Magnetic domain wall Skyrmions

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It is well established that the spin-orbit interaction in heavy metal/ferromagnet heterostructures leads to a significant interfacial Dzyaloshinskii-Moriya Interaction (DMI) that modifies the internal structure of magnetic domain walls (DWs) to favor Néel over Bloch type configurations. However, the impact of such a transition on the structure and stability of internal DW defects (e.g., vertical Bloch lines) has not yet been explored. We present a combination of analytical and micromagnetic calculations to describe a new type of topological excitation called a DW Skyrmion characterized by a 360° rotation of the internal magnetization in a Dzyaloshinskii DW. We further propose a method to identify DW Skyrmions experimentally using Fresnel mode Lorentz TEM; simulated images of DW Skyrmions using this technique are presented based on the micromagnetic results.

Introduction.—The discovery of a large Dzyaloshinskii-Moriya Interaction (DMI) [1, 2] in both bulk magnetic crystals [3, 4] and thin films with structural inversion asymmetry [5–8] has led to a fervent rebirth of research on magnetic bubble domains in the form of smaller particle-like features called Skyrmions, which are minimally defined as having an integer-valued topological charge \( C \), computed from \( 4\pi C = \int \mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) \mathrm{d}x \mathrm{d}y \), where \( \mathbf{m} \) is the unit magnetization vector. Although non-trivial to calculate, there is necessarily an energy barrier associated with the annihilation of such an object when \( C \) goes to 0 — something widely referred to as topological protection. The combination of a large DMI, which yields smaller, more stable Skyrmions, and a related spin-orbit coupling phenomenon, the spin Hall effect[9–12], makes the prospect of using Skyrmions for energy-efficient memory and computing attractive [13, 14].

We present a manifestly different type of topologically protected excitation called a domain wall (DW) Skyrmion [15, 16], which is described by a 360° wind of the DW’s internal magnetization along the wall profile and has a topological charge of ±1. In the absence of DMI, DWs in thin films with perpendicular magnetization tend to form the Bloch configuration [17]. It is common to encounter topological defects (\( C = \pm \frac{1}{2} \)) in these walls characterized by 180° transitions called vertical Bloch lines (VBLs), as shown in Fig. 1a-b [18, 19], which were once considered in their own right for computer memory [20, 21]. The interfacial DMI leads to a transition from a Bloch-type to a Néel-type DW with preferred chirality, known as the Dzyaloshinskii DW [5]. If a VBL is present during this transition, it could simultaneously transition into a DW Skyrmion as schematically illustrated in Fig. 1c-d. However, relatively little is known about the DW Skyrmion, including its formation energy, stability, and detection. As noted later, the interfacial DMI reduces the exchange length along the DW resulting in a DW Skyrmion that is much smaller than its VBL predecessor; an observation analogous to 2D Skyrmions and magnetic bubbles. Moreover, while conventional Skyrmions may propagate along any direction in 2D and are subject to the Skyrmion Hall effect [22], the network of magnetic DWs that can exist in thin films with perpendicular anisotropy now define reconfigurable 1D channels through which a DW Skyrmion can propagate. It is worth noting that unlike the conventional 2D Skyrmions that can form a lattice as the ground state, DW Skyrmions can only be metastable excitations. Their existence in systems with a strong DMI has not yet been investigated.

This Letter serves to describe the static properties of DW Skyrmions and propose a methodology to identify...
them experimentally. We begin with an analytical solution of the DW Skyrmion profile obtained by minimizing the energy functional. This solution is found to match very well with micromagnetic energy minimization performed using the M³ software package [23, 24]. Based on the micromagnetic output, Lorentz Transmission Electron Microscopy (LTEM) image simulations are performed, showing that DW Skyrmions should present a striking signature when viewed in the Fresnel observation mode.

**Analytical calculations.**—We choose Cartesian coordinates such that the DW normal is along \( \hat{x} \) and the film normal is \( \hat{z} \) as illustrated in Fig. 1. Assuming that the system is uniform through the film thickness, we can write down the free energy in the continuum limit as

\[
E = \int d\sigma \left\{ A|\nabla m|^2 - Km^2 + Dm \cdot \left[ (\hat{z} \times \nabla) \times m \right] \right\} + \frac{1}{2} \sigma_0 M_s^2 |\mathbf{n}(y) \cdot m|^2,
\]

where \( d\sigma = dx dy \), \( t_F \) is the film thickness, \( A \) is the exchange stiffness, \( D \) is the DMI, \( \mu_0 \) is the magnetic permeability, \( M_s \) is the saturation magnetization, and \( K \) is the effective perpendicular anisotropy with \( K_u \) the intrinsic magneto-crystalline anisotropy. In the last term, \( \mathbf{n}(y) \) is a *local* normal vector of the DW line that may depend on \( y \). To solve for \( m = m(x, y) \), we parameterize the magnetization vector in spherical coordinates as

\[
m = \{ \sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta \}.
\]

In the absence of DMI (\( D = 0 \)), minimizing the energy functional leads to a standard soliton profile: \( \theta = 2 \arctan \exp(x/\lambda) \) with \( \lambda = \sqrt{A/K} \) being the exchange length [25] and \( \phi = \pm \pi/2 \) representing a Bloch wall of either chirality.

Adding a strong DMI will overcome the demagnetization effect and twist Bloch walls into Néel walls where the internal magnetization prefers to align perpendicular to the DW. Depending on the sign of DMI, a Néel wall with either \( \phi = 0 \) or \( \pi \) is preferred; here we choose \( D > 0 \), thus \( \phi = \pi \) at \( y = \pm \infty \). During this process, any VBLs (Figure 1a-b) will smoothly evolve into DW-Skyrmions (Figure 1c-d). Similar to the deformation of the DW profile in a VBL due to the demagnetization effect [26], the presence of a DW-Skyrmion also deforms the DW profile due to DMI. Because the internal magnetization is inevitably tilted away from the DW normal in a DW Skyrmion, there is a driving force for the DW itself to bend locally in an attempt to recover this energy; this phenomenon is similar to that identified in [7, 27, 28]. To capture this effect, we adopt the Slonczewski ansatz for the profile function

\[
\theta = 2 \arctan \exp \frac{x - q(y)}{\lambda},
\]

\[
\phi = \phi(y),
\]

where \( \phi(y) \) is the azimuthal angle of the in-plane component of \( m \) and \( q(y) \) denotes the deviation of the DW center from its location in a straight homochiral DW without a VBL or DW Skyrmion; \( q(y) \) and \( \phi(y) \) are two collective coordinates to be solved by minimizing the total energy. We have neglected a possible \( y \)-dependence of the \( \lambda \), which is found to contribute only slightly to a difference between analytic and numerical results. Inserting Eqs. (3) and (4) into the energy functional Eq. (1), noting that the local normal vector \( \mathbf{n} = \{1, q', 0\}/\sqrt{1 + q'^2} \), and integrating out \( x \) from \(-\infty \) to \( \infty \), we obtain

\[
E = \frac{2t_F A}{\lambda} \int dy \left[ q'^2 + \lambda^2 \phi'^2 + 2\xi (\cos \phi - q' \sin \phi) \right.
\]

\[
\left. + 2\eta (\cos^2 \phi - q' \sin^2 \phi) \right],
\]

where \( \eta = (\ln 2) t_F \mu_0 M_s^2 / 8 \sqrt{A K} \) and \( \xi = \pi D / 4 \sqrt{A K} \) are two dimensionless parameters characterizing the relative strengths of the demagnetization and of the DMI, respectively. In deriving the demagnetization term, we have taken into account the film thickness \( t_F \) dependence of the demagnetizing factor of a Néel wall [5, 29].

Minimizing the energy in Eq. (5) through the Euler-Lagrange equations \( \delta E = 0 \) and \( \delta \phi = 0 \) gives

\[
-\lambda^2 \phi'' = \xi (\sin \phi + q' \cos \phi) + \eta (\sin 2\phi + 2q' \cos 2\phi),
\]

\[
q' = \xi \sin \phi + \eta \sin 2\phi,
\]

which are two coupled nonlinear differential equations that can only be solved numerically. However, when both \( \xi \ll 1 \) and \( \eta \ll 1 \), which is generally true using typical material parameters, Equation (6) on \( \phi \) is effectively decoupled from Eq. (7) and reduces to a double Sine-Gordon equation that, despite high non-linearity, can be solved analytically. After a tedious calculation, we obtain the central results in the Letter as

\[
\phi = \begin{cases} \pm \arctan \left( \frac{2\pi \pm \xi}{2\eta - \xi} \right) \tanh \left( \frac{1}{2} \sqrt{1 - \frac{\xi^2}{4\eta^2}} \frac{\pi}{\lambda_s} \right) & \text{if } \xi < 2\eta \\ \pm \arctan \frac{\xi}{\lambda_s} & \text{if } \xi = 2\eta \\ \pm \arctan \left( \frac{\xi}{\lambda_s - 2\eta} \sinh \left( \frac{\xi}{2\eta} - 1 \right) \right) & \text{if } \xi > 2\eta \end{cases}
\]

and

\[
q = \begin{cases} \frac{\eta (y/\lambda_s)^2}{1 - (y/\lambda_s)^2} & \text{if } \xi < 2\eta \\ \sqrt{2\xi \eta} \left[ 1 + \frac{(\phi - 1) \cosh \left( \frac{\sqrt{1 - \frac{\xi^2}{4\eta^2}}}{\lambda_s} \right)}{1 - \frac{\phi}{\lambda_s} \cosh^2 \left( \frac{\sqrt{1 - \frac{\xi^2}{4\eta^2}}}{\lambda_s} \right)} \right] & \text{if } \xi > 2\eta \end{cases}
\]
where \( \lambda_s = \lambda / \sqrt{2} \eta \) is the Skyrmion width along \( y \) at the threshold \( \xi = 2\eta \), and the \( + (-) \) sign represents the Skyrmion (anti-Skyrmion) solution with positive (negative) topological charge \( C \). The critical condition \( \xi = 2\eta \) is where the Néel wall is formed at \( y \to \pm \infty \) and a DW skrymion with \( \pm=\pm 1 \) is formed at the center. For \( \xi < 2\eta \), only a partial skrymion with \( |C| < 1 \) exists \((|C| = 1/2 \text{ at } \xi = 0)\). Correspondingly, the boundary conditions are: \( \phi(\pm \infty) = \pm \pi - \arccos(\xi/2\eta) \) for \( \xi \leq 2\eta \), and \( \phi(\pm \infty) = \pm \pi \) for \( \xi > 2\eta \). When converted into original units, the critical condition reads

\[
D_c = \frac{\ln 2}{\pi} t_F \mu_0 M_s^2.
\] (10)

**Micromagnetic calculations.**—We used our MATLAB based finite differences code M\(^3\) [23, 24]. The code implements the Dzyaloshinskii-Moriya interaction for thin films and the corresponding boundary conditions [31] together with the exchange interaction for micromagnetics [31]. As can be seen in Fig. 2 the magnetization profile of the analytic solutions agrees well with the full micromagnetic results, including the notch-like deformation near the center which ascribes to an increasing \( D \). Parameters used in these calculations are as follows: \( t = 2 \text{ nm, } K = 3 \times 10^5 \text{ J/m}^3, A = 1.6 \times 10^{-11} \text{ J/m, and } M_s = 600 \text{ kA/m}. \) In regard to future applications, the size of a Skyrmion plays an important role. A conventional Skyrmion, i.e., a Néel or Bloch type Skyrmion, in a thin film, consists of an inner and outer domain as well as a DW separating them. The Skyrmion size is often given by its radius which is defined by the inner area bounded by the contour for which the out of plane magnetization vanishes, thereby neglecting the wall width [32]. Because the DW Skyrmion is confined within a distorted DW (Figure 2), the conventional definition of a single Skyrmion radius is not applicable. However, one can use the DW width \( W_{m,x} \) at the Skyrmion center and the width of the DW substructure \( W_{m,y} \) along the wall to obtain an estimate of the size of the DW Skyrmion (for details, see supplemental materials). As shown in Fig. 3 both quantities decrease with increasing DMI. For the analytical solution, \( \lambda \) appearing in Eq. (3) and (4) is assumed to be independent of \( D \). It is simply given by \( \lambda = \sqrt{A/K} \), which provides an upper bound for the width \( W_{m,x} \). From the micromagnetic simulations. As shown in Fig. 3, the analytical value \( W_{m,y} \) provides a good approximation for the width determined from micromagnetic calculations. However, while these two quantities can be helpful for transmission electron microscopy studies they do not capture the unique shape of DW Skyrmyons. We therefore propose an alternative way to define the Skyrmion size and shape using the topological charge density defined by \[ \rho_{\text{top}} = \frac{1}{4\pi} \mathbf{m} \cdot (\partial_x \mathbf{m} \times \partial_y \mathbf{m}) . \] (11)

The size of an arbitrary Skyrmion can now be defined as the area enclosing a certain percentage of the topological charge. Normalized plots of topological charge density are shown in Fig. 2. The core of the DW Skyrmion defined by \( W_{m,x} \) and \( W_{m,y} \) contains about 20% of the topological charge of the DW Skyrmion.

**Lorentz TEM simulations.**—To support future experimental imaging of DW Skyrmyons, we employ Fresnel mode Lorentz TEM calculations on the micromagnetic output of Fig. 2. Fresnel mode Lorentz TEM is an out-of-focus imaging technique in which a through-focus series of bright field images is recorded; details regarding the simulation of relevant image contrast can be found in [34]. Numerical profiles of an isolated VBL (\( D = 0 \text{ mJ/m}^2 \))

**FIG. 2:** (a)-(e) Analytical solutions Eq. (8) and (9). (f)-(j) full micromagnetic solutions and (k)-(o) topological charge densities, here the contour lines enclose the topological charge indicated. The DMI strength is indicated at the bottom of each column. With \( A = 1.6 \times 10^{-11} \text{ J/m, } K = 3 \times 10^5 \text{ J/m}^3 \) and \( M_s = 600 \text{ kA/m}. \) The areas shown are \( 100 \text{ nm} \times 250 \text{ nm} \).
FIG. 3: DW Skyrmion width $W_{m,x}$ (blue) across and $W_{m,y}$ (red) along the domain wall as a function of DMI strength. Solid lines are the results of micromagnetic calculation, whereas the dashed lines are the analytical results. For the analytical results the wall width was assumed to be constant and is given by $W_{m,x}^{ana} = 2\lambda = 2\sqrt{A/K}$. The critical DMI strength $D_c$ is shown as a dotted magenta line.

FIG. 4: a & d) Fresnel mode LTEM, b & e) phase map, and c & f) in-plane magnetic induction map of a a - c) vertical Bloch line (D = 0 mJ/m$^2$) and d - f) DW Skyrmion (D = 0.5 mJ/m$^2$) calculated from the micromagnetic output of figures 2f and 2i.

FIG. 5: a - e) Fresnel mode LTEM images and f - j) corresponding in-plane magnetic induction maps of an isolated DW Skyrmion (D = 0.5 mJ/m$^2$) at varied states of tilt calculated from micromagnetic outputs illustrated in figure 2i.

and an isolated DW Skyrmion (D = 0.5 mJ/m$^2$) are illustrated in Fig. 2f and i, respectively, which are used in the calculations of Fig. 4. In the absence of DMI, Bloch walls are present which display a sharp magnetic contrast that reverses at the location of the VBL in Fresnel mode images (figure 4a). In the presence of DMI, Néel walls become the preferred configuration; they do not display any magnetic contrast in Fresnel mode images in the absence of sample tilt. However, strong magnetic contrast is still observed at the location of the DW Skyrmion in Fig. 4d. This dipole-like contrast originates from the Bloch-like portions of the DW in the 360° rotation of magnetization across the DW Skyrmion. Thus, DW Skyrmions would be the only contributor to magnetic contrast in systems that exhibit DMI when examined with Lorentz TEM in the absence of sample tilt.

As experimental Fresnel-mode Lorentz TEM images do not offer explicit directional information regarding the magnetic induction, phase reconstruction is typically employed using the Transport of Intensity Equation (TIE) to calculate the integrated in-plane magnetic induction [35, 36]. The resultant phase map for D=0 displays contrast along the domain wall which reverses at the location of the VBL similar to that observed in the Fresnel mode image. The color map shows the direction of in-plane induction matching those in the output of the micromagnetic simulation with a discontinuity at the location of the VBL. Because the center of the VBL is fully Néel, it exhibits no intensity in the Fresnel mode images and does not contribute in TIE calculations. The phase map of the DW Skyrmion also displays contrast similar to that observed in its corresponding Fresnel mode image. The magnetic induction takes on a distinct braided appearance centered around the DW Skyrmion with no signal from the surrounding DW. This signature takes on a larger footprint than that of magnetic contrast in the calculated Fresnel mode image which may assist in locating DW Skyrmions in experimental images.

As mentioned previously, Néel walls do not display magnetic contrast in the absence of a sample tilt in Fresnel mode imaging. When a tilt is applied to the sample, an effective Bloch-type induction emerges from the perpendicular induction of neighboring domains giving rise to contrast at a Néel wall. This too is observed in our calculated Fresnel mode images (Figure 5a-e); as sam-
ple tilt increases, magnetic contrast becomes more apparent along the DW surrounding the DW Skyrmion. Additionally, the contrast from the DW Skyrmion itself remains strong with respect to the surrounding DW contrast which will be useful for confirming the presence of a DW Skyrmion experimentally. This contrast remains constant on either side of sample tilt which display different contrast along the surrounding DW. The corresponding in-plane magnetic induction maps (Figure 5f-j) further support this notion as the braid-like feature from the DW Skyrmion remains visible even at larger tilts where a strong signal is observed around the DW due to the Bloch-like contributions of the surrounding perpendicular domains.

In summary, we have introduced a new kind of topological magnetic excitation called a DW Skyrmion characterized by a 360° transition of the internal magnetization within a chiral DW and defined by a topological charge of ±1. The DW Skyrmion analysis presented here builds off prior work on VBLs in much the same way the recent surge in Skyrmion research is rooted in decades of research on magnetic bubble memory. The static properties were calculated both analytically and micromagnetically with excellent agreement on the resulting size and profile. Although open questions remain about their thermal stability and dynamic properties, DW Skyrmions provide an alternative strategy for leveraging topological protection in magnetic systems with a strong interfacial DMI. The reconfigurable nature of the DWs that host these excitations could open the door to new kinds of memory and computing schemes based on topological charge. To this end, we have proposed an experimental methodology to unequivocally image DW Skyrmions using Fresnel mode Lorentz TEM to support future work in this area.

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[1] I. Dzyaloshinsky, Journal of physics and chemistry of solids 4, 241 (1958).
[2] T. Moriya, Physical Review 120, 91 (1960).
[3] X. Z. Yu, Y. Onose, N. Kanazawa, J. H. Park, J. H. Han, Y. Matsui, N. Nagaosa, and Y. Tokura, Nature 465, 901 EP (2010).
[4] S. X. Huang and C. L. Chien, Physical Review Letters 108 (2012).
[5] A. Thiaville, S. Rohart, E. Jue, V. Cros, and A. Fert, EPL 100 (2012).
[6] A. Hrabec, N. A. Porter, A. Wells, M. J. Benitez, G. Burnett, S. McVitie, D. McGrouther, T. A. Moore, and C. H. Marrows, Physical Review B 90 (2014).
[7] J. P. Pellegrin, D. Lau, and V. Sokalski, Phys. Rev. Lett. 119, 027203 (2017).
[8] D. Lau, J. Price Pellegren, H. Nembach, J. Shaw, and V. Sokalski, ArXiv e-prints (2018), arXiv:1808.05520 [cond-mat.mtrl-sci].
[9] J. E. Hirsch, Physical Review Letters 83, 1834 (1999).
[10] L. Q. Liu, C. F. Pai, Y. Li, H. W. Tseng, D. C. Ralph, and R. A. Buhrman, Science 336, 555 (2012).
[11] S. Emori, U. Bauer, S.-M. Ahn, E. Martinez, and G. S. D. Beach, Nature Materials 12 (2013).
[12] A. Hoffmann, Ieee Transactions on Magnetics 49, 5172 (2013).
[13] W. J. Jiang, P. Upadhyaya, W. Zhang, G. Q. Yu, M. B. Jungfleisch, F. Y. Fradin, J. E. Pearson, Y. Tserkovnyak, K. L. Wang, O. Heinonen, S. G. E. te Velthuis, and A. Hoffmann, Science 349, 283 (2015).
[14] S. Woo, K. Litzius, B. Kruger, M.-Y. Im, L. Caretta, K. Richter, M. Mann, A. Krone, R. M. Reeve, M. Weigand, P. Agrawal, I. Lemesh, M.-A. Mawass, P. Fischer, M. Klau, and G. S. D. Beach, Nat Mater 15, 501 (2016).
[15] P. Jennings and P. Sutcliffe, Journal of Physics a-Mathematical and Theoretical 46 (2013), Artn 465401 10.1088/1751-8113/46/46/465401.
[16] S. B. Gudnason and M. Nitta, Physical Review D 89 (2014), ARTN 085022 10.1103/PhysRevD.89.085022.
[17] A. Thiaville, Journal of Magnetism and Magnetic Materials 140-144, 1877 (1995).
[18] A. P. Malozemoff and J. C. Slonczewski, Physical Review Letters 29, 952 (1972).
[19] J. C. Slonczewski, Journal of Applied Physics 45, 2705 (1974).
[20] S. Konishi, Ieee Transactions on Magnetics 19, 1839 (1983).
[21] S. Konishi, M. Matsuyama, I. Chida, S. Kubota, H. Kawahara, and M. Ohbo, Ieee Transactions on Magnetics 20, 1129 (1984).
[22] W. Jiang, X. Zhang, G. Yu, W. Zhang, X. Wang, M. Benjamin Jungfleisch, J. E. Pearson, X. Cheng, O. Heinonen, K. L. Wang, Y. Zhou, A. Hoffmann, and S. G. E. te Velthuis, Nature Physics 13, 162 EP (2016).
[23] “Micromagnetic code M3,” http://micromagneticslab.ua.edu/micromagnetics-code.html.
[24] J. B. Mohammadi, K. Cole, T. Mewes, and C. K. A. Mewes, Phys. Rev. B 97, 014434 (2018).
[25] A. Hubert and R. Schaefer, Magnetic Domains: The Analysis of Magnetic Microstructures (Springer-Verlag Berlin Heidelberg, 1998).
[26] A. V. Nikiforov and E. B. Sonin, JETP 63, 766 (1986).
[27] O. Boulle, S. Rohart, L. D. Buda-Prejbeanu, E. Jué, I. M. Miron, S. Pizzini, J. Vogel, G. Gaudin, and A. Thiaville, Phys. Rev. Lett. 111, 217203 (2013).
[28] D. Lau, V. Sundar, J.-G. Zhu, and V. Sokalski, Phys. Rev. B 94, 060401 (2016).
[29] S. Tarasenko, A. Stankiewicz, V. Tarasenko, and J. Ferr, Journal of Magnetism and Magnetic Materials 189, 19 (1998).
[30] S. Rohart and A. Thiaville, Phys. Rev. B 88, 184422 (2013).
[31] M. Donahue and D. Porter, Physica B: Condensed Matter 343, 177 (2004), proceedings of the Fourth International Conference on Hysteresis and Micromagnetic Modeling.
[32] X. S. Wang, H. Y. Yuan, and X. R. Wang, Communications Physics 1, 31 (2018).
[33] S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer, and S. Blugel,
Nature Physics 7, 713 (2011).

[34] M. De Graef, in Magnetic Microscopy and its Applications to Magnetic Materials, Experimental Methods in the Physical Sciences, Vol. 36, edited by M. De Graef and Y. Zhu (Academic Press, 2000) Chap. 2.

[35] D. Paganin and K. A. Nugent, Physical Review Letters 80, 2586 (1998).

[36] M. Beleggia and Y. Zhu, Philosophical Magazine 83, 1045 (2003).