Current-induced switching in Co/Cu/Co spin valves: The effect of interdiffusion

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(Received 8 March 2005; revised manuscript received 9 June 2005; published 19 August 2005)

The effect of interdiffusion at the Co/Cu interfaces on current-induced switching in $Co/Cu_n/Co$ spin valves, $n=21$, 25, and 33, with the interdiffusion concentration varying between 0 and 10%, is described theoretically in terms of *ab initio* calculations using the relativistic screened Korringa-Kohn-Rostoker method and the Landau-Lifshitz-Gilbert equation. It is found that interdiffusion forces the system to form a noncollinear ground state such that switching to both kinds of collinear final states is possible. Furthermore, it is shown that (i) this behavior is caused by magnetic anisotropy effects, and (ii) by decreasing the interdiffusion, the current necessary to achieve switching to such a final state (critical current) can be reduced substantially.

DOI: 10.1103/PhysRevB.72.054431 PACS number(s): 75.30.Gw, 75.70.Ak, 75.70.Cn

I. INTRODUCTION

Although suggested theoretically by Slonczewski,[1] current-induced switching is now thought to be of enormous technological interest,[2,3] since in principle it is much easier to switch the orientation of the magnetization in the free layer of a spin-valve-type system by a current applied in the CPP (current perpendicular to the planes of atoms) geometry than by an external magnetic field. Ultimately, current-induced switching can perhaps replace most giant magnetoresistance (GMR) devices, now used in many commercial applications, provided, however, that the critical current, namely, the current that has to be applied to perform switching, can be reduced by at least one order of magnitude. At present, mostly nanopillars are investigated experimentally, i.e., systems that because of the preparation techniques used, necessarily show macroscopic roughness and chemical disorder (interdiffusion at interfaces), a fact that has to be taken into account also in theoretical descriptions.

In the present paper, the effect of interdiffusion on current-induced switching has been studied theoretically by investigating systems of the type $Co(100)/Co_{m_1}/Cu_{1-c}Co_c/Cu_{1-c}Co_c/Cu_n/Cu_{1-c}Co_c/Cu_{1-c}Co_c/Co_{m_2}/Co(100)$, with m_1, $m_1 \geqslant 11$ serving as buffer layers to the semi-infinite leads and c varying between 0 and 0.10, i.e., by assuming at the Co/Cu interfaces an interdiffusion profile extending over two adjacent atomic layers. The $n=19$, 23, and 31 interdiffused Cu spacer layers correspond in turn to a spacer thickness of 36.4, 43.24, and 57.18 Å. It should be noted that for $c=0$, the composition of the investigated spin-valve systems is simply of the form $Co(100)/Co_{m_1+1}/Cu_{n+2}/Co_{m_2+1}/Co(100)$.

The orientation of the magnetization in the left Co lead and the left half of the Cu spacer is kept fixed to point along the surface normal (see Fig. 1), whereas that of the right Co lead and the remaining spacer is rotated continuously around an axis perpendicular to the surface normal until the ground state $\Theta_0 \in [0, \pi]$ is reached. If $\Theta_0 \neq 0$ or π (collinear magnetic configurations) then a noncollinear magnetic configuration characterizes the ground state.

II. CONCEPTUAL AND COMPUTATIONAL DETAILS

In defining the twisting energy[4] $\Delta E(\Theta;\mathbf{c},N)$ as

$$\Delta E(\Theta;\mathbf{c},N) = E(\Theta;\mathbf{c},N) - E(\Theta_0;\mathbf{c},N), \tag{1}$$

$$\Theta = \Theta_0 + \Delta\Theta,$$

$$N = m_1 + m_2 + n, \tag{2}$$

Θ_0 serves as the zero point of eventual (further) rotations. $\Delta\Theta = -\Theta_0$ corresponds then to the parallel configuration, and $\Delta\Theta = 180 - \Theta_0$ to the antiparallel configuration (see Fig. 1). In principle, $\mathbf{c}$ is an N-dimensional vector that contains layerwise the concentrations of Co and Cu. It should be noted that only by applying an external magnetic field or a current does the system assume a magnetic configuration Θ other than Θ_0, since $\Delta E(\Theta;\mathbf{c},N) \geqslant 0$.

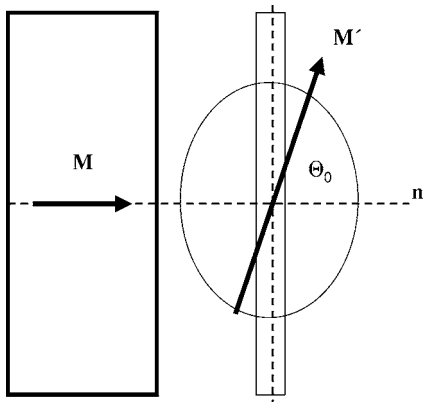

FIG. 1. Noncollinear ground state of two magnetic slabs separated by a nonmagnetic spacer. The orientation of the magnetization **M** in the thick magnetic layer is pointing along the surface normal **n**. In the so-called free layer, the orientation of the magnetization **M′** forms an angle Θ_0 with **n**.

Provided that in a CPP geometry the corresponding sheet resistance[5] $r(\Theta;\mathbf{c},N)$ is also evaluated, a current $I(\Theta;\mathbf{c},N)$ can be defined[4,6] as

$$I(\Theta;\mathbf{c},N) = \sqrt{A_0/|\tau(\Theta;\mathbf{c},N)|}I_0(\Theta;\mathbf{c},N), \quad (3)$$

$$I_0(\Theta;\mathbf{c},N) = \mathrm{sgn}[\tau(\Theta;\mathbf{c},N)]\sqrt{\Delta E(\Theta;\mathbf{c},N)/r(\Theta;\mathbf{c},N)}, \quad (4)$$

where $\tau(\Theta;\mathbf{c},N)$ is the time needed to accomplish a rotation by $\Delta\Theta$, and A_0 is the unit area in the relation $r(\Theta;\mathbf{c},N) = A_0 R(\Theta;\mathbf{c},N)$, with $R(\Theta;\mathbf{c},N)$ being the resistance. In the following, $I_0(\Theta;\mathbf{c},N)$ will be referred to as *reduced current*.

The (positive definite) twisting energy $\Delta E(\Theta;\mathbf{c},N)$ can be expressed in terms of a power series in $\cos(\Theta)$,

$$\Delta E^{(k)}(\Theta;\mathbf{c},N) = \sum_{s=0}^{k} a_s^s(\mathbf{c},N)\cos(\Theta)^s. \quad (5)$$

The expansion coefficients thereof are then used to solve the Landau-Lifshitz-Gilbert equation[4] in order to obtain for a given Θ the corresponding characteristic time $\tau(\Theta;\mathbf{c},N)$. In choosing a Gilbert damping factor of one, so-called minimal switching times are obtained.[4] Clearly enough, the unit area A_0 in Eq. (3) is an experiment-dependent parameter.

For all systems investigated, the parallel configuration (the orientation of the magnetization points uniformly along the surface normal) was calculated self-consistently by using the fully relativistic screened Korringa-Kohn-Rostoker method[7] and the density functional parametrization of Vosko *et al.*[8] The problem of interdiffusion was dealt with using the (inhomogeneous) coherent potential approximation.[9] The twisting energies were then obtained via the magnetic force theorem[10] by calculating the grand potentials $E(\Theta;\mathbf{c},N)$ in Eq. (1) using a sufficient number of $\mathbf{k}$ points in the surface Brillouin zone in order to guarantee stable convergence with respect to $\mathbf{k}$. The sheet resistances $r(\Theta;\mathbf{c},N)$ were evaluated in terms of the fully relativistic Kubo-Greenwood equation,[5,9] using again a sufficiently large enough $\mathbf{k}$ set. In both types of calculations, the angle Θ was varied between 0° and 180° in steps of at most 20°. The expansion in Eq. (4) was restricted to $k=3$, and the coefficients thereof were determined numerically in terms of a least-squares fitting procedure,[11] the fitting errors being typically of the order of 10^{-5} meV.

III. RESULTS

A. Probability for interdiffusion at the interfaces

It is well known that in the binary bulk system Co/Cu, the solubility of Co in Cu (and oppositely) is at best 1–2%. As this percentage not necessarily also applies for a possible interdiffusion at Co/Cu interfaces, total-energy calculations within the atomic sphere approximation (ASA) were performed for $n=19$ (spacer thickness 36.4 Å), with the orientations of the magnetizations in the magnetic parts being aligned parallel and pointing along the surface normal (see Fig. 1) in order to determine a realistic range of interdiffusion concentrations. In Fig. 2, the following difference in total energies:

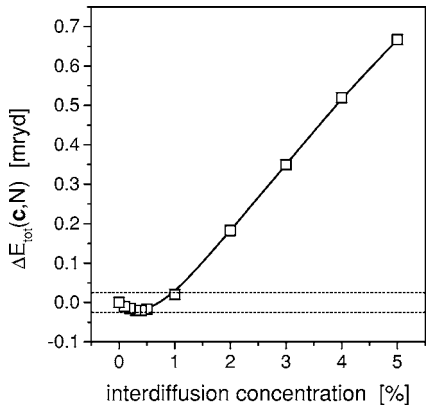

FIG. 2. Total energy difference with respect to the interdiffusion concentration for $n=19$ (spacer thickness 36.4 Å); see also Eq. (6).

$$\Delta E_{tot}(\mathbf{c},N) = E_{tot}(\mathbf{c},N) - E_{tot}(\mathbf{c}=0,N) \quad (6)$$

is displayed, since by forming total-energy differences, most of the inherent errors in the ASA can be avoided. As can be seen in this figure, by assuming an error of about ±0.025 mryd (indicated by horizontal dashed lines), $\Delta E_{tot}(c,N) \sim 0$ for all interdiffusion concentrations below about 1.5%. Figure 2 clearly indicates that in Co/Cu/Co spin valves interdiffusion at the interfaces definitely has to be considered with interdiffusion concentrations between about zero and 2%. It should be noted that Fig. 2 can only serve as an argument that interdiffusion at the interfaces is very likely to occur also in cases of noncollinear ground states.

B. Orientation dependence of the magnetization

In the top part of Fig. 3, it is shown that for the present purposes, the orientation of the magnetization was correctly assumed to point along the surface normal. As the energy difference between a uniformly perpendicular and a uniformly parallel to the surface normal magnetic configuration (the so-called band-energy part in a magnetic anisotropy energy calculation[7]) is very small, this quantity was analyzed with respect to the $\mathbf{k}$ convergence. As can be seen in this figure, if the number of $\mathbf{k}$ points used in the irreducible part of the surface Brillouin zone is above about 2000, this energy difference settles down at 0.05 meV, indicating that in the noninterdiffused system, indeed a magnetic configuration is preferred with the magnetization pointing uniformly along the surface normal. In the lower half of this figure, this energy difference is displayed with respect to the interdiffusion concentration. The very meaning of this dependency on the interdiffusion concentration and of the second curve displayed will be discussed in the Sec. III D.

C. Reduced currents and magnetoresistance

It is quite well known that the interlayer exchange coupling energy—and, therefore, also the more general twisting energy—is mostly determined by contributions from the interfaces. It is, therefore, not at all surprising that interdiffusion produces an almost dramatic effect on $\Delta E(\Theta;\mathbf{c},N)$ and consequently on the reduced current $I_0(\Theta;\mathbf{c},N)$ [see Eq. (4)].

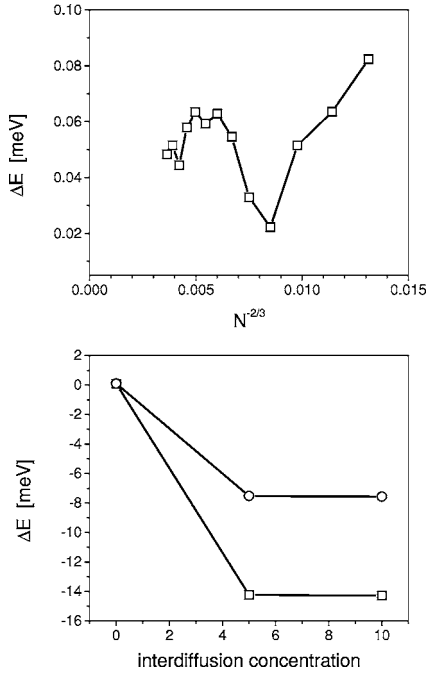

FIG. 3. (a) Band energy part of the magnetic anisotropy energy for $n=23$ (spacer thickness 43.24 Å) with respect to $N^{-2/3}$, where N is the number of $\mathbf{k}$ points used in the irreducible part of the surface Brillouin zone.(b) Band-energy part of the magnetic anisotropy energy (squares) and twisting energy for a perpendicular arrangement of the orientations of the magnetization (circles) with respect to the interdiffusion concentration (see also Fig. 1).

This is depicted in Fig. 4. While in the absence of interdiffusion for $n=21$ (spacer thickness 36.4 Å) the parallel magnetic configuration corresponds to the ground state, with increasing interdiffusion, a perpendicular arrangement of the orientations of the magnetization in the magnetic slabs is preferred, i.e., a noncollinear ground state is formed. As compared to the twisting energy, the changes in the sheet resistance caused by interdiffusion (not shown here) are much less spectacular—$r(\Theta;c)$ is predominantly proportional to $(1-\cos\Theta)$ for all concentrations investigated.

In order to recover the "traditionally" well-known definition of the magnetoresistance,

$$MR(\mathbf{c},N)=[r(\pi;\mathbf{c},N)-r(0;\mathbf{c},N)]/r(\pi;\mathbf{c},N), \qquad (7)$$

in Fig. 4 also the magnetoresistance, defined as

$$MR(\Theta;\mathbf{c},N)=[r(\Theta;\mathbf{c},N)-r(0;\mathbf{c},N)]/r(\Theta;\mathbf{c},N),$$

is displayed in this particular case, however, as an implicit function of the applied reduced current

$$MR(\Theta;\mathbf{c},N)=f[I_0(\Theta;\mathbf{c},N)].$$

It should be noted that in the left half of Fig. 4, the reduced current is displayed with respect to $\Delta\Theta$ [see Eq. (2)], since $\Delta\Theta=0$ refers to the ground state.

It is worthwhile to mention that $MR(\mathbf{c},N)$ [see Eq. (7)], does decrease with increasing interdiffusion concentration and also slightly with respect to the thickness of the spacer—for $n=19$, the magnetoresistance $MR(c,N)$, changes linearly

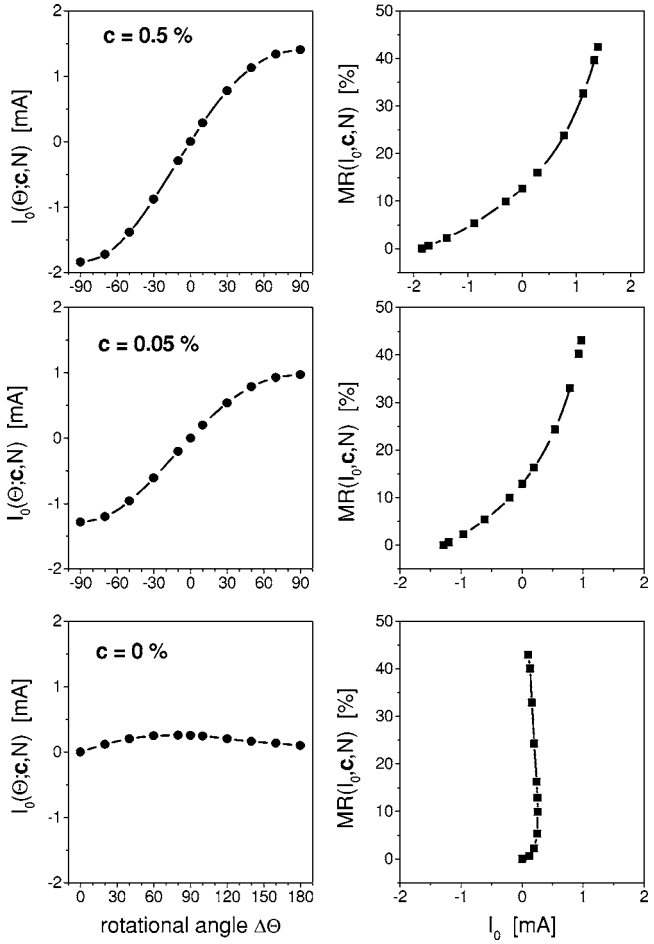

FIG. 4. Reduced current with respect to $\Delta\Theta$ (left column), and magnetoresistance with respect to the reduced current (right column) for $n=19$ (spacer thickness 36.4 Å). In each row, the interdiffusion concentration is marked explicitly. It should be noted that for matters of comparison in both columns, the scale on the ordinate is kept constant.

from 36.3% at 5% interdiffusion to 42.9% for the noninterdiffused system.

For $n=23$ and 5% interdiffusion, $MR(\mathbf{c},N)$ drops to about 32.8%, i.e., at a constant interdiffusion concentration of 5%, by increasing the spacer thickness by about 7 Å, the magnetoresistance decreases by about 3.5%.

In Fig. 5, again the magnetoresistance is shown vs the reduced current; however, this time for $n=31$ (spacer thickness 57.18 Å). In this figure, the switching from the ground state ($I_0=0$) to the parallel final state is indicated by open symbols, and the switching to the antiparallel final state by solid symbols. One can easily see (i) that the current needed to switch the system is bigger in the first case than in the second one and (ii) that with decreasing interdiffusion, this current is decreasing. A switching to the parallel state (negative current) yields a change in the magnetoresistance of about 12.5%, and to the antiparallel state (positive current), a change of about 22.5%. Figure 5 proves that the formation of a noncollinear ground state by interdiffusion effects is not the property of a particular spacer thickness. For $n=23$ (spacer thickness 43.24 Å), very similar results (not shown here) are obtained.

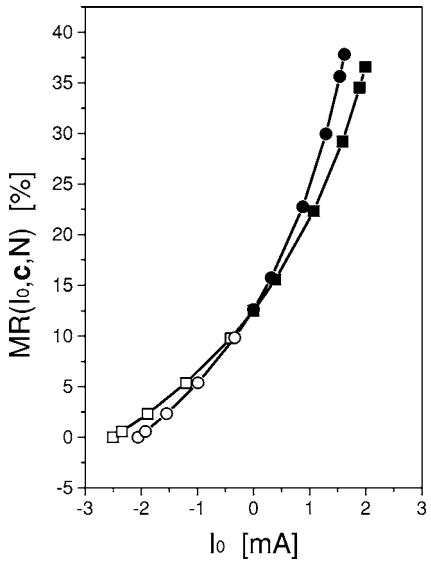

FIG. 5. Magnetoresistance vs reduced current for $n=31$ (spacer thickness 57.18 Å) and 1% (circles) and 2% (squares) interdiffusion. Open symbols refer to a switching to the parallel final state, and solid symbols to the antiparallel final state.

D. Expansion coefficients and switching times

The explanation for the formation of a noncollinear state in the interdiffused systems can be read directly from Fig. 6. As can be seen, there the coefficient of $\cos^2(\Theta)$, the so-called anisotropy term, increases sharply with increasing interdiffusion, while all other coefficients are very close to zero. Only for vanishing interdiffusion ($\mathbf{c}=0$) do the first two coefficients start to grow and the anisotropy term changes sign. This then yields the results shown in Ref. 4, namely, that the twisting energy has a maximum for a perpendicular arrangement of the orientations of the magnetization. Going back now to the lower part of Fig. 3, it is evident that it is indeed only the anisotropy term that causes the existence of a noncollinear ground state—the band-energy part of the anisotropy energy (difference in grand potentials between a uniform perpendicular and a uniform in-plane orientation of the magnetization) is nearly twice as big as the twisting energy for $\mathbf{M}'$ in Fig. 1, being perpendicular to the surface normal $\mathbf{n}$. Figures 3 and 6 prove that in the presence of interdiffusion at the interfaces, anisotropy effects not only change the twisting energy dramatically, but they in turn change the size of the reduced current.

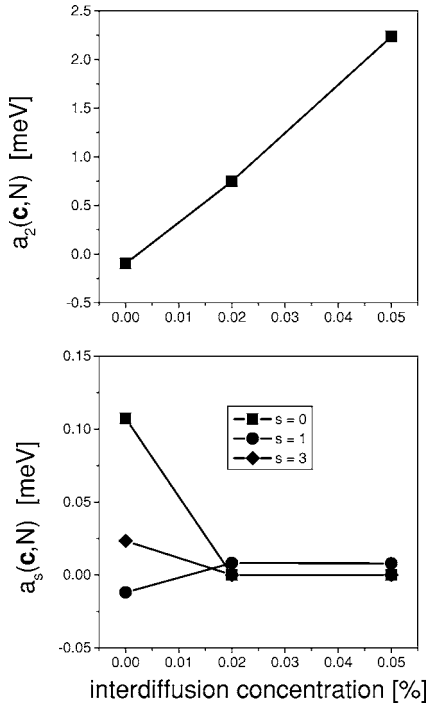

FIG. 6. Expansion coefficients for the twisting energy for $n=19$ (spacer thickness 36.4 Å) vs the interdiffusion concentration [see also Eq. (5)].

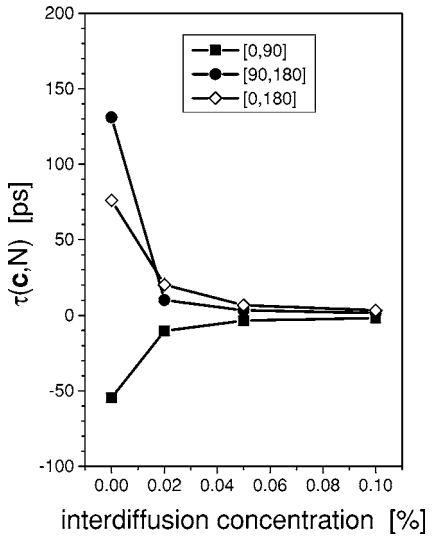

FIG. 7. Minimal switching times for $n=19$ (spacer thickness 36.4 Å). Squares denote switching from the ground state to the parallel, circles denote switching to the antiparallel magnetic configuration, and diamonds refer to the sum of both. Only in the case of a collinear ground state does this sum reflect the correct switching time.

In Fig. 7, the minimal switching times are depicted vs the interdiffusion concentration by displaying the more interesting low-interdiffusion regime. The squares in this figure refer to a switching from a perpendicular arrangement of the orientations of the magnetization (ground state in the presence of interdiffusion) to the parallel magnetic configuration, the circles refer to the antiparallel configuration, and the diamonds to the sum of both, which only in the noninterdiffused case yields the correct (minimal) switching time. It is interesting to note that with decreasing interdiffusion, the switching times increase strongly. For $n=19$ (spacer thickness 36.4 Å) and 2% interdiffusion, the minimal switching time from the ground state to either of the two collinear final states is only about 1 ps, while in the noninterdiffused system, the switching times is larger by at least one order of magnitude.

IV. DISCUSSION

From the entry for the reduced currents in Fig. 5, one can immediately determine that in the interdiffused systems, the

current needed to switch from the ground state to the antiparallel alignment is smaller than that needed to switch to the parallel alignment. This was the case for all interdiffusion concentrations and spacer thicknesses investigated and seems to confirm recent experimental evidence.[3] It is also evident in this figure that in the presence of interdiffusion, the reduced currents are larger by one order of magnitude than in the absence of interdiffusion. Assuming an interdiffusion concentration of 0.5%, which according to Fig. 2 is quite realistic, a unit area of 100 nm $\times$ 100 nm, and taking into account for $n=19$, the corresponding calculated reduced critical currents and switching times, then according to Eq. (3), the current needed to switch to the parallel (antiparallel) magnetic configuration amounts to 0.21 (0.17) mA. For a unit area of 500 nm $\times$ 500 nm, one would get 1.05 and 0.85 mA, respectively, which is already within the scale of experimentally observed critical currents. This simple example suggests strongly that in all experimental studies based on Co/Cu-related spin valves, interdiffusion at the interfaces (of unknown degree) was present.

The results displayed in Figs. 4 and 5 not only indicate that current-induced switching (formation of noncollinear ground-states induced by interdiffusion) is perhaps even more complicated than originally thought, but also that models based only on spin-up and spin-down electrons (strict collinearity) most likely are not suitable, to describe this kind of situation, since quite obviously strong anisotropy effects have to be taken into account. This was also found for current-induced switching in spin valves with Permalloy serving as magnetic slabs.[6]

Clearly, different interdiffusion profiles can be assumed, extending over several atomic layers, and different spacer thicknesses can be investigated. The main conclusions from the present results, however, are that (i) in principle, a well-defined noncollinear ground state is formed by interdiffusion effects, and (ii) the reduced current and the switching time(s) depend crucially on the amount of interdiffusion. Applying, e.g., a small external magnetic field as proposed in Ref. 3 simultaneously with the current automatically changes Θ_0 and therefore the critical current(s). Clearly, the present results also show that in principle the critical current can be reduced by reducing interdiffusion effects either by using suitable thin metallic layers (Ru, Ta) between the magnetic slabs and the nonmagnetic spacer or by means of other experimental "tricks" in order to prevent interdiffusion. Lower critical currents, on the other hand, imply slower switching times. It seems, therefore, that a technologically relevant compromise between these two aspects of current-induced switching is needed.

ACKNOWLEDGMENTS

Financial support from the Austrian Ministry for Economics and Labour (Zl 98.366) and the TU Vienna are gratefully acknowledged. We also want to thank the computing center IDRIS at Orsay, since part of the calculations were performed using their facilities.

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