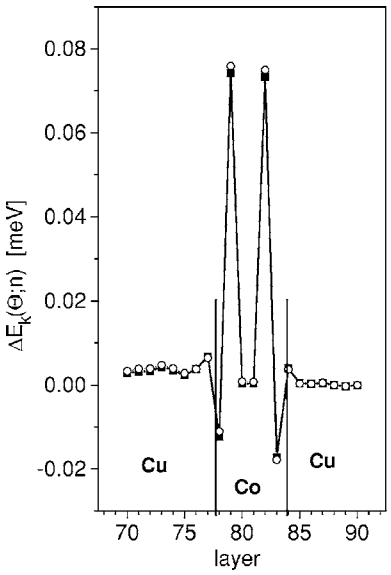

FIG. 8. Layer-resolved twisting energies $\Delta E_k(\Theta;n)$ [see Eq. (4)] for $\Theta=90°$ and $n=23$ in the vicinity of the free layer (see also Fig. 4). Circles: no interdiffusion. Squares: 1% interdiffusion.

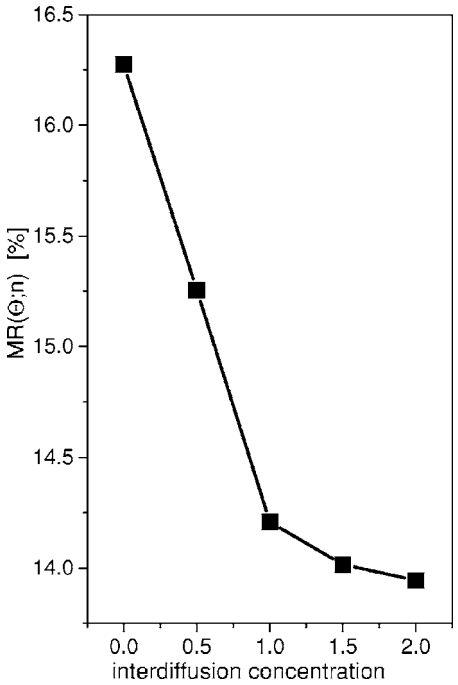

FIG. 9. Magnetoresistance for $n=23$ and $\Theta=180°$ as a function of the interdiffusion concentration for the case that all Co/Cu interfaces are interdiffused.

likely, e.g., the application of time-dependent density functional theory is needed in this case. The question of evaluating the size of the spin torques on an appropriate *ab initio* level and the problem of judging the importance of these torques versus the "traditional" torque term (the cross product of magnetization and effective field) in the phenomenological Landau-Lifshitz equation remains up to now unresolved and is subject of heated discussions.

It should be noted that this traditional torque term can directly be evaluated from the twisting energies, since only the derivative of $\Delta E(\Theta;n)$ with respect to $\cos\Theta$ is needed.[13] In using for the critical current the formulation given Ref. 13—namely, $I(\Theta;n)=\sqrt{A/\tau(\Theta;n)}I_0(\Theta;n)$, where A is the unit area, $\tau(\Theta;n)$ is the time needed to rotate the orientation of the magnetization in the free layer from the ground-state magnetic configuration to the one characterized by Θ, and $I_0(\Theta;n)=\sqrt{\Delta E(\Theta;n)/r(\Theta;n)}$. For $n=23$, $I_0(\pi;n)$ amounts to 0.178 [mA]. Within this admittedly phenomenological description for $n=23$ the time to switch from the parallel to the antiparallel configuration is 0.61 [ns]. It is important to recall that the above-quoted values are based on the use of a Landau-Lifshitz equation adapted for layered systems[13] and Ohm's law. Furthermore, since all sheet resistances were calculated in terms of the Kubo-Greenwood equation, they refer thus to a linear response formulation.

It was the main emphasis of this investigation to show for a realistic spin-valve system with an antiferromagnetic part and a sufficiently thick pinned magnetic layer that anisotropy effects in the energetic path corresponding to the rotation of the orientation of the magnetization in the free layer from the parallel to the antiparallel configuration are indeed important and that in this particular type of systems interdiffusion effects only matter if the interdiffusion concentration were much larger than 2%, which, however, is unlikely because of the very restricted solubility of Co in Cu (less than 2%).

ACKNOWLEDGMENT

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