Orientation and internal structure of domain walls in ferromagnetic films with anisotropic Dzyaloshinskii-Moriya interaction

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A R T I C L E   I N F O

A B S T R A C T

We present an analytical study of domain-wall internal structure and orientation in a ferromagnetic film with out-of-plane anisotropy and the anisotropic interfacial Dzyaloshinskii-Moriya interaction (iDMI). The term "anisotropic" means that the iDMI constant is different for different in-plane directions. The interplay between the magnetostatic interaction and the iDMI in a domain wall defines both its structure and orientation. In the case of the isotropic iDMI there is no preferable orientation of the DW in the film plane leading to formation of labyrinth domain structure with random shapes of the domains. In the case of the anisotropic iDMI an oriented domain stripe structure and zigzag domains appear. Depending on system parameters, either the Bloch domain walls, or the Néel ones or the hybrid canted walls realize in the magnetic film. The spatial orientation of the DW and the orientation of the magnetization rotation plane in the DW are intimately related by a simple linear ratio. The analytical results are corroborated by micromagnetic simulations.

Domain walls (DWs) in thin-film ferromagnets have been intensively studied over the last decades both experimentally [1–3] and theoretically [4–6]. This interest arises since the DWs are considered as promising candidates for information bit carriers in a racetrack memory [7], data transfer [8] and processing spintronic devices [9]. Static and dynamic properties of a DW depend on the interplay between exchange coupling, magneto-crystalline anisotropy and magnetostatic interaction [10,11]. In ultrathin films the spatial inversion symmetry is broken at the interface and strong interfacial DMI (iDMI) appears [12]. The iDMI favours formation of DWs and skyrmions in the thin films. To date, the chiral magnetic structures caused by the iDMI was experimentally observed in Mn/W [13,14], Fe/Ir [15], Co/Pt [16–19], and Fe/Ni/Cu [20,21] films with an out-of-plane anisotropy. The iDMI in transitional metal ferromagnet (FM)/ heavy metal (HM) bilayers leads to formation of the Néel walls [22]. This has been experimentally verified by a spin-polarized low-energy electron microscopy [20] and the Lorentz transmission electron microscopy [18]. The DWs in artificial ultrathin ferromagnetic films are attractive for spintronic application and recently get into the focus of many experimental studies [18,23–26].

A domain wall separates two regions with different magnetization orientation. Since the width of the domain wall is often much smaller than the domain size, people consider it as a plane separating magnetic

domains. Such a plane can be characterized by certain orientation in space. Further we will refer the orientation of the DW plane simply as DW orientation.

Note that in spite of small thickness, the domain wall has an internal magnetic structure. Usually, two types of DW are considered:

1) the Bloch one (in which magnetization rotates in the plane of the domain wall);
2) the Néel one (in which magnetization rotates in the plane made by the vector perpendicular to the domain wall plane and the vector of magnetization in the domain).

Generally, there could be an intermediate type of DW structure in which the magnetization rotates in the plane oriented by some angle with respect to the DW plane. Finally, the DW can be described by two angles defining orientation of the domain wall itself (β) and defining the orientation of the rotation plane of magnetization inside the DW (φ).

In the case of the strong isotropic iDMI (when the magnetostatic energy of the DW can be neglected) the analytical model gets the Néel type of the DW [27,28]. A competition between the iDMI and magnetostatic energies causes a fluent transition from the Bloch wall to the Néel one via a canted wall state with increase of iDMI [29].

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At that, due to the isotropy of the iDMI there is no preferable orientation of the DW itself. Therefore, the isotropic labyrinth domain structure or stripe domains with arbitrary orientation appear in such films (see for example, Ref. [20] where Co/Ni/Ir/Pt layers are studied).

Nevertheless, it is known that sometimes DWs are strictly oriented in a ferromagnetic layer with iDMI [22,30]. This can be attributed to the anisotropy of the iDMI in the film plane. This anisotropy may appear due to the crystalline structure at the FM/HM interface (for example, in Fe/W [22] and Co/W [31] systems), or can be induced by a strain, as it is observed in the bulk FeGe crystals [32]. Recently, the strong strain induced anisotropy of iDMI in Co/Pt is observed also [33]. It was shown in [33] that iDMI may have a different sign along different direction and the ratio of the iDMI constant along x (D_x) and y (D_y) axes can be as high as $D_x/D_y \approx -1$. This observation motivates studies of the systems with strongly anisotropic iDMI.

It is also theoretically demonstrated that the anisotropic iDMI may lead to formation of anti-skyrmions [31,34,35] (which were soon after observed experimentally [36]). However, the previously considered models of the anti-skirmions [31] neglect the DW magnetostatic energy, which plays decisive role in DW structure formation, especially in thin films [29].

In the current work we take into account both the in-plane magnetostatic energy and anisotropic character of the iDMI and obtain the analytic solution for the straight isolated DW. The solution demonstrates that the iDMI anisotropy orients the DWs in the FM film plane.

In a bilayer structure FM/HM the orientation and internal structure of domain walls is defined by the competition between the four energy contributions: exchange interaction, magnetic anisotropy, magneto-dipole interaction, and interfacial Dzyaloshinskii-Moriya interaction. Consider a thin magnetic film of the thickness t and with the saturation magnetization M_s. The film lays in the (x,y)-plane (Fig. 1). Usually, the iDMI interaction is studied in the FM layers with the thickness of few nms (much smaller than the exchange correlation length). Therefore, the magnetization is uniform across the layer. The magnetic anisotropy is out-of-plane, which may occur due to the interfacial effects (as in Co/Pt films, for example). The surface energy density of the anisotropy is defined by Km_z^2 (where **m** is the unit vector along the local magnetization and K is the anisotropy constant). Then the volume density of the anisotropy energy is given by Km_z^2/t. One can also introduce the effective out-of-pane anisotropy constant $K_{eff} = K/t - \mu_0 M_s^2/2$ (μ_0 is the vacuum permeability). It takes into account the magnetostatic demagnetizing factor of a thin film. The exchange stiffness in the film is A giving the exchange energy density $A((\partial \mathbf{m}/\partial x)^2 + (\partial \mathbf{m}/\partial y)^2 + (\partial \mathbf{m}/\partial z)^2)$. There is also the anisotropic iDMI in the considered film. Choose a coordinate system in which the surface density of the iDMI energy takes the form

$$W_{DMI} = D_x\left(m_x\frac{\partial m_z}{\partial x} - m_z\frac{\partial m_x}{\partial x}\right) + D_y\left(m_y\frac{\partial m_z}{\partial y} - m_z\frac{\partial m_y}{\partial y}\right). \quad (1)$$
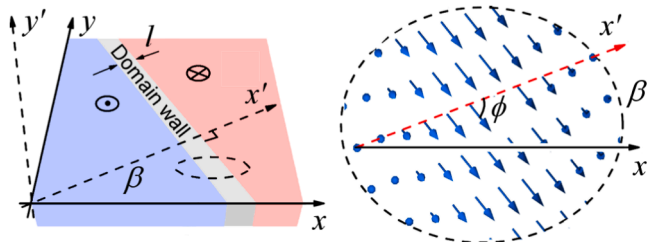

Fig. 1. Left panel: domain wall oriented along the x'-axis rotated by the angle β with respect to the x-axis. The domain wall width is denoted l. Right panel: magnetization distribution inside the domain wall. ϕ is the angle defining the orientation of the magnetization rotation plane with respect to the DW plane (x'-axis).

If the iDMI constants along both directions are the same $D_x = D_y$, then the interaction becomes isotropic and one gets a usual expression for the iDMI.

Lets find the orientation of a DW and its inner magnetic structure in the studied film. Consider a DW oriented by the angle β with respect to the x-axis (see Fig. 1). Introduce a new coordinate system (x',y') rotated around the z-axis at the angle β (the x'-axis coincides with the DW orientation). According to the q-ϕ model [37], the magnetization distribution within the DW is described by the expressions

$$\begin{aligned} m_z &= m_z(x') = \tanh(x'/l), \\ m_x &= m_x(x') = \cos(\phi)/\cosh(x'/l), \\ m_y &= m_y(x') = \sin(\phi)/\cosh(x'/l). \end{aligned} \quad (2)$$

Here ϕ is the angle defining the orientation of the magnetization rotation plane with respect to the DW plane (see Fig. 1). This angle is the same across the DW. The width of the DW is denoted by $l = \sqrt{A/K_{eff}}$. The expression (2) is also can be used in the presence of the DMI if it is small enough [38,29].

In the new coordinate system (x',y') the expression for the iDMI interaction takes the form

$$\begin{aligned} W_{DMI}^{\phi} = &D_{x'}\left(m_{x'}\frac{\partial m_z}{\partial x'} - m_z\frac{\partial m_{x'}}{\partial x'}\right) + \\ &+ D_{y'}\left(m_{y'}\frac{\partial m_z}{\partial y'} - m_z\frac{\partial m_{y'}}{\partial y'}\right) + \\ &+ D_{\perp}\left(m_{x'}\frac{\partial m_z}{\partial y'} + m_{y'}\frac{\partial m_z}{\partial x'} - m_z\frac{\partial m_{y'}}{\partial x'} - m_z\frac{\partial m_{x'}}{\partial y'}\right), \end{aligned} \quad (3)$$

where

$$\begin{aligned} D_{x'} &= D_x\cos^2(\beta) + D_y\sin^2(\beta), \\ D_{y'} &= D_x\sin^2(\beta) + D_y\cos^2(\beta), \\ D_{\perp} &= (D_y - D_x)\cos(\beta)\sin(\beta). \end{aligned} \quad (4)$$

The additional term (the last line in Eq. (3)) occurs due to the anisotropy of the iDMI. This term is zero when $D_x = D_y$. Introducing Eq. (2) into Eq. (3) and integrating Eq. (3) along the x'-axis one obtains the iDMI energy of the DW per unit length

$$W_{DMI} = -\pi t(D_{x'}\cos(\phi) + D_{\perp}\sin(\phi)). \quad (5)$$

Finally, the total energy of the DW per unit length is given by

$$\begin{aligned} W_{dw} = &t\left(\frac{2A}{l} + 2K_{eff}l + \frac{1}{2}k(t/l)\Omega\cos^2(\phi) + \right. \\ &\left. - \pi D_{x'}\cos(\phi) - \pi D_{\perp}\sin(\phi)\right). \end{aligned} \quad (6)$$

The first two terms are the exchange interaction and the effective magnetic anisotropy. The third term describes the magneto-dipole contribution to the DW energy. The derivation of the expression for the dipole-dipole interaction can be found in Ref. [29]. The thickness dependent factor $k(t/l)$ can be simplified in the case of thin films $k(t/l) \to 2\ln(2)/\pi \approx 0.44$. The characteristic magneto-dipole energy is denoted $\Omega = \mu_0 M_s^2 t$. In this limit the DW thickness l is defined by the exchange interaction and magnetic anisotropy and is given by $l = \sqrt{A/K_{eff}}$. The first two terms in Eq. (6) in this case can be replaced by $4\sqrt{AK_{eff}}$. The two terms in the second line are the iDMI contributions. The first one is taken into account in previous studies. It exists in films with isotropic iDMI. The second one appears only in the anisotropic films for the DW oriented along the direction not aligned with a main axis. Note that this energy contribution tends to turn the magnetic moments perpendicular to the DW plane x'. So, it "prefers" the Bloch-type DW.

To study the system ground state and find equilibrium DW orientation and magnetization rotation plane we minimize the energy Eq. (6) with respect to angles β and φ.

The orientation of the magnetization rotation plane (ϕ) is defined by the competition between the iDMI and the magneto-static interaction. In the absence of the iDMI the DW is of the Bloch type with $\phi = \pi/2$. In the case of isotropic iDMI at high $D_{x'}$ the DW is of the Néel type ($\phi = 0$).

In the case of the isotropic iDMI there is a degeneracy with respect to the DW orientation. The DW energy W_{dw} is independent of β. In contrast, the anisotropic iDMI introduces the dependence of the DW energy on it's orientation, $W_{dw} = W_{dw}(\beta, \phi)$. Therefore, one needs to optimize not only the magnetization rotation angle ϕ but also the DW orientation β to find the system ground state.

Introducing new parameters $D_+ = (D_x + D_y)/2$ and $D_- = (D_x - D_y)/2$ one gets for the DW energy

$$W_{dw} = t\left(\ldots - \pi D_+\cos(\phi) - 2\pi D_-\cos(2\beta - \phi) + \right.$$
$$\left. + \frac{1}{2}k\Omega\cos^2(\phi)\right). \tag{7}$$

Only the second term depends on β in Eq. (7). This immediately gives a rigid connection between the DW orientation β and the canting angle of the magnetization rotation plane ϕ

$$\beta = \phi/2. \tag{8}$$

Introducing ϕ into Eq. (7) one gets

$$W_{dw} = t\left(\ldots - \pi D_+\cos(\phi) - 2\pi D_- + \frac{1}{2}k\Omega\cos^2(\phi)\right). \tag{9}$$

From the equation one finds for the equilibrium canting angle ϕ

$$\cos(\phi) = \begin{cases} \frac{\pi D_+}{k\Omega}, \frac{\pi D_+}{k\Omega} \leqslant 1, \\ 1, \frac{\pi D_+}{k\Omega} > 1 \end{cases} \tag{10}$$

This extremum point is a minimum as both

$$\frac{\partial^2 W_{dw}}{\partial\phi^2} = k\Omega + 2\pi D_- - \frac{(\pi D_+)^2}{k\Omega} \tag{11}$$

and the Hessian

$$H = \frac{\partial^2 W_{dw}}{\partial\phi^2}\frac{\partial^2 W_{dw}}{\partial\beta^2} - \left(\frac{\partial^2 W_{dw}}{\partial\beta\partial\phi}\right)^2 = 8\pi D_-\left(k\Omega - \frac{(\pi D_+)^2}{k\Omega}\right) \tag{12}$$

are positive at this point. Note that second derivatives of the energy defines the rigidity of the corresponding ground state. The higher the derivatives the more stable the ground state is with respect to the variation of β and ϕ.

Fig. 2 shows the angles ϕ and β corresponding to the system ground state as a function of D_x and D_y. Rotation of the coordinate system by the angle $\pi/2$ changes $D_x \rightarrow D_y$ and $D_y \rightarrow D_x$. Therefore, the system phase diagram can be plotted in a single quadrant of the (D_x, D_y)-plane.

In the isotropic case ($D_x = D_y, D_- = 0$) the ground state is a neutral equilibrium (the Hessian is equal to zero) with respect to variations of the DW orientation angle β. There is no preferable orientation of domain walls. The magnetization rotation angle is still defined by Eq. (10). When $D_x = D_y > k\Omega/\pi$ the DW is of the Néel type ($\phi = 0$). Below the critical iDMI value the angle $\phi > 0$ and smoothly grows to $\pi/2$ (Bloch wall) while one decreases $D_{x,y}$.

The highest anisotropy appears at the line $D_y = -D_x$. In this case the DW orientation is $\beta = \pi/4$. This can be understood as follows. The isotropic part of the iDMI has the magnitude $D_{x'} = 2D_x/\sqrt{2}$. The anisotropic iDMI energy reaches its maximum ($D_\perp = 2D_x$) and dominates. To minimize this contribution one needs to take the magnetization rotation angle $\phi = \pi/2$. Such a choice of ϕ also minimizes the magneto-static interaction. Finally, the Bloch-type DW is oriented by the angle $\pi/4$ with respect to the system main axes. Note that the DW energy is the same for $\beta = -\pi/4$. Therefore, we expect zig-zag domains
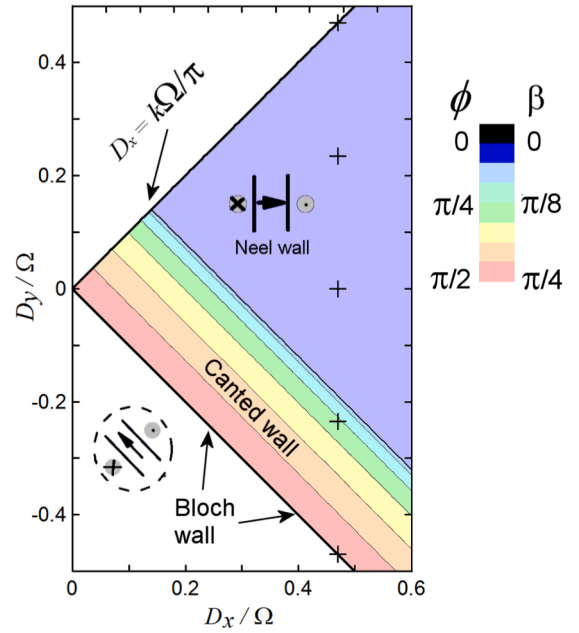

Fig. 2. Equilibrium orientation of the DW plane (β) and equilibrium orientation of the magnetization rotation plane (ϕ) as a function of D_x and D_y. Only the sector $|D_y| < D_x$ is shown. Crosses show the parameters corresponding to the numerically simulated domain structures represented in Fig. 3.

(or the stripe structure with a specific orientation) appearing in the case of strong iDMI anisotropy.

The region in the phase diagram between the lines $D_x + D_y = 4k\Omega/\pi$ and $D_x + D_y = 0$ corresponds to the canted type of DWs. As indicated in Eqs. (10) and (8) (and seen in Fig. 2) the system state is independent of D_-. However, the stiffness of the system ground state (defined by the second derivatives Eq. (11) and the Hessian Eq. (12)) depends on D_-. The closer the system parameters to the isotropic case ($D_x = D_y$) the smaller the second derivatives are and the less stable the ground state is according to random local fluctuations of the parameters in the system.

We corroborate our analytic approach with micromagnetic simulations utilizing the OOMMF code [39]. This code is based on a numerical solution of the system of Landau-Lifshitz-Gilbert (LLG) equations for the magnetization of the system. The simulated system is the rectangular plate with the width of 762 nm and the thickness of $t = 1$ nm. Periodical boundary conditions in the plane of the film are used. For our calculations we use the material parameters typical for ferromagnetic films with a perpendicular anisotropy and the iDMI $M_s = 1.3 \times 10^6$ A/m, $A = 1.6 \times 10^{-11}$ J/m, $K_v = 1.075 \times 10^6$ J/m^3 ($K_v = K/t$). The iDMI constants D_x, D_y varies from -10^{-3} to 10^{-3} J/m^2 which is also typical for FM/HM bilayers. The mesh element size $1.5 \times 1.5 \times 1$ nm^3 is much smaller than the DW width. The simulations start with a uniformly magnetized film ($M_z = \pm M_s$) and run until the system relaxes to a stationary state (at the zero external field). A small random anisotropy ($K_r = K \times 0.001$) is distributed over the film to initialize magnetization reversal. The typical domains configurations are represented in Fig. 3.

Evidently, the system with $D_x = D_y = 1$ mJ/m^2 demonstrates a labyrinth domain structure with the Néel DWs. There is no preferable orientation of the DWs in this case. With the decrease of D_y down to 0.5 mJ/m^2 the DW obtains a preferable orientation perpendicular to the x-axis. They are not straight because their stiffness characterised by the Hessian (9) is not high enough to overcome local metastable state caused by interplay of the DWs energy and global magnitostatic energy. Decreasing D_y down to zero increases the iDMI anisotropy up to 1 mJ/m^2. In this case the strictly oriented stripe domain structure is observed in the simulations. In the case of the $D_y = -0.5$ mJ/m^2 the stripe domain structure inclined to the x-axis should appears. However, due to

| $D_x = 1,\ D_y = 1$ | $D_x = 1,\ D_y = 0.5$ | $D_x = 1,\ D_y = 0$ | $D_x = 1,\ D_y = -0.5$ | $D_x = 1,\ D_y = -1$ |
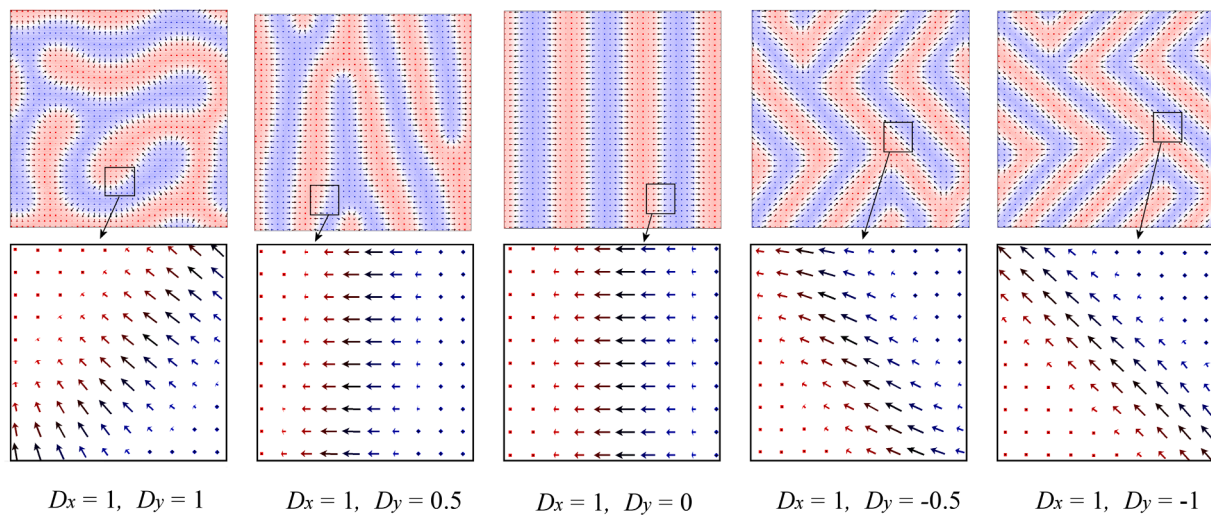
Fig. 3. Upper row: simulated domain structures for different iDMI constants. Bottom row: close view of the DWs. The values of the iDMI constants are shown in mJ/m^2.

some randomness in a domain nucleation process we observe zigzag domains instead (which correspond to the system metastable state). Note that the energy of the DW is the same for the two orientations, β and $-\beta$. The DWs have canted inner structure with intermediate orientation of the magnetization rotation plane. Finally, for $D_x = -D_y = 1$ mJ/m^2 the DWs become of the Bloch type and are oriented at 45° to the system axis. The iDMI constants corresponding to the simulated domain structures represented in Fig. 3 are shown in the phase diagram Fig. 2 by crosses, the similarity of the analytically and numerically calculated data is evident.

Experimentally, the anisotropic iDMI can be realized in the magnetic films grown on the initially anisotropic substrates or by applying a strain to the initially isotropic system. Changing the strain it is possible to manipulate the iDMI anisotropy (and therefore the structure and orientation of domain walls).

On the other hand, the iDMI anisotropy can be observed and estimated through studying of the domains structure in a magnetic film. Magnetic force microscopy can be used for this purpose. If the labyrinth domain structure has isotropic distribution of the walls orientation the iDMI is isotropic. If DWs have preferable orientation there should be the anisotropic iDMI in the system.

So, in our work we analyses the internal structure and orientation of domain walls in a thin ferromagnetic film with a perpendicular magnetic anisotropy and anisotropic interfacial DMI. It is shown that the DWs has a preferable orientation due to iDMI anisotropy. The orientation of the DW and the magnetization rotation plane inside the DW are related by a simple linear ratio.

CRediT authorship contribution statement

O.G. Udalov: Conceptualization, Methodology, Writing - original draft, Writing - review & editing, Investigation. **M.V. Sapozhnikov:** Conceptualization, Methodology, Writing - original draft, Writing - review & editing, Investigation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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