Current-induced switching in Py/Cu/Py spin valves

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Current-induced switching in Py/Cu/Py spin valves with the Cu spacer thickness varying between 20 and 30 monolayers is described theoretically in terms of a multiscale approach based on *ab initio* calculations using the fully relativistic screened Korringa-Kohn-Rostoker method and the Landau-Lifshitz-Gilbert equation. It is found that in all investigated cases a perpendicular arrangement of the magnetic slabs is lowest in energy and that therefore the critical current refers to a switching from this initial magnetic configuration to a collinear magnetic configuration, the switching time being about 30 ps. Because the twisting energy as well as the corresponding sheet resistance, both of them entering as key quantities the expression for the current, can be viewed layer resolved, very clear conclusions can be drawn with respect to possible reductions of the critical current.

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The concept of current-induced magnetization reversal was first suggested theoretically by Slonczewski[1] in 1996 and led to intensive experimental investigations in many academic and industrial research institutions. It was stated very recently by Grollier *et al.*[2] that "from the application point of view, current induced reversal of the magnetization can be of great interest to switch spintronic devices (MRAM for example), if especially the required current density—presently 10^7 A/cm^2—can be reduced by approximately an order of magnitude." Clearly enough, since in present magnetic devices or media the magnetic moments are switched via externally generated magnetic fields, it would be much simpler to switch these moments by applying a current pulse perpendicularly through the magnetic layer itself. In the present paper the system Py/Cu/Py is investigated theoretically by making use of a recent suggestion[3] to relate the twisting energy—i.e., the energy necessary to rotate the orientation of the magnetization in the thin magnetic slab—and the corresponding sheet resistance in a spin-valve-type system to the current needed for such a switching process. As the time scale of the switching enters the description of the current, this approach combines in a kind of multiscale manner *ab initio* calculations based on the Kohn-Sham-Dirac Hamiltonian with the Landau-Lifshitz-Gilbert equation. It will be shown that this conceptually rather simple approach not only can be used to evaluate critical currents and switching times, but can also provide ideas of how to reduce the size of the critical current.

Systems of the type $Cu(100)/Cu_{m_1}/Py_{24}/Cu_m/Py_6/Cu_{m_2}/Cu(100)$, Py: $Ni_{85}Fe_{15}$, have been investigated with m varying between 18 and 30 monolayers (ML)—i.e., with a Cu spacer thickness between about 32 and 54 Å—using as lattice spacing that of the Cu leads (interlayer spacing 1.8094 Å). Note that the total number n of atomic layers considered in the calculations[4] amounts to $n=m_1+m_2+m+30$. The orientation of the magnetization in the thick permalloy slab (about 43 Å) is kept fixed to point along the surface normal, whereas that of the thin permalloy slab (10.8 Å) is rotated continuously around an axis perpendicular to the surface normal by an angle $\Theta \in [0,\pi]$. The parallel magnetic configuration then corresponds to $\Theta=0$, the antiparallel to $\Theta=\pi$. In defining the twisting energy[3] $\Delta E(\Theta;m)$ as

$$\Delta E(\Theta;m) = E(\Theta;m) - \min[E(\Theta;m)], \tag{1}$$

this quantity is positive definite for all Θ and can be regarded as a magnetic contribution to the Joule's heat. Provided that in a current perpendicular to the planes of atoms (CPP) geometry the sheet resistance[5] $r(\Theta;m)$ is also evaluated, and a corresponding current $I(\Theta;m)$ can be defined[3] as

$$I(\Theta;m) = \sqrt{\frac{A_0 \Delta E(\Theta;m)}{\tau(\Theta;m) r(\Theta;m)}} = \sqrt{\frac{\langle A_0\rangle}{\langle \tau(\Theta;m)\rangle}} I_0(\Theta;m), \tag{2}$$

where $\tau(\Theta;m)$ is the time needed to accomplish such a rotation by Θ and A_0 is the unit area in the relation $r(\Theta;m)=A_0 R(\Theta;m)$ with $R(\Theta;m)$ being the resistance. In Eq. (2), $\langle A_0\rangle$ and $\langle \tau(\Theta;m)\rangle$ denote the magnitude of the corresponding quantities within the international system of units; $I_0(\Theta;m)$ will be referred to in the following as the reduced current, which just depends on the twisting energy and the sheet resistance.

Furthermore, since $\Delta E(\Theta;m)$ can be expressed in terms of a kth-order power series in $\cos(\Theta)$,

$$\Delta E^{(k)}(\Theta;m) = \sum_{s=0}^{k} a_s(m)[\cos(\Theta)]^s, \qquad (3)$$

this expansion can be used to solve the Landau-Lifshitz-Gilbert equation along the lines discussed in Ref. 3 in order to obtain for a given Θ the corresponding minimal time[6] $\tau(\Theta;m)$. It should be noted that the only quantity in Eq. (2) that cannot be determined theoretically is the unit area A_0, since it is an experimental parameter, which of course depends very much on the design of the prepared samples.

For all systems investigated the parallel configuration 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] Chemical disorder (the alloy problem) was treated in terms of the (inhomogeneous) coherent potential approximation.[7] The twisting energies were then obtained via the magnetic force theorem[9] by calculating the grand potentials[5,7] $E(\Theta;m)$ in Eq. (1) using a sufficient number of **k** points in the surface Brillouin zone in order to guarantee stable convergence. The sheet resistances $r(\Theta;m)$ were evaluated in terms of the fully relativistic Kubo-Greenwood equation[5,10] using again a sufficiently large enough **k** set. In both types of calculations the angle Θ was varied between 0° and 180° in steps of 15°. Contrary to the analytic ansatz chosen in Ref. 3 in here the derivative of $\Delta E(\Theta;m)$ with respect to $\cos(\Theta)$, $d\Delta E(\Theta;m)/d\cos(\Theta)$ [see Eq. (3)], was determined numerically by a linear least-squares fitting procedure,[11] since then $\tau(\Theta;m)$ can easily be calculated sufficiently accurate for any value of Θ between 0 and π.

In Fig. 1 a characteristic case is depicted—namely, for 20 ML of the spacer. In this figure in the top row the twisting energy $\Delta E(\Theta;m)$ and the sheet resistance $r(\Theta;m)$ are displayed versus the rotation angle Θ, in the bottom row the reduced current $I_0(\Theta;m)$ [see Eq. (2)] and magnetoresistance $MR(\Theta)$, defined as $MR(\Theta;m)=[r(\Theta;m)-r(0;m)]/r(\Theta;m)$. Since in all other investigated cases the variation of $\Delta E(\Theta;m)$ and $r(\Theta;m)$ with Θ is of similar shape, for a characterization of $\Delta E(\Theta;m)$ only the necessary and sufficient expansion coefficients $a_s(m), s\leqslant 3$ [see Eq. (3)] are shown in Fig. 2 with respect to the number of spacer layers m. The value of $MR(\pi;m)$ merely drops by about 2% from 20 ML to 30 ML and need not to be shown graphically. From Fig. 2 one can see that $a_0(m), a_1(m) \ll a_2(m)$—i.e., that the coefficient for the $(\cos\Theta)^2$ term, which has to be regarded as an "anisotropy" term, is by far leading.

Since according to the plot for the reduced current $I_0(\Theta;m)$ in Fig. 1 applying a current does not necessarily switch one collinear configuration for the other, this indicates that current-induced switching is perhaps even more complicated than originally thought and that models based on spin-up and spin-down electrons (strict collinearity) most likely are not suited to describe this kind of situation.

A distinction between the various cases to be possibly encountered can easily be made by recalling the expression for the current in Eq. (2) and the fact that for solving the Landau-Lifshitz-Gilbert equation[3] the first-order derivative of $\Delta E(\Theta;m)$ with respect to $\cos\Theta$ is needed. Let Θ_0 characterize the ground state $[\Delta E(\Theta_0;m)=0]$—i.e., the state lowest in energy—and $t(\Theta_i,\Theta_j;m)$ the minimal time needed to force the system from the state corresponding to Θ_i into the state corresponding to Θ_j. Then at present it seems that in principle the following situations can occur:

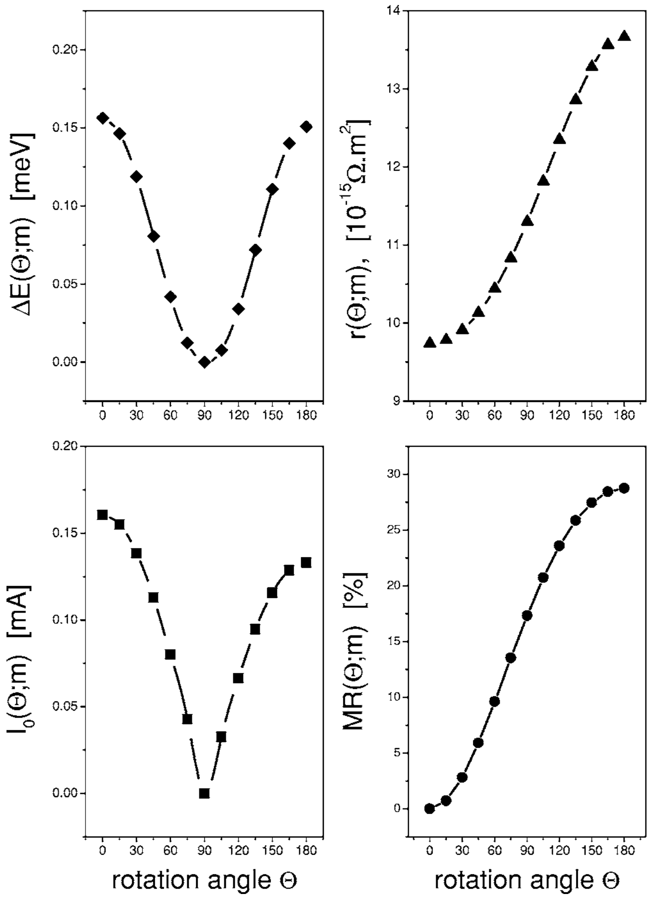

FIG. 1. Twisting energy $\Delta E(\Theta;m)$, sheet resistance $r(\Theta;m)$ (top row), reduced current $I_0(\Theta;m)$, and magnetoresistance $MR(\Theta;m)$ (bottom row) for $m=20$ ML of Cu.

$$\Theta_0 = 0,\pi:\ \tau(m) = |t(0,\Theta_1;m)| + t(\Theta_1,\pi;m);$$

$$\Theta_1:\ \Delta E(\Theta_1;m) = \max\{\Delta E(\Theta;m)\}, \qquad (4)$$

$$\Theta_0 \neq 0,\pi:\ \tau(m) = \begin{cases} t(0,\Theta_0;m), \\ |t(\Theta_0,\pi;m)|, \end{cases} \qquad (5)$$

where $\tau(m)$ is the actual minimal switching time—namely, the minimal time[6] needed to excite the system from the ground state to a collinear final state. It should be noted that the condition $\Theta_0 \neq 0,\pi$ in Eq. (5) is rather important, since in the absence of interdiffusion this condition does not apply for most spacer thicknesses of the system Co/Cu/Cu.[3] If, however, Eq. (5) applies, then the two possible solutions can be distinguished by introducing the convention

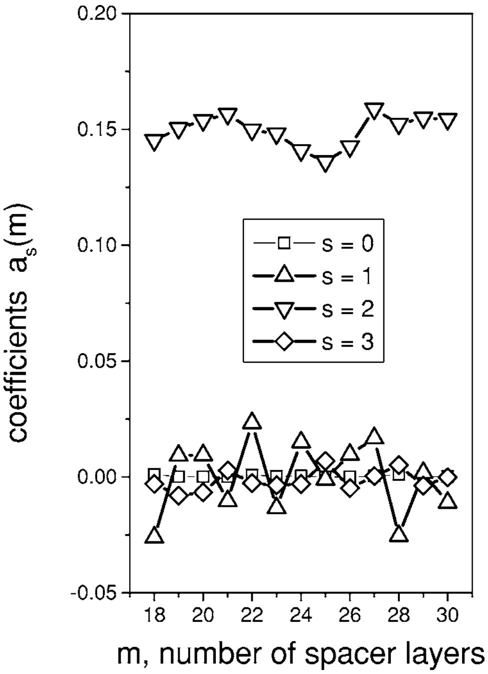

FIG. 2. Expansion coefficients a_s [see Eq. (3)] for $s \leqslant 3$ versus the number of spacer layers.

$$I(\Theta;m) = \begin{cases} +\sqrt{\langle A_0/\tau(\Theta;m)\rangle} I_0(\Theta;m), & \Theta \leqslant \Theta_0, \\ -\sqrt{\langle A_0/|\tau(\Theta;m)|\rangle} I_0(\Theta;m), & \Theta \geqslant \Theta_0. \end{cases} \quad (6)$$

A definition of the critical current I_{crit}—namely, the current needed to switch the system from the ground state into a final collinear state—has to take into account all possibilities: namely,

$$\Theta_0 = 0, \pi\colon\ I_{crit}(m) = \max\{I(\Theta;m)\},$$

$$\Theta_0 \neq 0, \pi\colon\ I_{crit}(m) = \begin{cases} I^{+}_{crit}(m) = \max\{I(\Theta;m) | \Theta \leqslant \Theta_0\}, \\ I^{-}_{crit}(m) = \min\{I(\Theta;m) | \Theta \geqslant \Theta_0\} \end{cases} .$$

All these different cases are immediately evident, considering the anisotropy term in the following (more traditional) definition for the twisting energy:

$$\Delta E(\Theta;m) = E(\Theta;m) - E(0;m) = b_1(m)[1-\cos(\Theta)] + b_2(m)[\cos(\Theta)]^2 + \cdots,$$

since then

$$\Theta_0 = 0, \pi, \quad b_2(m) \geqslant 0,$$

$$\Theta_0 \neq 0, \pi, \quad b_2(m) < 0,$$

provided, of course, that $|b_1(m)| \leqslant 2|b_2(m)|$—i.e., that the first term, the so-called interlayer exchange coupling term, is small enough, which definitely is the case for reasonably thick spacers.

In Fig. 3 the two critical currents $I_0(0;m)$ and $I_0(\pi;m)$ and the minimal times $t(0,\pi/2;m)$ and $t(\pi,\pi/2;m)$ are shown versus the number of Cu spacer layers. It is interesting to note that in all investigated cases $I_0(\pi;m) \leqslant I_0(0;m)$, which seems to be an intrinsic property.

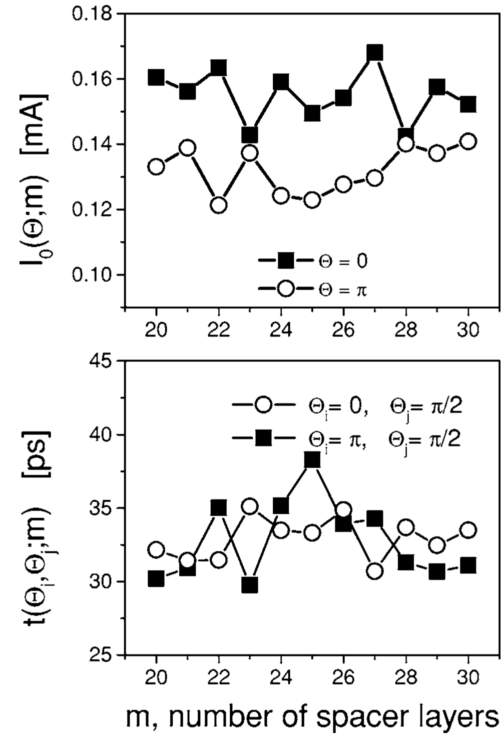

FIG. 3. Reduced critical current $I_0(\Theta;m)$ (top) and minimal time $t(\Theta_i,\Theta_j;m)$ (bottom) versus the number of Cu spacer layers.

From Eq. (2) it is evident that the size of the critical current is determined by (1) the unit area, which is an experimental parameter, (2) the minimal time, and (3) the reduced critical current. As discussed in Ref. 3 the minimal time depends in a rather complicated way on the change of the twisting energy with respect to $\mathbf{M}/|\mathbf{M}| = \cos\Theta$, where $\mathbf{M}$ is the magnetic moment averaged over all layers of the thin magnetic slab—i.e., offers only an indirect way to manipulate the critical current. Therefore, it seems that in order to reduce the critical current—besides reducing interdiffusion—one has to concentrate on the ratio of the twisting energy and the sheet resistance. Both quantities can be expressed as a sum over layer-dependent quantities (for details see also Refs. 5 and 7),

$$\Delta E(\Theta;m) = \sum_{i=1}^{n} \Delta E_i(\Theta;m) = \Delta E_L(\Theta;m) + \Delta E_R(\Theta;m), \quad (7)$$

$$r(\Theta;m) = \sum_{i=1}^{n} r_i(\Theta;m) = r_L(\Theta;m) + r_R(\Theta;m), \quad (8)$$

where for matters of simplicity L comprises all atomic layers of the thick magnetic slab and the adjacent half of the spacer layers and R the other half of the spacer layers and the thin magnetic slab. It is well known that both $\Delta E(\Theta;m)$ and $r(\Theta;m)$ are mostly determined by the interfaces between the magnetic slabs and the spacer. Therefore, the simplest way to reduce the critical current is to increase the contribution to the sheet resistance from the left part of the system, $r_L(\Theta;m)$—i.e., from the thick magnetic slab—since there (the orientation of the magnetization is kept fixed) the contribution to the switching energy is negligible. $r_L(\Theta;m)$ can be increased either by increasing the chemical disorder in this part of the system (small effect) or by putting in additional interfaces in terms of an additional number of layers of a different material such as, for example, Co_xFe_{1-x} (large effect). In manipulating only the right part of the system—i.e., the thin magnetic slab—by adding additional interfaces, $\Delta E(\Theta;m)$ also increases and therefore the net effect might turn out to be very small or even unwanted.

Assuming an area of 400×100 [nm^2] as described very recently[12] for $Cu/Co_{90}Fe_{10}$ nanopillars and using a switching time of about 0.03 [ns] and a reduced critical current of about 0.15 [mA] (see Fig. 3), the critical current amounts to about 1.6×10^{-3} [mA], which clearly is by a factor of about 1000 smaller than for the cited nanopillars. It should be noted, however, that in the calculations neither the additional Ru spacer nor the IrMn pinning layer or the Ta cap present in the experimental samples is included, all of them adding to both the twisting energy and the sheet resistance. Furthermore, most likely at the various interfaces in the experimental system interdiffusion effects and macroscopic roughness apply, the latter being rather difficult to deal with in a quantitative manner. It also should be noted that only at zero temperature can total energy differences such as defined in Eq. (1) be related to the free energy appearing in the Landau-Lifshitz-Gilbert equation.

Despite these drawbacks a few surprising features of the experimental data[12] can indeed be deduced from the present results: namely, (1) the size of the measured negative current (in the notation of Ref. 12 leading from antiparallel to parallel) is smaller than the positive one (see in particular the top part of Fig. 3) and (2) when applying a small external magnetic field the negative current is reduced while the positive current remains more or less unchanged. The latter feature can easily be understood if the angle $\Theta_0(H)$ that defines the ground state in the presence of a magnetic field H is increased in comparison to the case of a vanishing external field—i.e., if $\Theta_0(H)>\Theta_0(0)$ (see, e.g., Fig. 1).

In conclusion it can be said that (1) the initial state in current-induced switching does not necessarily have to be a collinear state (either parallel or antiparallel) and (2) that theoretical concepts based on spin-up and spin-down electrons only might be misleading in the case of noncollinearity, since obviously anisotropy effects can be rather important. Furthermore, the results shown suggest a promising way to reduce the critical current for current-induced switching in spin-valve-related systems by simply manipulating the composition and the design of the thick magnetic slab.

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