Micromagnetic modeling of magnetization switching driven by spin-polarized current in magnetic tunnel junctions

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This paper presents results of micromagnetic simulations of magnetization switching driven by spin-polarized current in magnetic tunnel junctions. For the studied structures, and for all the simulated currents, the switching occurs via nucleation process. A complete study of how a misalignment of the applied field and nonidealties in the shape of the sample affect the switching behavior has also been performed. The main results are as follows: (a) The switching mechanism does not change qualitatively by introducing a misalignment and (b) In contrast, the switching mechanism changes qualitatively when a nonideal shape is introduced. Lastly, simulations that include the effects of a 77 K thermal bath are presented; these indicate that the switching times are shorter than for zero temperature simulations (sometimes also less than 50%).


I. INTRODUCTION

A sufficiently large spin-polarized current (SPC) can apply a torque to a nanoscale ferromagnet that can either invert the magnetization of the ferromagnet or excite persistent dynamics.\textsuperscript{1,2} These behaviors have been experimentally observed in both spin valves (SVs) and magnetic tunnel junctions (MTJs).\textsuperscript{4} The latter shows promise as high performance magnetic random access memory. A MTJ is composed of two ferromagnetic layers separated by a thin insulator. One of the ferromagnetic layers [pinned or fixed layer (PL)] is either thicker than the other [free layer (FL)] or exchanged biased with an antiferromagnetic material.\textsuperscript{5,6} The resistance of the device depends on the relative orientation of the magnetization of the ferromagnets, giving rise to a tunneling magnetoresistance (TMR) defined as \((R_{AP}−R_{P})/R_{P}\), where \(R_{AP}\) and \(R_{P}\) are the resistances of the antiparallel (AP) and parallel (P) configurations of the magnetization of the two layers, respectively.\textsuperscript{4} While the SPC necessary to invert the magnetic state in MTJs is comparable with that of SVs, there is a more restrictive physical limit on the maximum value of applied current due to the breakdown voltage of the tunnel barrier.\textsuperscript{4} In addition, the possibility to excite microwave oscillations in MTJs opens important potential applications such as high impedance spin-transfer-driven oscillators.\textsuperscript{7} Furthermore, these could form the basis of a nanometer scale radio frequency detector.\textsuperscript{1,4,6}

From the technological point of view, MgO tunnel barriers in CoFe/MgO/CoFe pillars show the best performance so far (e.g., with respect to an AlO\textsubscript{2} tunnel barrier), presenting a high TMR (of the order of 200%) and an efficiency larger than 60% for the spin polarization.\textsuperscript{6,8}

This paper presents the results of micromagnetic simulations of MTJs patterned from thin films consisting of CoFe(8 nm)/Al\textsubscript{2}O\textsubscript{3}(0.8 nm)/Py(4 nm) with an elliptical cross section \((90×35 \text{ nm}^2)\), where the CoFe and the Py are the PL and the FL, respectively. We consider the easy axis of the ellipse as the \(x\) axis and the in-plane hard axis as the \(y\) axis. This device has been chosen because it is possible to identify its model parameters by means of the results presented in Ref. 9, which show experimental data related to these structures when a copper spacer and a third ferromagnetic layer (which acts as a second fixed layer) have been added. We use the model parameters for the torque and the thermal behavior determined from experimental data presented in Ref. 9 for each magnetic configuration of the fixed layers. We will begin by describing the behavior of this more complex structure and then we will present our simulations of the simple MTJ structures.

Section II describes the numerical details of the model. Sections III and IV present results of micromagnetic simulations of magnetization reversal driven by SPC in MTJs either with one or two PLs. Also, simulations were performed to study (a) the effects of a misalignment of the applied field with respect to the easy axis, (b) the effect of nonidealties in the elliptical shape at zero temperature, and (c) the thermal effects at a bath temperature of 77 K. Conclusions are presented in Sec. V.

II. MODEL AND NUMERICAL DETAILS

From the theoretical point of view, both macrospin\textsuperscript{10,11} or full micromagnetic model\textsuperscript{12-14} can be used to explain the

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results of experiments related to magnetization reversal and dynamics driven by a SPC in a ferromagnet. The former is able to reproduce the experimental behavior in some cases qualitatively, either numerically or analytically. On the other hand, the micromagnetic model also provides spatial information about the magnetization configuration, and therefore gives a deeper understanding of switching processes and magnetization dynamics. We present micromagnetic simulations of the magnetization reversal driven by SPC computed by numerically solving the Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation,14

\[
(1 + \gamma^2) \frac{d\mathbf{m}}{d\tau} = - (\mathbf{m} \times \mathbf{h}_{\text{eff}}) - \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{h}_{\text{eff}}) - \frac{g|\mu_B|}{|e|} gT(\mathbf{m}, \mathbf{m}_p)[\mathbf{m} \times (\mathbf{m} \times \mathbf{m}_p)]
\]

where \(g\) is the gyromagnetic splitting factor, \(\gamma_0\) is the gyromagnetic ratio, \(\mu_B\) is the Bohr’s magneton, \(\alpha\) is the damping parameter, \(j\) is the current density (in this paper it is considered positive when flows from the PL to the FL), \(L_e\) is the thickness of the FL, \(e\) is the electron charge, \(\mathbf{m} = M/M_s\) is the normalized magnetization of the FL, \(\mathbf{m}_p = M_p/M_{SP}\) is the normalized magnetization of the PL, \(M_s\) and \(M_{SP}\) are the saturation magnetization of the FL and the PL, respectively, \(d\tau = \gamma_0 M_s dt\) represents the dimensionless time step, while for the scalar function \(g_T\) we have used the expression proposed by Slonczewski in 2005.

Starting from this experimental finding that a decreasing in TMR does not indicate a decrease in the spin polarization, we consider \(\eta_2\) constant in our simulations for both positive and negative current densities. A different case has been considered by others.16

The effective field \(\mathbf{h}_{\text{eff}}\) is given by the following equation:

\[
\mathbf{h}_{\text{eff}} = \mathbf{h}_{\text{exch}} + \mathbf{h}_{\text{anis}} + \mathbf{h}_{\text{ext}} + \mathbf{h}_M + \mathbf{h}_{\text{Amp}} + \mathbf{h}_{\text{AF}},
\]

where \(\mathbf{h}_{\text{exch}}, \mathbf{h}_{\text{anis}}, \mathbf{h}_{\text{ext}}, \mathbf{h}_M\) are the standard micromagnetic contributions from exchange, anisotropy, external, and demagnetizing fields, \(\mathbf{h}_{\text{Amp}}\) and \(\mathbf{h}_{\text{AF}}\) are the Ampere field due to the current and the magnetostatic coupling between the PL and the FL. These last two contributions cannot be taken into account in the macrospin approximation. Previous simulations show that both play a crucial role in reversal processes and magnetization dynamics.14,17

We do not consider magnetocrystalline anisotropy since it is expected to be very low in Py. We also use \(M_s = 644 \times 10^5\) A/m, \(M_{SP} = 1.15 \times 10^6\) A/m, \(\alpha = 0.01\), and an exchange constant of \(1.3 \times 10^{-11}\) J/m.

The thermal behavior of the structure has been modeled considering the experimental data of the MTJ when a copper spacer (6 nm) and a CoFe layer (5 nm) have been added.13 Predicted by Berger,18 this introduces an additional torque which can be modeled as in the SV using the polarizing function computed by Slonczewski in 1996.10

\[
g_{SV}(\theta) = \begin{cases} -4(1 + \eta^2) \cos(\theta)/4 & \text{if } \text{the two fixed layers are aligned} \\ 2(1 + \eta^2) \cos(\theta)/4 & \text{if } \text{the two fixed layers are antialigned} \\ 0 & \text{if } \text{the two fixed layers are } \theta = \pi - \theta \text{ and } \eta \text{ is the polarization factor which we consider 0.35 for the CoFe.} \end{cases}
\]

The total spin torque depends on the relative configuration of the magnetization of the two fixed layers. If they are aligned, the torques exerted by electrons transported from each fixed layer are in opposite directions, which reduces the overall spin torque exerted on the FL. On the other hand, when the two fixed layers are antialigned, the torques are exerted in the same direction, and the total effect is the sum. The total polarization function is \(g_T(\theta) = g_{SV}(\theta) + g_T(\theta)\) if the two fixed layers are aligned or antialigned, respectively. We have computed \(\eta_2 = 0.3\) by fitting the experimental values of the critical currents obtained at 5 K (two PLs antialigned), when a field of 26 mT is applied (we did not include thermal effects). Theoretical critical currents are around \(I_{AP} = 0.18\) mA and \(I_{P-AP} = -0.15\) mA, these are very close to the experimental ones. Figure 1 displays all the torques versus the angle \(\theta\) in unit of \(2\mu_B/L_e e\); SV is the torque in a spin valve CoFe(5 nm)/Cu(6 nm)/Py(4 nm) \((\eta = 0.35)\), MTJ is the one in a magnetic tunnel junction CoFe(8 nm)/AlO(0.8 nm)/Py(4 nm) \((\eta = 0.3)\), and MTJ2(AP) and MTJ2(P) are the torques in a magnetic tunnel junction with the second fixed layer \([\text{CoFe}(8 \text{ nm})/\text{AlO}(0.8 \text{ nm})/\text{Py}(4 \text{ nm})/\text{Cu}(6 \text{ nm})/\text{CoFe}(5 \text{ nm})]\) when the two fixed layers are antialigned or aligned (absolute value), respectively.

In our calculations, we use a time step of 28 fs. Simulations performed with shorter time step gave the same results exactly. The samples where discretized into cells of 2.5 \(\times 2.5 \times 4.0\) nm\(^3\). Simulations have also been performed (at zero temperature) with cells of 2.0 \(\times 2.0 \times 2.0\) and 2.5 \(\times 2.5 \times 2.0\) nm\(^3\), giving rise to very similar results, where the magnetization dynamics vary by less than 5%.

In order to take into account the effect of the temperature, we consider that the experimental data are well-de-
scribed by current dependent activation barriers that agrees with the prediction of the Landau-Lifshitz-Gilbert (LLG)-based models.21 We include in our micromagnetic simulations a thermal field \( h_{th} \) as an additive random field to the deterministic effective field [see Eq. (2)] for each cell, which leads to a definition of the stochastic Langevin-Landau-Lifshitz-Gilbert (LLLg) equation.21 In order to take into account the SPC terms in this formulation, we assume that the spin torque does not contain a fluctuating field, the fluctuating field is independent of the spin torque, and the magnetization configuration of the PLs does not depend on the temperature.22 The \( h_{th} \) is a random fluctuating three-dimensional vector quantity given by

\[
h_{th} = \frac{\xi}{M_s} \sqrt{\frac{2}{\mu_0 \gamma_0 \Delta V M_s \Delta t}} \tag{3}
\]

where \( K_B \) is the Boltzmann constant, \( \Delta V \) is the volume of the computational cubic cell, \( \Delta t \) is the simulation time step, \( T_s \) is the true temperature of the sample,19,22 and \( \xi \) is a Gaussian stochastic process.

The thermal field \( h_{th} \) satisfies the following statistical properties:

\[
\langle h_{th,k}(i) \rangle = 0
\]

\[
\langle h_{th,k}(i), h_{th,l}(i') \rangle = D \delta_{kl} \delta(t - t') \tag{4}
\]

where \( k \) and \( l \) represent the Cartesian coordinates \( x \), \( y \), and \( z \). According to this expression, each component of \( h_{th} = (h_{th,x}, h_{th,y}, h_{th,z}) \) is a space and time independent random Gaussian distributed number (Wiener process) with zero mean value. The constant \( D \) measures the strength of thermal fluctuations [it can be computed by means of Eq. (3)], and its value is obtained from the Fokker-Planck equation.21

The temperature of the sample has been computed using the results of Ref. 9. When the PLs are parallel, the total torque is reduced and it is possible to model the thermal behavior. Finally, the temperature of the sample \( (T_s) \) is given by the following equation:

\[
T_s = \sqrt{T_B^2 + \beta I^2} \tag{5}
\]

where the \( T_B \) is the bath temperature, \( I \) is the current, and \( \beta \) has been computed for both switching processes P \( \rightarrow \) AP and vice versa independently \( (\beta_{P\rightarrow AP} = 4.4 \times 10^5 \text{ K}^2/\text{mA}^2 \text{ and } \beta_{AP\rightarrow P} = 4.7 \times 10^5 \text{ K}^2/\text{mA}^2) \).9 Regarding the thermal behavior, here we will present simulations at a bath temperature of 77 K.

III. RESULTS OF MTJ WITH TWO FIXED LAYERS

First, we performed simulations to describe the behavior of two fixed layers MTJs (PLs antialigned). We simulated switching from both P \( \rightarrow \) AP and vice versa (with an applied field of 26 mT along positive \( x \) axis). Since all our simula-
tions show that magnetization reversal occurs in the same way qualitatively, we will present only one example in detail. Figure 2 shows the time evolution of the three components of the average magnetization $\langle m_x \rangle$ top (the insets are the zoom in the range of 6–9 and 10–14 ns), $\langle m_y \rangle$ bottom left (with a time range of 10–14 ns), $\langle m_z \rangle$ bottom right (with a time range of 10–14 ns]) for AP to P switching ($I$ =0.25 mA) that occurs at around 13 ns. Initially, there is an oscillation of the spins at the boundary of the structure [Fig. 3(a), 9.1 ns, phase 1] which increases [Fig. 3(b), 10.9 ns], eventually nucleating a stable 360° domain configuration [Fig. 3(c), 11.4 ns, phase 2]. In the last step, there is domain wall motion which gives rise to a 180° domain configuration [Fig. 3(d), 12.5 ns, phase 3] before total inversion. We note that switching occurs via a nucleation process, and that the switching mechanisms obtained with other currents in the range of 0.22–0.3 mA are qualitatively the same. The P →AP reversals also show similar phases magnetization dynamics (not shown).

We performed a systematic study considering a set of nonideal elliptical shapes [see Fig. 4 (right)], computed from scanning electron microscopy images directly [see Fig. 4 (left)]. Figure 5 shows a comparison among the temporal evolution of the $\langle m_x \rangle$ ($\langle m_y \rangle$ shape B offset+1 and $\langle m_z \rangle$ shape A offset+2) for the three nonideal shapes studied. The AP →P switching (with $I$=0.25 mA, and an applied field of 26 mT) occurs via a nucleation process, but in a longer time than in the ideal case and with a different spatial evolution of magnetization. For example, for shape A, after the 180° domain configuration forms, the defects at the boundary of the structure pin one side of the domain wall which sweeps back and forth (Fig. 6 top and bottom) until it is expelled in the bottom part of the structure. For larger currents, the switching time tends to be independent of the shape. A similar study performed for the P →AP switching, however, shows a different result. In particular, the simulations show that all of these nonidealities decrease the switching time as compared to the time for ideal elliptical shapes. In these cases, the switching also occurs via a complex nucleation process (in some cases there are also vortex configurations), indicating that the differences can be only observed by full micromagnetic modeling since the spatially averaged magnetization behavior is similar.

For the ideal elliptical shape, we have also performed simulations where we include the thermal effects at $T_B$ =77 K [the temperature of the sample has been computed by Eq. (5)]. We find that the reversal processes are thermally activated, giving rise to shorter switching times (less than 50% with respect to the zero temperature model). The inset of Fig. 5 shows the temporal evolution of the average $x$ component of the magnetization $\langle m_x \rangle$ (50 iterations) for the ideal shape (with an $I$=0.25 mA, $T_B$=77 K, and an applied field of 26 mT). It is to be noted that the temperature introduces a spread in the phase of magnetic oscillations. This causes the $\langle m_x \rangle$, averaged over 50 iterations of simulation, to appear smoother.

**IV. RESULTS OF SIMPLE MTJ**

A complete theoretical study of the magnetization reversal in the simple MTJ shows that the switching behavior is consistent with the experimental observations of quasistatic switching. The study has been performed at two different
fields (50 and 30 mT) applied along the x axis. Figure 7 shows the temporal evolution of the three average components of the magnetization \(\langle m_x \rangle\) top (the insets are the zoom in the range of 13–15, 48–50, and 60–65 ns), \(\langle m_y \rangle\) bottom left (with a time range of 53–67 ns), and \(\langle m_z \rangle\) bottom right (with a time range of 53–67 ns) for a switching process AP→P (with an applied field of 50 mT and \(I=0.3\) mA). It occurs via a nucleation process in \(\sim 65\) ns, in three main phases comparable to the case with two fixed layers described above, with timings as follows: (phase 1) 0–30 ns, (phase 2) 30–55 ns, and (phase 3) 55–65 ns.

In order to analyze the detailed mechanism of the switching, the spatial configuration of the excited modes has been studied by means of the micromagnetic spectral mapping technique (MSMT). The procedure consists of performing a fast Fourier transform (FFT) of the temporal evolution of magnetization for each computational cell and then plotting the two dimensional (2D) spatial distribution of the spectral density at the specific frequency of the mode to be analyzed. For each cell, the FFT is computed by the following equation:

\[
S_Y(x_i, y_m, z_n, f) = \sum_h m_Y(x_i, y_m, z_n, t_h) e^{-j2\pi f t_h},
\]

where the indexes \(l, m,\) and \(n\) identify a computational cell, \(t_h\) is the discretized time step, and \(f\) is the frequency. The total spectrum is

\[
S_T(f) = \frac{1}{N} \sum_{m,n} |S_Y(x_i, y_m, z_n, f)|^2
\]

where \(N\) is the number of the cells. Considering the switching shown in Fig. 7, the total spectra of \(m_x\) referred to phases 1, 2, and 3 are displayed in Fig. 8 from the bottom to the top, respectively. Only a single mode is present (phase 1, \(f_M=7.83\) GHz). As time progress, this mode decreases in frequency (phase 2, \(f_M=6.76\) GHz). Finally, before switching, the main peak widens and gives rise to an asymmetric spatial configuration of that mode (\(f_M=5\) GHz, phase 3). This shift in frequency is due to the nonlinear behavior of the LLG equation.

Figure 9 displays the spatial configuration of the main mode (\(f_M\)) for the phases 1, 2, and 3. A gray scale is used to describe the power spectral density of the mode for each cell (increasing from white to black) and it is proportional to \(S_T\) of that cell and that frequency.

In order to study the importance of the alignment of the device with the applied field, we performed a systematic study with the field (applied in plane) tilted 5° and 10° with respect to the easy axis. Figure 10 shows the temporal evolution of the average \(x\) component of the magnetization in presence of a tilted angle for the same switching of Fig. 7. For all of the simulated currents, the switching time is shorter when there is a misalignment of the field with respect to the easy axis. This is due to a large initial value of the torque. In these cases, the dynamics of the switching (in terms of excited mode) do not change qualitatively (not shown). We also performed a complete study of the effect of non ideal shapes in simple MTJs that shows the same results presented in the previous section for a MTJ with two fixed layers.

For an ideal ellipse, we also consider the effect of a finite temperature. As we observed previously, the simulations indicate that the switching processes are thermally activated (with switching times less than the 50% with respect to the
zero temperature). The inset of Fig. 10 shows the temporal evolution of the \( x \) component of the average magnetization \( m_x \) (with \( I = 0.3 \) mA and an applied field of 50 mT along \( x \) axis) at \( T_B = 77 \) K (50 iterations). As can be noted the reversal occurs in around 20 ns. The spread of the switching time due to the misalignment of the field decreases while the temperature increases, at \( T_B = 77 \) K it is negligible.

V. CONCLUSIONS

We have simulated the magnetization reversal driven by SPC in two different MTJs by means of a micromagnetic model. In all the simulations, the switching occurs via nucleation process. Magnetization reversal can be described in three main phases that are characterized by different magnetization motion and a different spatial configuration of the excited modes. The frequency of the main mode goes through a redshift due to the nonlinearity of the LLGS equation.

Misalignment of the applied field with respect to the easy axis does not qualitatively change the behavior of the switching, but it reduces the switching time because the initial torque is larger and the physical symmetry of the structure is broken by the existence of a nonzero \( y \) component of the applied field. On the other hand, a systematic study performed to determine the effect of nonidealities of the shape in the magnetization reversal reveals that the mechanism of inversion changes qualitatively depending on the shape. These nonidealities can either increase or decrease the switching time. Lastly, we showed that the switching is thermally activated giving rise to a smaller switching time increasing temperature.

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15J. Slonczewski, Phys. Rev. B 71, 024411 (2005). It should be noted that the denominator \( [1 + \eta \gamma \cos \theta] \) is an approximation in the limit of low TMR for the conversion of a torque proportional to voltage but independent of angle into a torque proportional to current, thus introducing an
angular term. If, however, the TMR is very high, the bias dependence of
the TMR should be included in the angular term explicitly.
16 Y. Zhang, Z. Zhang, Y. Liu, B. Ma, and Q. Y. Jin, J. Appl. Phys. 99,
08G515 (2006).
17 G. Finocchio, M. Carpentieri, B. Azzerboni, L. Torres, E. Martinez, and L.
(2004).
21 W. F. Brown, Jr., Phys. Rev. 130, 1677 (1963); J. L. Garcia-Palacios and F.
23 M. Grimsditch, L. Giovannini, F. Montoncello, F. Nizzoli, G. Leaf, H.
Kaper, and D. Karpeev, Physica B 354, 266 (2004); R. D. McMichael and
M. D. Stiles, J. Appl. Phys. 97, 10J901 (2005); G. Finocchio, I. Krivorotov,
M. Carpentieri, G. Consolo, B. Azzerboni, L. Torres, E. Martinez, and