Field-free spin–orbit torque perpendicular magnetization switching in ultrathin nanostructures

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Magnetic-field-free current-controlled switching of perpendicular magnetization via spin–orbit torque (SOT) is necessary for developing a fast, long data retention, and high-density SOT magnetoresistive random access memory (MRAM). Here, we use both micromagnetic simulations and atomistic spin dynamics (ASD) simulations to demonstrate an approach to field-free SOT perpendicular magnetization switching without requiring any changes in the architecture of a standard SOT-MRAM cell. We show that this field-free switching is enabled by a synergistic effect of lateral geometrical confinement, interfacial Dzyaloshinskii–Moriya interaction (DMI), and current-induced SOT. Both micromagnetic and atomistic understanding of the nucleation and growth kinetics of the reversed domain are established. Notably, atomically resolved spin dynamics at the early stage of nucleation is revealed using ASD simulations. A machine learning model is trained based on ~1000 groups of benchmarked micromagnetic simulation data. This machine learning model can be used to rapidly and accurately identify the nanomagnet size, interfacial DMI strength, and the magnitude of current density required for the field-free switching.

INTRODUCTION

Magnetization switching through spin–orbit torque (SOT) is of great recent interest due to its potential applications in SOT magnetoresistive random access memory (SOT-MRAM), which is expected to have faster write speed, lower write energy, and higher endurance than the currently used spin-transfer torque MRAM1,2. An SOT-MRAM cell integrates a magnetic tunnel junction (MTJ) on top of a heavy-metal layer. During writing, an in-plane charge current flowing into the heavy-metal layer is converted to a perpendicular spin current via the spin Hall effect (SHE)3–5, as schematically shown in Fig. 1a. The spin current then flows into the overlaying magnetic layer and switch its magnetization via the SOT. SOT has been used to switch both the perpendicular6 and in-plane7 magnetization, but perpendicular switching is more attractive for SOT-MRAM applications because it is faster8 and more scalable9. However, SOT-mediated perpendicular magnetization switching typically requires a simultaneous application of an in-plane bias magnetic field5,7. This in-plane magnetic field is not desirable for practical SOT-MRAM application, because it reduces the thermal stability of perpendicular magnetization and because it may cause crosstalk among neighboring SOT-MRAM cells.

Thus far, many approaches have been proposed for achieving a magnetic-field-free SOT-mediated perpendicular magnetization switching. An early proposed approach is to fabricate asymmetric multilayer stack, such as engineering a thickness gradient into the magnetic layer10 or its overlying oxide9 or heavy-metal layer underneath11. Such structural asymmetry generates a unidirectional effective perpendicular magnetic field, leading to a deterministic switching. Approaches proposed thereafter aim to introduce a built-in in-plane bias magnetic field, generated by an in-plane magnetized reference layer in the MTJ12,13 or an antiferromagnetic heavy-metal with in-plane magnetized sublattices14,15. Other approaches include (1) adding a ferroelectric layer below the heavy-metal to harness the effect of electric-field-switchable spontaneous polarization15 or piezoelectric strain16, (2) adding another heavy-metal layer to generate competing spin currents17; (3) applying an out-of-plane charge current from the top terminal of the MTJ to generate an assisting STT18; and (4) engineering the geometry of the ferromagnetic layer19,20. Most recently, micromagnetic simulations21,22 have suggested that a magnetic-field-free SOT perpendicular magnetization switching can also be achieved by simultaneously controlling the lateral size of the magnetic layer, the strength of the Dzyaloshinskii–Moriya interaction (DMI) arising from the ferromagnet/heavy-metal interface, and the magnitude of applied charge current density within an intermediate range. Compared with earlier proposed approaches, this approach does not require any changes in the architecture of a standard perpendicular SOT-MRAM cell, which is important to practical applications.

In this article, we use both micromagnetic and atomistic spin dynamics (ASD) simulations (see “Methods”) to study the nucleation of the reversed magnetic domain and its subsequent growth during the two-step switching. Notably, the ASD model enables predicting the evolution of atomistic spin moment of each atom based on the actual lattice structure of the material, which leads to a generally more accurate description of the nucleation process, especially at its early stage when embryos (clusters of several atoms) are too small to be accurately described by micromagnetic model. We show that the lateral geometrical confinement, interfacial DMI, and current-induced SOT synergistically lead to a deterministic nucleation and growth process. Accordingly, it is found that the field-free SOT perpendicular switching occurs when the lateral size of the nanomagnet, the interfacial DMI strength, and the magnitude of applied current are all within an intermediate range. Furthermore, a decision-tree-based machine learning model is trained using data from about 1000 groups of benchmarked micromagnetic simulations, which is then used to rapidly and accurately identify the regime of successful two-step switching from a ternary parameter space comprising the lateral size of magnetic layer, interfacial DMI strength, and magnitude of charge current density.

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Published in partnership with the Shanghai Institute of Ceramics of the Chinese Academy of Sciences
RESULTS

Field-free SOT perpendicular switching in a standard SOT-MRAM cell

Consider a 40 nm diameter MgO/CoFeB/MgO/CoFeB bilayer nanodisks on top of a Pt layer as an example. Figure 1b shows the evolution of the average perpendicular magnetization \(<m_z>\) of the 1.1-nm-thick CoFeB nanodisk under a time-invariant \(J_c\). When \(J_c\) is relatively small (top panel of Fig. 1b), the SOT is insufficient to rotate the initially upward magnetization significantly. When \(J_c\) is large (middle panel), the SOT is large enough to switch the magnetization by 90° to the direction of net spin polarization \(\alpha\) (which is along the +x-axis, see Fig. 1a). This is consistent with the conventional belief that the SOT alone typically cannot reverse the polarity of an out-of-plane magnetization due to the inability to break mirror symmetry. However, an unconventional SOT switching appears under a moderate magnitude of current, showing a reversal of the out-of-plane magnetization component. As shown in the bottom panel of Fig. 1b, \(<m_z>\) equilibrates at a negative value (approximately \(-0.17\)) under \(J_c = 1.4 \times 10^{13} \text{A/m}^2\). This indicates that a majority portion of local magnetization vectors were flipped from up to down, and thereby provides a basis for realizing a two-step switching under a pulsed charge current. Specifically, if turning off the current when \(<m_z>\) equilibrates at 3.5 ns after turning on the current (see Fig. 1c) or evolves to its lowest negative value (at 0.3 ns, see Fig. 1d), the magnetization state will deterministically relax to its new equilibrium state with a downward magnetization (\(<m_z>\) approximatively \(-1\)).

Deterministic > 90° perpendicular switching under a time-invariant current

Thus, flipping a major portion (>50%) of local magnetization vectors from up to down (and vice versa) in a deterministic manner using SOT is the basis for the two-step switching, and is called “>90° switching” hereafter for convenience. Figure 2a-\(c\) shows the local magnetization distributions at several key time stages, including the initially upward magnetization with tilted vectors along the disk edges (0 ns), where the tilting occurs due to the co-action of interfacial DMI and lateral geometrical confinement (ref.24, also see “Methods”); the nucleation of downward domain (0.07 ns); the critical state at which \(<m_z>\) ~ 0 (0.18 ns), and the equilibrium state (0.71 ns), all under the time-invariant \(J_c\). Starting from the initially quasiuniform state where inwards tilting edge magnetization, the domain nucleation always occurs in the bottom left region (the third quadrant) of the disk under a \(J_c\) flowing along the \(-y\) direction. This is because only in this region, the out-of-plane SOT \(r_z^{\text{SOT}}\) and the out-of-plane SHE effective field \(H_y^{\text{SHE}}\) are both negative (as shown in Fig. 2f and explained in “Methods”). Such a nucleation mechanism is similar to that in a conventional SOT perpendicular magnetization reversal in the presence of in-plane bias magnetic field25-27. However, the growth kinetics of the downward domain we present herein under zero magnetic field (Fig. 2b-\(d\)) is different. Specifically, the curvature of the domain wall changes from an initially negative value (Fig. 2b) to almost zero when \(<m_z>\) ~ 0 (Fig. 2c), and then to a positive value (Fig. 2d). Figure 2e shows the trajectories of the domain wall motion during the entire process of >90° switching. It can be seen that the growth of downward domain is more favorable in the second and third quadrants of the disk, which is due to the fact that the out-of-plane SOT \(r_z^{\text{SOT}}\) is...
negative in both regions (see Fig. 2f). For further analysis, the evolution of the total out-of-plane torque $\tau_{z}^{\text{tot}}$ are plotted. The spatial distributions of $\tau_{z}^{\text{tot}}$ in the entire disk are shown in Fig. 2g–i, while the evolution of site-specific $\tau_{z}^{\text{tot}}$ along the domain wall is shown in Fig. 2j. Two key observations are noted. First, the $\tau_{z}^{\text{tot}}$ is negative in the front of the domain walls for most of the time during the wall motion, which is mainly because the out-of-plane SOT torque $\tau_{z}^{\text{SOT}}$ in front of the domain wall is always negative (see complete torque analysis in Supplementary Fig. 1). This negative $\tau_{z}^{\text{SOT}}$ can be inferred from its formula $\tau_{z}^{\text{SOT}} = -\gamma H_{\text{SOT}} m_{y} m_{z}$ where (1) the local $m_{y}$ is always positive during the wall motion (see Fig. 2b–d) to maintain the left-chirality of the domain walls (caused by the positive interfacial DMI strength $D$); (2) the local $m_{y}$ is always positive in front of the domain wall (which is the unswitched area); and (3) $\gamma$ is positive and the coefficient $H_{\text{SOT}}$ is positive under a positive $J_{z}$ (see “Methods”). Since the total out-of-plane torque $\tau_{z}^{\text{tot}}$ is negative in front of the wall, local magnetization vectors therein rotate deterministically from up to down. As a result, the domain wall moves forwards in a unidirectional manner and drives the magnetization distribution across the critical state of $\langle m_{z} \rangle < -0$ (Fig. 2c). Second, for most of the time, the $\tau_{z}^{\text{tot}}$ at the two ends of the domain wall (point “1” and “3” in Fig. 2e) are larger than that in the center (point “2”), leading to the formation of a positive domain wall curvature at equilibrium.

Repetable 180° perpendicular switching induced by either unipolar or bipolar current pulses

The above analyses show that the nucleation and growth of the downward domain during the >90° switching (step 1) and the subsequent relaxation to $\langle m_{z} \rangle$ approximately $-1$ (step 2) are both deterministic. We note that achieving such a two-step SOT perpendicular switching does not require the breaking of mirror symmetry. This feature allows for switching a perpendicular magnetization repeatedly with either a unipolar or bipolar (Supplementary Fig. 2) current pulse, which is not possible to achieve with other field-free SOT switching approaches and therefore adds flexibility in the way of writing information. Figure 3a shows the evolution of both the $\langle m_{z} \rangle$ and the total magnetic free energy density change $\Delta f_{\text{tot}}$ (see “Methods”) under a unipolar current pulse. As seen, the forward switching (up to down, $\langle m_{z} \rangle$ changing from 1 to $-1$) and the backward switching (down to up, $\langle m_{z} \rangle$ changing from $-1$ to 1) show exactly the same profile of $\Delta f_{\text{tot}}(t)$. As seen from the zoom-in view of $\Delta f_{\text{tot}}(t)$ in Fig. 3b, for both the forward and backward switching, the realization of the >90° switching (step 1) requires overcoming an energy density barrier for the nucleation of an oppositely oriented domain and another barrier (albeit small for this particular case) for pushing the domain wall forward at the critical state of $\langle m_{z} \rangle < 0$, both driven by the out-of-plane SOT torque $\tau_{z}^{\text{SOT}}$ as discussed above. Figure 3c shows the magnetization distributions at the initial and final stage of the switching as well as the two transitional states (where $\Delta f_{\text{tot}}$ peaks). It can be seen that the evolution of magnetization distributions during backward switching is symmetric to that in the forward switching. This explains why the free energy evolution during the backward switching is exactly the same as that in forward switching as shown in Fig. 3b. However, for the backward switching, the magnetization is initially pointing down and the edge magnetization tilts outwards due to the interfacial DMI, which is exactly opposite to the initial state in the case of forward switching. Therefore, the domain nucleation occurs at the bottom right region (the fourth quadrant) of the disk where the out-of-plane SOT $\tau_{z}^{\text{SOT}}$ and the out-of-plane SHE effective field $H_{x}^{\text{SHE}}$ are both positive since the polarity of the current $J_{z}$ remains unchanged. Likewise, the growth of upward domain is more favorable in the fourth and the first quadrants where the $\tau_{z}^{\text{SOT}}$ is positive.

DISCUSSIONS

Below we show that achieving a >90° out-of-plane SOT switching under a time-invariant current requires a balanced combination of the geometrical confinement (disk diameter), interfacial DMI...
The evolution of both the \( <m_y> \) and the total magnetic free energy density change \( \Delta f_{\text{tot}} \) (see “Methods”) in a 1.1-nm-thick, 40 nm diameter Co20Fe60B20 disk. A unipolar current pulse (magnitude: \( 1.4 \times 10^{13} \) A/m²; duration: 5.31 ns) is applied to the Pt underlayer. 

(a) zoom-in view of the \( \Delta f_{\text{tot}}(t) \) when \( <m_y> \) changes from \(-1\) to \(+1\) (upper panel), and when \( <m_y> \) changes from approximately \(-1\) to \(+0.21\) (lower panel). 

(b) Magnetization distributions at several key stages, all indicated by vertical dashed lines in (a). These stages include the initial and final stage of the forward \( (<m_y> \) changes from approximately \(-1\) to approximately \(+1\) in the disk edge (see Fig. 4b), and the critical stage where the domain wall has an almost zero curvature (2.28 and 12.90 ns for the forward and backward switching, respectively). 

(c) The switching diagram as a function of the disk diameter (40–63 nm). At smaller disk diameters, the CoFeB disk has a larger perpendicular magnetic anisotropy (PMA), defined as \( K_{\text{PMA}} = \frac{K_{\text{inter}}}{\mu_0} + K_{\text{shape}} \), where \( K_{\text{inter}} \) is the magnetic interfacial anisotropy (\( \sim 1.3 \) mJ/m² for CoFeB) and \( d \) is the disk thickness; the out-of-plane magnetic shape anisotropy \( K_{\text{shape}} \) is larger in smaller disks due to stronger geometrical confinement (see “Methods”). The enhanced PMA facilitates the alignment of magnetization along the \( z \)-axis, thereby reducing the extent of interfacial-DMI-induced magnetization tilting along the disk edge. As shown in Fig. 4b, the magnitude of the normalized in-plane magnetization \( m_p \) along the disk edge (see schematic in the inset) decreases as the disk diameter reduces. 

This trend continues until \( m_p \) becomes smaller than a threshold (\( \sim 7.22 \times 10^{-2} \)), below which the nucleation of reversed domain is not possible. As the disk diameter increases, \( m_p \) also increases and gradually approaches its saturation value (\( \sim 7.31 \times 10^{-2} \)). The latter is linearly proportional to \( D^2 \). A larger \( m_p \) will make it easier for the reversed domain to nucleate and hence facilitate the \( >90^\circ \) switching, demonstrated by the increasing disk diameter, because the interfacial DMI primarily tilts magnetization along the outermost edge of the disk. When \( \gamma_f \), becomes smaller than a threshold (\( \sim 0.88\% \)), the domain nucleation is also disabled, in other words, the numbers of flipped magnetization vectors are too small to trigger a nucleation. This is analogous to a classical nucleation process where the size of the unstable embryo cluster cannot grow large enough to exceed the critical nucleus size.

Furthermore, the fact that there exists a lower and an upper bound for the disk diameter suggests that the desirable \( >90^\circ \) perpendicular SOT switching may be more robust when the disk diameter is far away from the two bounds. In that case, both the \( m_p \) and \( \gamma_f \) can maintain a sufficiently large value, which synergistically facilitate the nucleation and thereby lead to a more robust switching. To test this hypothesis, we compared the success rate of the switching in the presence of a thermal fluctuation field at room temperature (see “Methods”) for the cases of 40, 50, and 60 nm based on 100 groups of repeated simulations for each case. It is found that the success rate in the case of 50 nm is as high as 98%, which is much higher than that in the case of 40 nm (50%) and 60 nm (54%) (see Supplementary Fig. 3). In this regard, the switching diagram in Fig. 4a allows us to infer the robustness of the switching under other combinations of current densities and disk diameters. We also note that this finding (that is, higher success rate in an intermediate disk size) is different from the perpendicular magnetization switching driven by current-induced spin-transfer torques [28] or voltage-controlled magnetic anisotropy [29,30], where the switching in larger-volume single-domain nanomagnets generally has a higher success rate due to the enhanced thermal stability [31,32].

Figure 4c shows the switching diagram as a function of the interfacial DMI strength \( D \) and the \( J_c \) under a constant disk.
diameter of 40 nm. As seen, the desirable >90° switching only appears within an intermediate range of DMI strength $D$ (0.2–3.2 mJ/m²) and an intermediate range of $J_c$. When $D$ is relatively small ($\leq 1$ mJ/m²), increasing $D$ reduces the $J_c$. This is because the resultant increase in both the $m_{IP}$ and $V_t$, as shown in Fig. 4d, reduces the energy density barrier for the nucleation of reversed domain (Supplementary Fig. 4). However, when $D$ is relatively large ($1.2 \leq D \leq 3.2$ mJ/m²), increasing $D$ increases the $J_c$, despite that both the $m_{IP}$ and the $V_t$ still increase. We attribute the larger $J_c$ to the change in the domain wall structure and the kinetic switching path when $D$ is relatively large (Supplementary Fig. 5). Specifically, a large $D$ tends to destabilize both the initial upward (downward) magnetization and the domain wall, thereby making the domain wall motion more turbulent (Supplementary Video 1) which in turn reduces the mobility of the domain wall. As a result, a larger $J_c$ will be required to move the domain wall. This is reminiscent of the Walker breakdown for the magnetic field or current-induced motion of 180° magnetic domain walls, where domain wall exhibits lower mobility if the field or current is so large that the domain wall structure becomes less stable during motion. When $D$ is even larger ($\geq 3.4$ mJ/m²), the equilibrium spin structure under an intermediate range of DMI strength $D$ displays an almost pure Néel wall that separates upward and downward domains (note that mixed Néel and Bloch wall features appear at lower $D$ values). Once the current is turned off, this spin structure will relax to a metastable or stable (if $D$ is sufficiently large) Néel stripe domain, where upward and downward domains are roughly half and half with $<m_z> ~ 0$ (Supplementary Fig. 6), rather than relaxing to the desirable downward single-domain with $<m_z> \approx -1$.

We also simulated the $J_c$ vs. $D$ switching diagrams for other disk diameters in the range of 40–63 nm. It is found that the switching diagrams in the cases of other disk diameters all exhibit two features that are the same as the above-discussed 40 nm diameter case, due to similar physical mechanisms. First, as $D$ increases, the critical $J_c$ required for the >90° switching decreases (increases) when $D$ is relatively small (large). Second, the relaxation to single domain of reversed polarity in the second step is prohibited if $D$ is too large. The numerical calculation of such switching diagram is tedious because one needs to search for the desirable range of $J_c$ for each combination of $D$ and disk diameter. To accelerate the calculation of switching diagram, we
train a decision-tree-regression-based machine learning model (see "Methods") from about 1000 groups of micromagnetic simulation datasets. The machine learning model is then tested with 80 datasets. Each dataset is comprised of an input vector $X_i$ ($i = 1, 2, 3$, representing the disk diameter, $D$, and $J_c$, respectively) and an output scalar variable $Y$ representing the equilibrium value of $<m_z>$. The trained machine learning model can be used to rapidly regress the $Y$ as a function of $X_i$. As one example, Fig. 4e shows the machine-learning-model predicted $J_c$ vs. $D$ switching diagram for the disk diameter of 40 nm, which is well consistent with the diagram calculated via micromagnetic simulations except one outlier (c.f., Fig. 4c). Remarkably, the machine-learning-predicted diagram, which also contains many more data points than the micromagnetic-simulations-based diagram, was calculated in <2 min in a laptop. This is much faster than that by micromagnetic simulations, where the calculation of one switching diagram takes ~250 groups of simulations and each group typically takes ~4 h to complete with 16 cores running simultaneously on state-of-the-art supercomputers. The prediction accuracy of our machine learning model is >90% with running simultaneously on state-of-the-art supercomputers. The mean square error of ~0.01 (Fig.4f), and can be further improved with more training datasets. Such machine learning model is thus particularly suited for accelerating the prediction of such switching diagram, e.g., $J_c$ vs. $X$ (where $X$ = disk size, $D$, $K_{int}$, $M_u$, etc.), in which case large quantities of micromagnetic simulations are normally needed.

Having shown that the >90° perpendicular switching occurs through a deterministic nucleation and lateral growth of reversed domain (Fig. 2), we further perform ASD simulations to analyze the early-stage nucleation kinetics at which the embryos (clusters of several atoms) are too small to accurately describe with a continuum micromagnetic model. A multilayer stack (similar to the structure in Fig. 1a) with 50 nm diameter MgO/Co bilayer nanodisks on top of a Pt stripe is considered as the model system. There are two reasons for considering Co (instead of CoFeB) as the magnetic layer herein. First, since the goal is to reveal the nucleation and growth kinetics of the reversed domain (within which $m_z < 0$) at the atomic scale, a pure metal Co would be a better model system than the solid-solution CoFeB. Second, it will show that the proposed two-step switching is applicable to other ferromagnets.

We first present the micromagnetic simulations results on the >90° switching in Co as the baseline of the discussion. As shown in Fig. 5a, after a brief incubation period (during which $m_z > 0$), the volume fraction ($V_r$) of the reversed domain (within which $m_z < 0$) increases gradually from 0 to above 60% at saturation, when moderate charge currents are applied (the range of $J_c$ is from $1.1 \times 10^{13}$ to $1.5 \times 10^{13}$ A/m²). A larger $J_c$ yields a larger out-of-plane torque $T_{zz}$ which in turn leads to faster nucleation (that is, shorter incubation period) and faster growth. Notably, the growth of the reversed domain (described by the evolution of $V_r$ at later time stages) well fits the Kolmogorov–Avrami equation38,39, given by $V_r = V_0(1 - e^{-(t/t_c)^p})$, where $V_0$ is a fitting parameter; $t_c$ is the characteristic time for the $V_r$ to saturate, which decreases from 0.24 to 0.12 ns as $J_c$ increases; $n$ is the effective dimension of domain growth and is best fitted with values around 2, indicating a two-dimensional domain growth as expected.

Fig. 5 On the kinetics of reversed domain nucleation and growth during the >90° perpendicular magnetization switching. Both the a micromagnetic and b–e atomistic spin dynamics (ASD) simulations consider a 50 nm diameter MgO/Co(1.1 nm) bilayer nanodisks on top of a Pt layer. a Volume fraction of the reversed domain (regions where $m_z < 0$) as a function of time, calculated from micromagnetic simulations. $J_c$ increases from $1.1 \times 10^{13}$ to $1.5 \times 10^{13}$ A/m². b Percentage of atoms with flipped magnetization ($S_z < 0$) as a function of time, calculated from ASD simulations. $J_c$ increases from $4.5 \times 10^{12}$ to $5.0 \times 10^{12}$ A/m². In both a and b, the growth kinetics of the reversed domain well fits the Kolmogorov–Avrami equation (results plotted using lines). c Distributions of the normalized perpendicular atomic spin moment $S_z$ as a function of time, calculated from micromagnetic simulations. $S_z$ increases from $1000$ groups of micromagnetic simulations. The trained machine learning model can be used to rapidly regress the $Y$ as a function of $X_i$. As one example, Fig. 4e shows the machine-learning-model predicted $J_c$ vs. $D$ switching diagram for the disk diameter of 40 nm, which is well consistent with the diagram calculated via micromagnetic simulations except one outlier (c.f., Fig. 4c). Remarkably, the machine-learning-predicted diagram, which also contains many more data points than the micromagnetic-simulations-based diagram, was calculated in <2 min in a laptop. This is much faster than that by micromagnetic simulations, where the calculation of one switching diagram takes ~250 groups of simulations and each group typically takes ~4 h to complete with 16 cores running simultaneously on state-of-the-art supercomputers. The prediction accuracy of our machine learning model is >90% with running simultaneously on state-of-the-art supercomputers. The mean square error of ~0.01 (Fig.4f), and can be further improved with more training datasets. Such machine learning model is thus particularly suited for accelerating the prediction of such switching diagram, e.g., $J_c$ vs. $X$ (where $X$ = disk size, $D$, $K_{int}$, $M_u$, etc.), in which case large quantities of micromagnetic simulations are normally needed.

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Figure 5b shows the nucleation and growth kinetics of reversed domain simulated using ASD modeling, where a 2D hexagonal lattice of 36,096 atoms is used to approximately describe the 1.1-nm-thick hcp Co nanodisk. The evolution of the average atomic spin moment and free energy terms during the entire two-step switching process are also simulated by ASD modeling (see Supplementary Fig. 7). As shown in Fig. 5b, the nucleation and growth of the reversed domain display generally similar kinetic features to those obtained using micromagnetic modeling. Specifically, the percentage of atoms (Nt) with flipped atomic spin moment (Sz ≤ 0, see “Methods”) displays a similar saturation value. The growth kinetics of the reversed domain can likewise be fitted using the Kolmogorov–Avrami equation. For early nucleation stage (0.055 ns), Fig. 5c shows the density maps of the perpendicular atomic spin moment Sz at three different nucleation clusters (labeled as P1, P2, and P3, as indicated in Fig. 5d) at the same time stage. It can be seen that the switching is fastest at P3 and then P2, which is also indicated by the evolution trajectories of the atomic spin moment in the central atoms (marked by circles) at these three points from 0 to 0.06 ns (Fig. 5e). This locally variant switching speeds are mainly due to the fact that the downward-pointing effective SOT field, the magnitude of which is proportional to |Sz|, is the largest at cluster P2 while smallest at P3 at this early stage of nucleation. As a result, the magnetization at P3 can be flipped more quickly.

In summary, we have computationally demonstrated a field-free SOT-mediated perpendicular magnetization switching, the implementation of which does not require any changes in the standard architecture of an SOT-MRAM cell, thus being promising for practical applications. The full 180° switching is achieved through a >90° perpendicular switching (mz changes from −1 to <0, or vice versa from approximately −1 to >0) plus a subsequent precession relaxation to the reversed direction. The simulations indicate that there are two key critical steps for achieving the >90° perpendicular switching, including the nucleation of the reverse domain and its successful growth to exceed the critical "half-up half-down" spin state (e.g., Fig. 2c). Successful realization of both steps relies on striking the balance of the interfacial DMI, geometrical confinement, and SOT by tuning the interfacial DMI strength (D), lateral size of the magnetic layer, and magnitude of charge current density (Jc), respectively.

Our analyses show that the growth of the reversed domain is two-dimensional and can be well described by classical theory of growth kinetics, similarly to the growth of polarization domain in ferroelectric thin films. Our ASD simulations, which resolve the evolution of magnetic moment in every single magnetic atom in a confined system, provide an atomistic picture of the nucleation kinetics of SOT-mediated perpendicular magnetization switching in general. Last but not the least, we have trained a decision-tree-based machine learning model using about 1000 groups of micromagnetic simulations that were benchmarked using the open-source micromagnetic simulation package MuMax3. This machine learning model along with the datasets can evolve to an accurate and efficient computational design tool that can be used to quickly determine whether the field-free switching can occur and what are the values of average magnetization at equilibrium under a given set of design parameters (D, size, Jc, key magnetic parameters, etc.).

METHODS
Micromagnetic simulations using μ-Pro
Most of the micromagnetic simulations in this work are performed using the commercial μ-Pro package (mupro.co/contact), which is CPU (Central Processing Unit) based and parallelized using Message Passing Interface. Consider a MgO/CoFe2O4/Fe80B20(1.1)/Pt multilayer structure, where the CoFeB disk is discretized using a cuboid-shaped cell of 1 nm x 1 nm x 0.55 nm. We note that the thickness of the CoFeB (1.1 nm) is significantly smaller than the magnetic exchange length lex = 1/√(A/0.5μ0M_s^2) ~ 4.54 nm, where A is the Heisenberg exchange coefficient, μ0 is the vacuum permeability, M_s is the saturation magnetization. In combination with the fact that the interfacial DMI field does not modify the gradient of magnetization along the thickness direction (shown later), we expect the magnetization distribution to be spatially uniform along the thickness direction, which is confirmed by micromagnetic simulations. The simulations performed using a smaller cell size along the z-axis (i.e., 0.275 nm) yield the same results. Other magnetic nanostructures with sufficiently strong room temperature PMA, which can arise due to either the magnetic interface anisotropy (e.g., 0.5-nm-thick FePt/CoFeB, ref. 11) or the intrinsic magnetocrystalline anisotropy such as FePt12, can also be used to demonstrate the proposed field-free SOT perpendicular magnetization switching.

The magnetization in each cell M = M_s m, where m = (m_x, m_y, m_z) is the normalized magnetization vector. The evolution of the normalized magnetization m is obtained through solving the Landau–Lifshitz–Gilbert (LLG) equation with an SOT term tSOT:

\[ \frac{\partial \mathbf{m}}{\partial t} = -\gamma_0 \mathbf{m} \times (\mathbf{H}_{\text{eff}} + \alpha \mathbf{H}_{\text{SOT}}) \]

(1)

where \( \alpha \) is the Gilbert damping coefficient and \( \gamma_0 \) is the gyromagnetic ratio.

The effective magnetic field \( \mathbf{H}_{\text{eff}} = -\frac{\mu_0 m_s}{V} \mathbf{F}_{\text{ex}} - \frac{1}{\tau} \mathbf{F}_{\text{SOT}} \) is the total magnetic free energy density \( \mathbf{f}_{\text{tot}} = \mathbf{f}_{\text{mag}} + \mathbf{f}_{\text{anis}} + \mathbf{f}_{\text{DMI}} + \mathbf{f}_{\text{stray}} \), which is the sum of the densities of the magnetic stray field energy, perpendicular anisotropy energy, interfacial DMI energy, and Heisenberg exchange energy, respectively. Each energy density term is associated with an effective magnetic field. Therefore, one can also write \( \mathbf{H}_{\text{eff}} = -\frac{\mu_0 m_s}{V} \mathbf{F}_{\text{ex}} - \frac{1}{\tau} \mathbf{F}_{\text{SOT}} \) = \( \mathbf{H}_{\text{mag}} - \mathbf{H}_{\text{DMI}} - \mathbf{H}_{\text{exch}} \). Among them, the magnetic stray field \( \mathbf{H}_{\text{stray}} \) is obtained through solving magnetoostatic equilibrium equation \( \nabla \cdot \mathbf{m} = 0 \) under a finite-size boundary condition, using a Fast Fourier Transform accelerated convolution theorem42. The anisotropy field \( \mathbf{H}_{\text{ani}} = \frac{1}{V} \int_{\Omega} \mathbf{H}_{\text{ani}} d\Omega \) is the uniaxial magnetic anisotropy energy density \( f_{\text{ani}} = \frac{A}{V} (1 - m_z^2) \). For the ultrathin (1.1-nm thick) CoFeB in this work, it is the contribution from the magnetic interface anisotropy \( f_{\text{ani}} \) that outweighs the out-of-plane shape anisotropy \( K_{\text{shape}} \). The latter can be evaluated based on numerically calculated out-of-plane stray field. Experimentally, a room temperature thermally stable perpendicular magnetization has been demonstrated in ultrathin (1.3 nm or thinner) CoFeB nanodisks with diameter as small as 40 nm19 (down to 20 nm according to a very recent report12), where MgO is used as the overlayer, the same as in our structure. The interfacial DMI field \( \mathbf{H}_{\text{DMI}} = \frac{2D}{\Omega} \left( \frac{\partial H_z}{\partial y} \right) \), where D is the strength of the interfacial DMI24. When calculating the \( \mathbf{H}_{\text{DMI}} \) in a geometrically confined nanostucture, the boundary condition \( \mathbf{m} \cdot \mathbf{n} = 0 \) needs to be applied at the interface between the magnetic disk and nonmagnetic phase24, where n is the interface normal; e_z is the unit vector along the z-direction. The Heisenberg exchange field \( \mathbf{H}_{\text{exch}} = \frac{\partial H_z}{\partial y} \mathbf{e}_z \). The influence of thermal fluctuations is modeled by adding a thermal fluctuation field \( \mathbf{H}_{\text{therm}} \), given by \( \mathbf{H}_{\text{therm}} = \sqrt{8k_B T/\pi \eta} n_x \mathbf{e}_z \), where \( k_B \) is the Boltzmann constant, \( T = 298 \) K is the temperature, \( \Delta V \) is the volume of each simulation cell, \( \tau \) is the time interval in real unit. \( \mathbf{n} = (n_x, n_y, n_z) \), where \( n_x, n_y, n_z \) are Gaussian-distributed random numbers with a mean of zero, which are uncorrelated both in space and time.

Let us further consider that the input charge current flowing along the −y direction (\( J_{\text{in},-y} \)) of the Pt layer. Due to the SHE3, electrons with opposite spin orientations are deflected towards the top and bottom surfaces along the z-axis (yielding a spin current, denoted as \( J_s \), as well as the two lateral surfaces along the x-axis (yielding a spin current \( J_{x} \)). We note that the spin current is a flow of angular momentum, and that the net charge currents along both x and z are zero. Since the magnetic nanodisk is laid on the top surface of the Pt layer, only the z-axis spin current \( J_z \), which has a spin polarization \( \sigma \) along x according to the right-hand rule of the SHE3, can be injected into the nanomagnet (Fig. 1a). In this case, the transfer of angular momentum from the Pt to nanomagnet can only occur along the z-axis, and in turn switch the magnetization in the latter via the SOT44. Experimental demonstration of this switching scheme can be found in for example refs. 9,19,14,25.

The spin–orbit torque \( t_{\text{SOT}} \) is expressed as23,24:

\[ t_{\text{SOT}} = -\frac{\gamma_0}{1 + \alpha^2} \left( (m \times H_{\text{SOT}}) - \alpha H_{\text{SOT}} \right) \]

(2)

where the corresponding effective field \( H_{\text{SOT}} = H_0(m \times \mathbf{e}_z) \). Here, the

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\[ B_{\text{eff}} = -\frac{1}{\mu_y} \frac{\partial H_{\text{eff}}}{\partial t} + B_{\text{therm}}, \]

where \( \mathcal{H} \) is the total spin Hamiltonian; \( \mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{dipole}} + \mathcal{H}_{\text{anis}} + \mathcal{H}_{\text{exch}} + \mathcal{H}_{\text{therm}} \) is the sum of the Hamiltonians of magnetic dipole–dipole interaction, uniaxial magnetic anisotropy, interface DMI and Heisenberg exchange interaction of all atoms. Since each Hamiltonian is associated with an effective magnetic field, one can write

\[ B_{\text{dipole}} = \mathcal{H}_{\text{dipole}}, \quad B_{\text{anis}} = \mathcal{H}_{\text{anis}}, \quad B_{\text{exch}} = \mathcal{H}_{\text{exch}}, \quad B_{\text{therm}} = \mathcal{H}_{\text{therm}}. \]

Among them,

\[ B_{\text{dipole}} = \frac{\mu_y \mu_B}{4 \pi} \sum_{i,j} \left( 3(\mathbf{S}_i \cdot \mathbf{r}_{ij} - \mathbf{S}_i \cdot \mathbf{S}_j) \right). \]

where \( r_{ij} \) is the distance between atom site \( i \) and atom site \( j \), \( \mathbf{r}_{ij} \) is the unit vector along the direction of \( r_{ij} = r_{ij} - r_i \).

\[ B_{\text{anis}} = \frac{K_B}{\mu_y} \sum_{i} \mathbf{S}_i, \]

where \( K_B \) is the anisotropy constant, \( \mathbf{u} \) is the direction vector of the magnetic easy axis.

\[ B_{\text{exch}} = \frac{\mu_y}{\mu_B} \sum_i \mathbf{S}_i, \]

where \( \mu_y \) is the exchange parameter describing the Heisenberg-type exchange coupling between two spins at atom site \( i \) and \( j \). For interfacial DMI, \( D_{\text{DMI}} = D_{\text{DMI}} x \cdot \mathbf{r}_{ij} \), where \( D_{\text{DMI}} \) is the interfacial DMI constant.

\[ B_{\text{therm}} = \frac{2 \alpha B \mathbf{S}_i}{\mu_y \Delta t}, \]

where \( \alpha \) is the strength of field-like torque, \( \beta_{\text{DL}} \) is the strength of damping-like torque, \( \sigma \) is the orientation of spin polarization, which is along +x direction in our case.

The parameters in ASD simulations can be derived from their continuum-scale counterparts used in micromagnetic simulations as follows:

\[ J = \frac{1}{2} \left( \frac{1}{3} \right) \times 1.27 \times 10^{-22} J_0 = \frac{1}{\mu_y} = 1.18 \times 10^{-22} J_0 \]

\[ \mu_y = \frac{3}{4} \pi a M = 3.03 \times 10^{-23} J_{\text{Co}} = \frac{3}{4} \pi a_2 K = 3.14 \times 10^{-22} J_0, \]

where \( a_2 \) is 4.0 A. Note that these continuum-scale parameters \( (A, D, M, K) \) are values experimentally measured for 1.1-nm-thick Co film. Here, we are considering a 2D hexagonal lattice with a thickness of only one monolayer (\( \sim 4.0 \) Å) for reducing the computational cost (which is common for ASD simulations\(^{2,3}\)), by assuming the variation of magnetization along the thickness direction is negligible. This approximation would lead to significantly stronger demagnetization field (dipolar) field in the system than it is supposed to be in a 1.1-nm-thick Co sample, which in turn reduces the PMA. To balance the stronger demagnetization field, we use a larger anisotropy constant \( K_0 = 5.50 \times 10^{-23} J_0 \). It is shown that under this combination of parameters, the extent of edge magnetization tilting \((m_y \approx 0.3, \text{c.f., Fig. 4b})\) is the same as that in the micromagnetic simulations of 1.1-nm-thick Co film. Strength of field-like torque and damping-like torque is proportional to
the magnitude of charge current density $J_c$: $\beta_{Hc} = \frac{\mu_0}{Hc Hc} J_c$, $\beta_{HL} = -\frac{\mu_0}{1 + \frac{L_c}{L_{mag}}} J_c$, the pre-factors are derived corresponding to the SOT term of micromagnetic LLG equation. The LLG equation is solved using forth-order Runge-Kutta method with a time interval of 1 fs. Using a smaller time interval of 0.5 fs yields the same results.

**DATA AVAILABILITY**

The data that support the plots presented in this paper and its supplemental information files are available from the corresponding authors upon reasonable request. All training data for the machine learning model can be accessed via https://github.com/mdai26/ML-SOT.

**CODE AVAILABILITY**

The in-house open-source AtomMag package for performing the atomistic spin dynamics simulations can be accessed via https://github.com/jhu238/AtomMag. Open-source codes for the machine learning model can be accessed via https://github.com/mdai26/ML-SOT.

Received: 7 March 2020; Accepted: 22 May 2020;
Published online: 12 June 2020

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ACKNOWLEDGEMENTS
The work is supported by a start-up fund from the University of Wisconsin–Madison. The simulations were performed using Bridges at the Pittsburgh Supercomputing Center through allocation TG-DMR180076, which is part of the Extreme Science and Engineering Discovery Environment (XSEDE) and supported by NSF grant ACI-1548562.

AUTHOR CONTRIBUTIONS
J.-M.H. conceived the idea, designed and supervised the research. M.D. performed the research. Both authors analyzed the data and wrote the paper.

COMPETING INTERESTS
The authors declare no competing interests.

ADDITIONAL INFORMATION
Supplementary information is available for this paper at https://doi.org/10.1038/s41524-020-0347-0.

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