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Micromagnetic modeling of domain wall motion in sub-100-nm-wide wires with individual and periodic edge defects

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Reducing the switching energy of devices that rely on magnetic domain wall motion requires scaling the devices to widths well below 100 nm, where the nanowire line edge roughness (LER) is an inherent source of domain wall pinning. We investigate the effects of periodic and isolated rectangular notches, triangular notches, changes in anisotropy, and roughness measured from images of fabricated wires, in sub-100-nm-wide nanowires with in-plane and perpendicular magnetic anisotropy using micromagnetic modeling. Pinning fields calculated for a model based on discretized images of physical wires are compared to experimental measurements. When the width of the domain wall is smaller than the notch period, the domain wall velocity is modulated as the domain wall propagates along the wire. We find that in sub-30-nm-wide wires, edge defects determine the operating threshold and domain wall dynamics.

I. INTRODUCTION

Devices based on domain wall (DW) motion in magnetic nanowires are a promising alternative to conventional transistors for memory and digital logic applications with low switching energy.1–4 The logical state of the device depends on the position of a DW, which can be read back using, for example, a magnetic tunnel junction (MTJ), as shown in the elementary logic gate of Fig. 1(a).1 In DW-based devices, the DW must move predictably in the presence of a spin-polarized current or external magnetic field. However, in practice, DW motion can be affected by variations in nanowire width resulting from the lithography and pattern transfer processes, for example roughness with amplitude around 2-6 nm reported in Ref. 5. Consequently, the pinning of the DW by edge roughness is critical for determining the scalability of DW devices.

High-resolution patterning has enabled the fabrication of sub-100-nm-wide nanowires. At this scale, line edge roughness (LER) of even a few nm provides significant interactions with DWs. Studies have shown the effect of LER on DW depinning in both in-plane magnetic anisotropy (IMA) and perpendicular magnetic anisotropy (PMA) nanowires.6–11 A DW can also be pinned by local variations in anisotropy, which can arise from misorientation between grains in a polycrystalline film or from other perturbations in the nanowire anisotropy, due to inhomogeneous strain for example.7,12 On the other hand, LER can facilitate the nucleation of a DW or the confinement of a DW to a region within the nanowire, which can be useful in device applications.13

Micromagnetic simulations provide a tool to study the effect of edge roughness or anisotropy variations, subject to the limitations of the discretization cell size, which should be similar to the exchange length. LER can be introduced into a simulation by removing cells or blocks of cells from the edge of a nanowire in a model with cuboidal14,15 or tetrahedral cells.6 Other studies use a Voronoi...
FIG. 1. (a) Schematic of a logic device made from a magnetic IMA nanowire from Ref. 1 with LER added. Red and blue represent magnetization directions, the output is a tunnel junction with a fixed layer (blue), and the input and clock include an antiferromagnet (not shown) to pin the magnetization direction of the free layer. Simulation model image of DW motion in an (b) IMA nanowire with LER and (c) PMA nanowire with LER. (d) SEM image of CoFeB nanowire and its discretization, from which the shapes of (b) and (c) are derived. Pinning site A labeled in (b) is the strongest pinning site that defined the threshold for that nanowire.

Despite the differences in approach, edge defects can only be resolved when their sizes are larger than the cell size.16 To date, studies on DW motion in nanowires with edge roughness have focused on wires with widths over 100 nm. As the wire width increases, the DW also becomes larger in size, making it less sensitive to small-scale edge fluctuations, and LER contributes little to DW pinning in wires that are wider than 200 nm,12,17 within which artificial pinning sites are engineered in some cases.8,18 Studies have found that DW pinning fields increase linearly with LER, but narrower linewidths have not been explored.6,10,19,20 An analytical model has shown the effect of periodic pinning potentials on thresholds for DW traversal.21 Here, we examine the effects of defects in wires with linewidths below 60 nm, examining both edge roughness and anisotropy variations, on the threshold and on DW velocity. We begin with a description of the modeling techniques in Section II. In Section III, we analyze the effects of anisotropy and notch defects on DW pinning in IMA nanowires. We explain the effect of periodic LER on DW motion in IMA nanowires and PMA nanowires in Sections IV and V, respectively.

II. METHODS

We model magnetic nanowires with the Object-Oriented Micro-Magnetic Framework (OOMMF) software package.22 Figures 1(b) and 1(c) show a top-down view of the magnetization vectors in an IMA Co nanowire and a PMA CoFeB nanowire, respectively, each containing a DW, after relaxation at remanence. The shape of the wire in Figs. 1(b) and 1(c) is taken from Fig. 1(d), which shows the discretization of a scanning electron microscope (SEM) image of a 30-nm-wide CoFeB nanowire fabricated using a bilayer resist lithography process.5

We modeled field-driven DWs by initializing a DW in the wire, then measuring the threshold for DW traversal as a function of applied magnetic field, which is parallel to the wire for IMA or out-of-plane for PMA simulations. The threshold is defined as the magnetic field value that allows a DW to traverse the entire nanowire without being pinned. The simulations did not include any thermal effects, which require a much more computationally intensive model.9,23 Thermal effects are generally known to lower the threshold field,14,24–26 and thermally-induced changes in DW velocity can change the positions at which a DW could be trapped in a wire with LER.15 Once we determined...
the threshold, we calculated the DW velocity at a constant field that is 3% above the threshold field for that nanowire. The fields were below the Walker breakdown limit in IMA simulations.

In our simulations of IMA Co nanowires, the cell size was 3 nm × 3 nm × 2.5 nm, and the wire was 30, 45, or 60 nm wide with thickness 5 nm and length 900 nm, containing about 10^4 cells. The damping parameter, α, described in Ref. 15, was set to 0.018, and the saturation magnetization, \( M_{\text{sat}} = 1.40 \times 10^6 \text{ A/m} \). A uniaxial magnetocrystalline anisotropy of 4100 J/m^3 with random direction was present in each cell. This anisotropy value was 10% of the fcc-Co anisotropy, \( K_{\text{fcc-Co}} \), based on the assumption that the anisotropy of the thin film is less than that of bulk,27 and the weak crystalline texture leads to an approximately random anisotropy.28 \( K_{\text{fcc-Co}} \) is about 10% of the hcp-Co anisotropy, \( K_{\text{hcp-Co}} = 4.1 \times 10^5 \text{ J/m}^3 \).29,30 In some nanowire simulations we added anisotropy fluctuations, in addition to the preexisting random-direction anisotropy. An anisotropy fluctuation could correspond to a region where the crystallographic axes of several grains happen to align leading to a net anisotropy. It was modeled as a region of the wire with a local anisotropy increase that was up to \( K_{\text{fcc-Co}} \) (or 10% of \( K_{\text{hcp-Co}} \)), as suggested by the thin film microstructure.30,31 For simulations of IMA permalloy (\( \text{Ni}_{80}\text{Fe}_{20} \)), \( M_{\text{sat}} = 7.96 \times 10^5 \text{ A/m} \) and a randomly-directed uniaxial anisotropy of 100 J/m^3 were used with other parameters the same as IMA Co. We initialized the DW far enough from the wire ends to avoid the influence of their stray fields. The relaxed DW had a transverse structure in both Co and NiFe.

PMA nanowires were modeled corresponding to 5-nm-thick CoFeB, illustrated in Fig. 1(c). Studies report CoFeB nanowires can be fabricated with strong PMA.32,33 The cell size for PMA wires was 3 nm × 3 nm × 2.5 nm. We used \( \alpha = 0.01 \), \( M_{\text{sat}} = 7.96 \times 10^5 \text{ A/m} \) and an anisotropy in the out-of-plane direction of \( K_z = 7.82 \times 10^5 \text{ J/m}^3 \) with an additional random-direction anisotropy in each cell of 100 J/m^3.9

III. DEFECT PINNING IN IMA NANOWIRES

A. Triangular and Rectangular Notch Defects

In Fig. 2, we model the effect of an isolated notch, whose shape is (a) triangular or (b) rectangular, by setting zero magnetization in appropriate cells in the wire edge. The DW is initialized on the left of the wire and moves to the right as the in-plane field is applied. The DW core magnetization is oriented towards the top of the page such that the DW is wider at the upper edge of the wire where the notch

![Diagram](image-url)
Figure 2 shows the ranges of fields at which the DW is pinned or when it continues past the notch, for different notch depths, $d$, and wire widths, $w$. The notch width at the wire edge is $(2d – 3)$ nm for $d = 3, 6, 9 \ldots$ nm. The pinning fields increase by up to a factor of 2 as the wire width decreases from 60 nm to 30 nm.

As the notch depth increases, the pinning field increases, in agreement with the trend seen in Ref. 11. For a given notch depth, the rectangular notch has a higher pinning field than the triangular notch in wires that are 45 nm and 60 nm wide, but the difference is smaller in 30-nm-wide wires. Rectangular notches have a steeper profile in our model, and their higher pinning field in wider wires agrees with the observation in Ref. 20 that in 1.4-µm-wide wires the depinning field is higher for steeper-profile notches. In the depinning process, the DW oscillates as seen in Ref. 9 and then breaks free of the notch.

Reversing the orientation of the transverse core of the DW, or, equivalently, moving the notch to the opposite side of the wire, increases the pinning field as predicted by Ref. 23. The different pinning in the cases of notch depths around 3 to 9 nm is shown in Fig. 2 for the 30 nm wide wire. This leads to a chirality filtering effect as described in Ref. 34, where within a certain field range, DWs with one core chirality pass but DWs with the opposite chirality are pinned because the pinning is greater when the narrower side interacts with the notch.

### B. Anisotropy Defects

We simulate anisotropy defects as regions of the wire with an increase in anisotropy, $\Delta K$, of up to 10% of $K_{\text{hcp-Co}}$. Anisotropy defects consisted of sections of the wire that are 9 nm long, similar to the grain size. Each section of an anisotropy defect is treated as a row of cells with higher anisotropy, which spans across the entire width and entire thickness of the magnetic nanowire, shown in the red-shaded region of the top panel of Fig. 3.

In Fig. 3, we plot the pinning field vs. $\Delta K$ for each nanowire width. Although the pinning strength of anisotropy defects nearly doubles when halving the nanowire width, the overall pinning strength of anisotropy defects is almost an order of magnitude smaller than that of the notch defects described earlier, and hence is not expected to be the dominant factor in determining the depinning fields for the geometry and IMA material parameters studied here.

**FIG. 3.** (a) Moving DWs are pinned by an anisotropy defect, shown as a shaded rectangle in the top panel. This pinning is modeled for various anisotropy magnitudes. (b) Comparison of the range of depinning fields for experimental 60-nm-wide and 80-nm-wide Co nanowires and simulated 60-nm-wide Co nanowires with a rectangular notch, varying the notch depth and including anisotropy increases of up to 10% of $K_{\text{hcp-Co}}$, shown as shaded rectangles around the notch in the top panel. The ranges of depinning fields for the experiment and model are comparable at notch depths around 6 – 14 nm.
C. Comparison to Experimental Results

The depinning fields observed in experimentally fabricated 5-nm-thick and 60-nm-wide or 80-nm-wide Co nanowires are in the range of 16 kA/m to 32 kA/m. The LER amplitude is up to ~7 nm, or 10% of the wire width, found by analyzing nanowire SEM images using the method of Ref. 5.

The experimental depinning fields can be compared with modeled depinning fields for a 60-nm-wide Co wire with a single notch and distributed anisotropy defects, shown in Fig. 3(b). Distributed anisotropy defects were modeled as blocks of 3 cells × (3 to 11 cells), i.e. 9 nm wide and 9 to 33 nm long, subject to an increased anisotropy ΔK = 1% to 10% of $K_{hcp-Co}$ in the direction along the wire length. Ten of these defects with varying size and ΔK were placed within the wire around the notch. Notch depths of 6 – 14 nm resulted in depinning fields that were comparable to the range of measured values.

Furthermore, we model Co nanowires with an edge profile determined from discretized SEM images such as the nanowire in Fig. 1(d), with and without local anisotropy variations modeled as blocks of cells of size (2 to 4 cells) × (2 to 11 cells) within the nanowire with ΔK values uniformly distributed from 1% to 10% of $K_{hcp-Co}$. The pinning field for such nanowires increases by about 2 kA/m, from 25 kA/m to 27 kA/m, as a result of adding the local anisotropy variations. Hence, based on Figs. 2 and 3, LER is confirmed to be a significant source of pinning in nanowires that are 30 to 60 nm wide while anisotropy defects increase the pinning field by a lesser amount.

IV. DW MOTION IN IMA WIRES WITH PERIODIC NOTCHES

To understand how a DW interacts with the series of notches present at a rough edge, we identify the peak spatial frequencies along the nanowire edge from a spectral analysis of the edge deviation seen in an SEM image of a nanowire. The peak spatial periods for our example nanowire are 200 nm with the highest peak, 91 nm with a smaller peak, 47 nm, 29 nm, and below, determined from the analysis of a micrograph with a resolution of 1.4 nm. We then model DW motion in wires with an array of notches, each with one spatial period and compare the DW velocity in nanowires with monochromatic edge spatial frequencies with the DW velocity in the discretized nanowire with a range of frequencies.

In simulations of NiFe nanowires with periodic notches of depth $d = 3$ nm, the threshold field is 2 to 15 kA/m, well below the Walker breakdown field, which we determined to be 185 kA/m. The threshold in the 36-nm-wide wires with LER is higher than the thresholds in Ref. 36 around 0.3 kA/m reported for NiFe nanowires that are 100 to 300 nm wide, whose ratio of edge roughness to width is an order of magnitude smaller.

Figure 4 shows the modeling results for DW movement under a field, $H_x$, that is 3% greater than threshold, as well as a definition of the notch array geometry. A smooth wire with no defects has a threshold close to but not exactly zero due to the random-direction anisotropy.

In periodically notched wires, the DW velocity varies periodically with distance, higher as the DW encounters a narrow section where the DW area decreases, and lower as it encounters a wider section of the wire where its area increases. The DW width, which is defined as the full width at half maximum of the magnetization component transverse to the wire at the wire midpoint, is 29, 40, and 50 nm for smooth Co wires that are 30, 45, and 60 nm wide, respectively. When the spatial period of the notches is smaller than the DW width, the DW velocity shows less variation, as seen in the 6-nm-period and 18-nm-period cases. In the 36-nm-wide wire, the DW width varied from 29 nm in narrow sections to 32 nm in wide sections. The DW is wide enough to average over the fluctuations in wire width for high frequency roughness, leading to less effective pinning. In these IMA nanowires, the DW does not change chirality and retains its transverse structure while moving through the narrow and wide sections.

When $d$ and $w$ are increased by the same amount, oscillations in DW velocity are seen but the threshold is higher because more energy is needed for the DW to expand into a larger increase in volume. We also plot the DW velocity for a simulated nanowire whose shape is taken from a discretized SEM image, shown in Fig. 1(b) and 1(d). The DW velocity is minimum when the DW reached a deep notch and then expanded into a wider section of the wire.
V. DW MOTION IN PMA WIRES WITH PERIODIC NOTCHES

Figure 5 shows an analogous model study of CoFeB PMA nanowires with a periodic notch structure with \( d = 3 \) nm and \( w = 36 \) nm. The Walker breakdown field is 10 kA/m for a smooth wire. The threshold field is close to zero in the smooth wire, but the threshold field exceeds the Walker breakdown field when there are periodic notch defects. The DW is therefore moving in the precessional regime with its core orientation changing, in Fig. 5.
FIG. 5. The DW velocity in PMA nanowires driven at a constant magnetic field. The same field is applied in all wires, higher than Walker breakdown. There are small fluctuations in velocity with position along the wire except for a period of 6 nm and below.

The velocity varies periodically as the DW encounters changes in width, but the changes in velocity are less than 20% for the notch geometries examined here, a smaller modulation than seen in the IMA model of Fig. 4. The velocity modulation is similar across the range of periods. The DW velocity decreases when \(d\) and \(w\) are increased by the same amount, not shown in Fig. 4. The velocity modulation is consistent with Ref. 6, which shows oscillations in DW velocity when a DW in a rough PMA nanowire is driven above Walker breakdown.

Since the DW is in Walker breakdown in the PMA nanowires, the DW core orientation rotates. In a smooth wire, this rotation has a period of 20 nm and the DW velocity is constant, increasing with width. Due to the rotation of the DW, the DW is more likely to get pinned in one orientation compared to another. This means that even if a DW continues past one notch period, it could be pinned in a subsequent period depending on its core orientation there. We drive the DW at \(H_z = 200\, \text{kA/m}\) in all PMA wires, which is sufficient to avoid any pinning. Hence, the changes in DW velocity are not only due to the periodic notches but also due to the rotating DW. Figure 5 shows that the DW velocity varies by about \(\pm 3\, \text{m/s}\) as the DW traverses the larger period notched wires.

In Fig. 5, we plot the DW velocity for a simulated nanowire with the same shape as the discretized SEM image in Fig. 1(c) and 1(d). Its threshold field, which is determined by the most effective pinning site along the wire labeled as Pinning site A, is higher than that for the periodic notches, but the fluctuations in velocity are similar to those of the longest period notch array.

Our modeling shows that for the parameters explored here, LER leads to smaller fluctuations in the velocity of DWs under an applied field in the PMA case compared to the IMA case. Comparing the same discretized geometry wires for IMA (Fig. 1(b)) and PMA (Fig. 1(c)), the lowest DW velocity...
occurs at the same location, labeled as Pinning site A in Fig. 1(b). However, the velocity dip associated with Pinning site A is an 82% reduction for the IMA case and only a 7% reduction for the PMA case.

VI. CONCLUSIONS

In Co nanowires with IMA, we find with micromagnetic modeling that the line edge roughness is an important source of pinning as the linewidth decreases to 30 nm, while fluctuations in anisotropy also contribute to pinning. The pinning increased as linewidth decreased and depended on the notch shape. In NiFe wires with a periodic array of shallow notches, the DW velocity fluctuated with a periodic oscillation as the DW encountered the changes in linewidth. In these IMA wires, the DW became less sensitive to roughness as the period of the notches decreased below the DW width. In the PMA case for CoFeB, the DW was narrower and interacted even with high frequency roughness. The micromagnetic modeling of Co nanowires with defects predicted pinning fields of similar magnitude to those measured experimentally, showing that our modeling can be applied to physical devices. Models with discretized wire images could further explain actual pinning sites observed in experiment. Further fabrication advances that lower LER will lower the threshold field or current density needed to translate DWs.

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