Editor's Choice

Effects of anisotropic exchange on the micromagnetic domain structures

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We have investigated the influence of anisotropic exchange on the micromagnetic domain structure. Three-dimensional simulations based on the Landau–Lifshitz–Gilbert equation were performed incorporating a generalized tensor representation of the exchange following a phenomenological approach. In comparison to isotropic exchange, which is usually used in micromagnetic simulations, anisotropic exchange significantly affected the equilibrium distribution of the magnetization. The formation of slanted domain walls aligning in the direction of stiffest exchange and the deformation of edge domains were the most prominent consequences. In general, we found that anisotropic exchange may have profound effects on magnetic nanostructures.

1 Introduction

In recent years magnetic materials have become very important in information technology. The ability to produce magnetic nanostructures opened the door for future applications, like spin electronics or magnetic memory devices (MRAMs) [1]. The knowledge of the magnetization distribution is important from a scientific and technological point of view because the domain structure of the material governs the capabilities for applications. Computational micromagnetics gives a quantitative treatment of the influence of the micromagnetic structure on basic macroscopic magnetic properties like magnetization reversal and hysteresis.

In the continuum theory of micromagnetism, the exchange energy density is the term that represents the quantum mechanical coupling originating from the collective character of magnetism. It imposes an energy constraint on any change in magnetization direction. An isotropic model is typically used in micromagnetic simulations [2–5]. However, this is only suitable for cubic crystals, as lower symmetry crystals exhibit a bond anisotropy leading to an anisotropic exchange stiffness [6]. Examples of practically relevant, anisotropic magnets are PtCo, PtFe, Co, and SmCo5 [7]. Furthermore, modern fabrication techniques have extended the classes of magnetic materials. In particular, alloys and oxides with non-cubic crystal structure, disordered and partially ordered magnets, magnetic nanostructures, and multilayers exhibit coupling phenomena that are highly anisotropic. In addition, the strain of epitaxially grown films can lead to an exchange-striction effect causing an anisotropy in the magnetic exchange [8].
To generalize the exchange stiffness energy density, a tensor rather than a scalar should be used [9, 10]. The coefficients of this tensor can be determined experimentally, for example by the long-wavelength part of the magnon spectrum [11]. Although for some selected tetragonal and hexagonal crystals the principal components of the exchange stiffness tensor have been calculated using a spin-spiral formulation of the tight-binding linear muffin-tin orbital method [12], the experimental and theoretical determination of the components are not commonly performed. Moreover, the effects of anisotropic exchange on the micromagnetic domain structure have not been explored yet and are the focus of this paper. It will be shown that a strong anisotropy of exchange stiffness can significantly affect the domain structure.

For magnetic materials, where the magnetocrystalline easy axis is collinear with the direction of the stiffest exchange, a stable solution of a domain transition is trivial. In this case, i.e., the direction normal to the domain wall perpendicular to both the direction of the stiffest exchange and the magnetocrystalline easy axis, the respective energies are minimum. However, in case the direction of the stiffest coupling is not parallel to the magnetocrystalline easy axis, the energy minimum of a domain transition is non-trivial [12]. A domain wall along the stiffest coupling decreases the exchange energy by simultaneously increasing the magnetocrystalline anisotropy energy and the demagnetization energy.

We have implemented anisotropic exchange in a micromagnetic simulator based on the finite difference method [13] and optimized it for parallel computing using the message passing interface (MPI) [14]. In the following, we introduce a phenomenological model for the anisotropic exchange tensor and discuss the effects of anisotropic exchange phenomena on the domain structures.

2 Phenomenological model of the exchange stiffness tensor

As mentioned in the introduction, the exchange energy term is typically assumed to be isotropic in micromagnetism. This is a convenient approximation for cubic crystals [15]. For all non-cubic crystals, anisotropic exchange can be present and the implementation of the exchange stiffness tensor is needed. Here, the exchange anisotropy is solely related to the different bonding in the crystal. This must not be confused with the rather weak relativistic anisotropies, which involve spin-orbit coupling and depend on the angle between magnetization and the crystal axes. For the exchange stiffness energy density, we use the general expression [9, 10]:

$$\varepsilon_{\text{exch}}(x, y, z) = \sum_{i,j} A_{ij} \frac{\partial m^k(r)}{\partial x_i} \frac{\partial m^k(r)}{\partial x_j},$$

where $A_{ij}$ is the exchange stiffness tensor. The isotropic case is given for $A_{ij} = A \delta_{ij}$, which reduces Eq. (1) to the usually used exchange stiffness expression $\varepsilon_{\text{exch}} = A [\nabla \cdot \mathbf{m}(r)]^2$. Equation (1) is isotropic with respect to the magnetization, but anisotropic with respect to the nabla operator $\nabla = \partial/\partial x$, reflecting a bonding-related anisotropy [6].

As discussed by Döring [10], the symmetry of the crystal defines the principal axes of the exchange stiffness. For cubic crystals, the exchange coefficients have to be of the same amplitude, resulting in isotropic exchange. For hexagonal, rhombohedral, and tetragonal crystals, one principal axis coincides with the crystallographic main axis, whereas the other two lie in a plane perpendicular to it with equal coefficients, which differ from that for the main axis direction. The directions of all principal axes of the matrix are arbitrary for triclinic crystals, whereas for monoclinic crystals one principal axis has to point along the symmetry axis of the crystal. Moreover, for exchange coupling phenomena where the direction does not coincide with the crystal symmetry, the exchange stiffness tensor cannot be used directly in the principal-axis representation. This situation can occur for magnetic materials where double exchange, superexchange, or indirect exchange couples the magnetic moments.

The exchange interaction tensor is defined to be positive to ensure an increase of the energy with a change in the magnetization. It is assumed to be symmetric, because an antisymmetric part is canceled out in Eq. (1) due to the permutation of the derivatives. If the matrix is transformed to the principal axis representation, only the coefficients of the trace are nonzero and positive.
These considerations lead us to the following phenomenological model of the anisotropic exchange stiffness tensor $A$ that can be employed for micromagnetic simulations. The Curie temperature provides an estimate for the maximum principal value of $A$ [6]. For a completely generalized tensor, two exchange stiffness anisotropies, defined as the ratio of the maximum value with the other principle values, are needed to account for the three different eigenvalues of the matrix. Two rotation angles for an azimuthal and a polar rotation are needed to transform the exchange tensor to the coordinate system of the simulator.

### 3 Results and discussion

We investigate the effects of anisotropic exchange in an artificial material system, starting from the known parameters of MnAs on GaAs(001) [16, 17]. MnAs is a hexagonal crystal in its ferromagnetic phase, which exhibits two phase transitions, one of first order at $T_1 = 40^\circ$C from ferromagnetic to non-ferromagnetic [18], and one of second order at $T_2 = 130^\circ$C to a paramagnetic state [19, 20]. The phase transition at $40^\circ$C can be attributed to a change in the lattice constant of the basal plane and a corresponding change of magnetic coupling in this direction. The phase transition at $130^\circ$C is, on the other hand, a result of a change in the $c$ lattice constant of the hexagonal structure (normal to the basal plane) with associated changes in magnetic coupling along that direction.

The phenomenological exchange coupling tensor is characterized by two different eigenvalues, $A_{\text{min}}$ and $A_{\text{max}}$, and a possible rotation. The rotation is restricted within the $x,y$-plane and the rotation angle $\theta$ is defined between a principal axis with the largest eigenvalue $A_{\text{max}}$ and the $x$-axis. The tensor is then given by:

$$
A = \begin{bmatrix}
a_{11} & a_{12} & 0 \\
a_{12} & a_{22} & 0 \\
0 & 0 & a_{33}
\end{bmatrix}
$$

with

$$a_{11} = A_{\text{max}} \left( \cos^2 \theta + \gamma \sin^2 \theta \right) ,$$

$$a_{12} = A_{\text{max}} \left( 1 - \gamma \right) \left( \cos \theta \cdot \sin \theta \right) ,$$

$$a_{22} = A_{\text{max}} \left( \gamma \cos^2 \theta + \sin^2 \theta \right) ,$$

$$a_{33} = A_{\text{min}} \text{ or } A_{33} = A_{\text{max}} .$$

The ratio of the two eigenvalues defines the exchange stiffness anisotropy $\gamma = A_{\text{min}}/A_{\text{max}}$. For $\gamma = 1$, the tensor reduces to the isotropic exchange $a_{ij} = A_{\text{max}} \delta_{ij}$. For $\gamma \neq 1$ and $\theta = 0^\circ$, the tensor results in an anisotropic exchange with the principal axis along the crystallographic symmetry. For $\theta \neq 0^\circ$, the off-axis elements are nonzero according to the rotation.

$A_{\text{max}}$ and $\gamma$ can be estimated in a very approximate manner from the phase transition temperatures. For the simulation, we have chosen $A_{\text{max}} = 1 \times 10^{11} \text{ J/m}$ for the isotropic case and $\gamma = 0.1$. Because an indirect exchange mechanism between Mn atoms via As sites may govern the coupling in MnAs [21], the principal axis assigned to the maximum principal value has to be rotated by $\theta = 52^\circ$ in the direction of strongest coupling. Under these assumptions an exchange stiffness tensor was calculated according to Eq. (3).

Thus, the elements of the tensor are $a_{11} = 6.6 \times 10^{12} \text{ J/m}$, $a_{12} = 4.4 \times 10^{12} \text{ J/m}$, $a_{22} = 4.5 \times 10^{12} \text{ J/m}$, and $a_{33} = 1 \times 10^{12} \text{ J/m}$. MnAs exhibits a uniaxial anisotropy with an easy plane, and thus the first magnetocrystalline anisotropy constants $K_u$ is negative and has a value of $-7.2 \times 10^3 \text{ J/m}^3$. The absolute value for the constant was taken from Ref. [22]. The second constant was assumed to be $K_{2u} = -3.6 \times 10^3 \text{ J/m}^3$.

Given the exchange lengths $l_{\text{ex}} = 5 \text{ nm}$ and $l_{\text{ex}} = 5.2 \text{ nm}$ (assuming a saturation magnetization $M_s = 8 \times 10^4 \text{ A/m}$), the cell size was set to $5 \text{ nm}$. It has to be noted that in the $z$-direction the exchange length is smaller than $5 \text{ nm}$ ($\sqrt{0.1 \times 5.2 \text{ nm}^2} = 1.6 \text{ nm}$), thus, in principle, requiring a smaller grid size in this direction. Given our computing power, a simulation for both a cubic grid size $\leq 1 \text{ nm}$ and for ex-
tended geometries is not feasible due to an increase in the cell number by a factor 125. On the other hand, using a rectangular grid of $5 \times 5 \times 1 \text{ nm}^3$ results in artifacts due the strongly distorted geometry of the cells [23].

The $x$-axis of the simulation is parallel to the $c$-axis of MnAs, which is the magnetic hard axis. The calculations were performed on a $128 \times 64 \times 16$ grid that corresponds to a volume of length $\times$ width $\times$ thickness $= 640 \times 480 \times 80 \text{ nm}^3$. The simulated sample geometry was chosen such that the two-domain state, as shown in Fig. 1, is a stable configuration.

The initial magnetization distribution of a two-domain state, separated by a $180^\circ$ Bloch wall [9] where the magnetization vector rotates in the easy plane ($y$,$z$-plane) and is independent of $z$, was calculated from the analytical formula by Landau [24]. The wall profiles are given by:

$$
\begin{align*}
    m_y &= \tanh\left( \sqrt{|K_u|/A} (x + y \tan \phi) \right), \\
    m_z &= \cosh\left( \sqrt{|K_u|/A} (x + y \tan \phi) \right),
\end{align*}
$$

with $m_z = 0$ due to the constraint $|m| = 1$. The tilted domain walls were modeled using the angle $\phi$ between the $x$-axis and the normal direction of the wall. The magnetization components of the initial magnetization are shown in Fig. 1.

The relaxation of the magnetization towards the energy minimum was performed for various walls with different normal directions. Our simulation results were independent of the stopping criterion, thereby assuring correct convergence. To investigate the influence of anisotropic exchange when compared to isotropic exchange, we discuss in each case the two scenarios of a slanted domain wall with an angle of $\phi = 52^\circ$, and of a straight domain wall ($\phi = 0^\circ$).

Fig. 1 Visualization of the initial magnetization distributions according to Eq. (4) with $\phi = 38^\circ$ for the $y$-component $m_y$ (a) and for the $z$-component $m_z$, respectively. The legend indicates the magnitude of the two magnetic components. The orientation of the domain wall is along the direction of stiffest coupling for the assumed anisotropic exchange tensor.

Fig. 2 Relaxed magnetization distribution of the straight domain wall ($\phi = 0^\circ$) assuming isotropic exchange. The magnetization component $m_y$ is represented in grayscale on the side faces, with arrows to indicate the magnetization direction.
3.1 Isotropic exchange

The relaxed magnetization configuration (Fig. 2) shows that the domain wall oriented along the direction of magnetization remains stable. In addition, closure-like domains in the $y$-direction evolve at the edges, thereby reducing the demagnetization energy. They are spatially structured, exhibiting a conical shape along the $z$-axis. Along the $x$-direction, the cones are alternately opened towards the top and the bottom, and are located near the edges.

Furthermore, the magnetic pattern also exhibits long-range ordering along the $y$-direction. A cone on the front edge is associated with a cone on the back edge with the same orientation of magnetization but an opposite direction of opening. Edge effects along the $x$-direction can affect this long-range ordering.

The minimum energy configuration of magnetization for the slanted domain wall with $\phi = \infty$ is shown in Fig. 3. Now, the shape of the domain wall is slightly altered. The domain wall is broadly straight, but in the vicinity of the closure domains is bent towards the opening cone of the oppositely magnetized closure domains [cf. Fig. 3(a) and (c)].

In summary, the energy minimum state for the two initial magnetization distributions – assuming isotropic exchange – is characterized by a domain wall with $\phi = 0^\circ$ in the absence of spatially structured closure domains (cones).

3.2 Anisotropic exchange

Relaxing the initial configurations with the constraint of anisotropic exchange revealed that the domain structures differ significantly from the initial magnetization. The relaxed state of the domain wall with an initial inclination of $\phi = 52^\circ$ is shown in Fig. 4. Here, a new type of domain transition is found, where the underlying domain configuration in the easy plane translocates through the structure, giving rise to an apparent domain wall on the surface. As the underlying closure domain pattern in the easy plane is a diamond state with an out-of-plane magnetization in its center [see Fig. 4(b)], well-known from thin permalloy elements [9], the surfaces of the sample show an apparent in-plane domain transition (under an angle of $\phi = 22^\circ$). Farther away from the domain transition, a Landau state governs the easy plane magnetization pattern [see Fig. 4(a) and (c)].

The relaxed magnetization distribution for an initial domain wall at angle of $\phi = 0^\circ$ is shown in Fig. 5. Again, flux-closure domains are formed in the easy plane. In contrast to the initially slanted domain wall, now diamond states are found in the $y,z$-plane (easy plane) [see Fig. 5(a) and (c)], most notably a triple diamond state where the domain wall intersects the $y,z$-plane, [i.e. at $x = 61$, see Fig. 4(b)]. It should be
noted that the neighboring opposite magnetization on the surface is a result of the underlying diamond state. For the straight domain wall ($\phi = 0^\circ$), the extended edge domains remain in the relaxed state and form a diamond state in the easy plane [Fig. 5], which again leads to an efficient demagnetization. The initial domain wall is tilted by an angle of $\phi = 20^\circ$ towards the direction of stiffest exchange.

In comparison to the isotropic exchange, the presence of the anisotropic exchange leads to a completely different domain structure. The anisotropy allows for the formation of flux-closure patterns in the easy plane and, as a result, the character of the domain transition is governed by these patterns. In both cases, we found slanted, apparent domain walls on the surface in the relaxed state, independently of the initial magnetization.

Fig. 4 Explosion sketch of the relaxed magnetization distribution of the slanted domain wall ($\phi = 52^\circ$) assuming anisotropic exchange. The magnetization component $m_z$ is represented in grayscale with arrows to indicate the magnetization direction. Panel (a) shows the top, front and right faces, and panel (c) shows the bottom, back and left faces, respectively. Panel (b) shows the cross-sectional view in the $y,z$-plane (easy plane) at $x = 64$. The spatial coordinate is given in units of the simulation grid.

Fig. 5 Explosion sketch of the relaxed magnetization distribution of the straight domain wall ($\phi = 0^\circ$) assuming anisotropic exchange. The magnetization component $m_z$ is represented in grayscale with arrows to indicate the magnetization direction. Panel (a) shows the top, front and right faces, and panel (c) shows the bottom, back and left faces, respectively. Panel (b) shows a cross-sectional view in the $y,z$-plane (easy plane) at $x = 61$. The spatial coordinate is given in units of the simulation grid.
3.3 Domain wall energetics

To quantify the influence of the exchange energy and to avoid the formation of closure domains, we reduced the saturation magnetization by an order of magnitude to $M_s = 8 \times 10^4$ A/m. The result is shown in Fig. 6 and a comparison of the energies is given in Table 1.

The total energy of the initial state with the slanted domain wall is twice as large as the energy of the straight domain wall. The increase of the demagnetization energy can be attributed to the additional interface charge on the slanted domain wall. For a domain wall separating two domains with antiparallel magnetization, an interface charge builds up when the wall is not parallel to the magnetization direction of the domains. In addition, there are two contributions that increase the exchange energy of slanted domain walls. First, the domain wall is longer. Second, the exchange energy not only included the change of magnetization in the $x$-direction, but also in the $y$-direction. For the domain wall with $\phi = 52^\circ$, both contributions increased the domain wall energy by a factor of 1.6 and 1.7, thus increasing the exchange energy by 2.6. The values estimated this way are in good agreement with the simulated exchange energy ratio given in Table 1.

The magnetization distribution for the isotropic case corresponding to the minimum energy state is shown in Fig. 6(c) and (d). The domain wall of the relaxed state was along the $y$-direction, independent of the initial direction. As expected, no edge domains or closure domains were formed. This is in agreement with the analytic solution of domain wall transitions in uniaxial materials, whereby the energy of the wall $\gamma_w = 4\sqrt{AK}$ is given by the exchange constant $A$ and the anisotropy constant $K$ [24]. During relaxation the wall becomes significantly broadened due to the smaller saturation magnetization. Since the magnetocrystalline anisotropy only permits magnetization within the easy plane, the sample geometry determined the magnetic easy axis. If we consider the demagnetization to simply be a shape anisotropy, the anisotropy constant $K_s$ is proportional to $M_s^2$ [9]. Since the domain wall width scales as $\sqrt{A/K_s}$, the broadening was due to a smaller saturation magnetization.

For anisotropic exchange, the slanted domain wall relaxes to a smaller angle of $\phi = 36^\circ$ as illustrated in Fig. 6(f). The straight domain wall also tends to tilt in the direction of stiffest exchange. However, the

![Diagram]

**Fig. 6** Top view of the out-of-plane magnetization component $m_z$ of (a) a straight and (b) a slanted domain wall ($\phi = 52^\circ$). The relaxed magnetization distributions for these initial configurations are given in (c) and (d) assuming isotropic exchange, and respectively in (e) and (f) assuming anisotropic exchange. The grayscale legend is the same as in Fig. 1.
Table 1 Contributions to the total energy $E_{\text{tot}}$, exchange energy $E_{\text{exch}}$ and demagnetization energy $E_{\text{demag}}$, for the initial and relaxed states, respectively. The magnetocrystalline anisotropy energy contribution is negligible. In the legend, iso = isotropic, ani = anisotropic. In the anisotropic case, starting with $\phi=\infty$, the listed state is not fully relaxed and mentioned for completeness of the table only (denoted relaxed*) (see text for details). The energies are given in reduced units, i.e., normalized to $\mu_0/2\cdot M_s^2 = 4.0 \times 10^3 \text{ J/m}^3$.

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<th>$E_{\text{demag}}$</th>
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initial magnetization did not result in an energy minimum despite a long computation with 120000 iteration steps, the domain wall was inclined by $\phi=11^\circ$, see Fig. 6(e).

The exchange energies of the two domain walls are different (see Table 1). The exchange energy of the domain wall with $\phi=36^\circ$ is smaller although the domain wall is longer. This can only be explained by an orientation-dependent expression of the exchange energy.

In the case of anisotropic exchange, the domain wall energy is now given by $\gamma_{\alpha} = 4\sqrt{A_{\alpha}K}$, where $A_{\alpha} = A_{\alpha\alpha} \gamma (\cos(\theta - \phi) + \sin(\theta - \phi))$ is the scalar projection of the exchange stiffness tensor onto the normal direction of the domain wall and $\theta = 90^\circ - \phi$. The wall normal direction of $\phi=36^\circ$ [see Fig. 6(f)] agrees well with the direction of smallest exchange for the given exchange tensor $\theta = 52^\circ$. This lead to $A_{\alpha} = 0.13A_{\alpha\alpha}$ whereas for the domain wall with $\phi=11^\circ$, $A_{\alpha} = 0.54A_{\alpha\alpha}$. To estimate a ratio of the exchange energies, the product of domain wall length and exchange constant normal to the domain wall were taken into account, yielding $E_{\text{exch}}(\phi=11^\circ)/E_{\text{exch}}(\phi=36^\circ) = 5/3$. The exchange energy ratio calculated by the simulator is 4/3 (cf. Table 1). The small deviation in the estimated ratio was due to the assumption that the domain wall was completely aligned along the stiffest exchange. The magnetization distribution in Fig. 6(f) shows that the ends of the domain wall are bent, which results in a higher exchange energy of the simulated structure and thus in a smaller exchange energy ratio.

Furthermore, a closer inspection of the domain wall width in Fig. 6(e) and (f) reveals that the width also depends on the direction of the wall. According to anisotropic exchange, the width scales as $\sqrt{A_{\alpha}/K_{\alpha}}$. For a small $A_{\alpha}$, the wall width is narrow whereas a deviation from the direction of smallest exchange results in a wider domain transition. This is in agreement with the exchange energy, which is lower for the domain wall in Fig. 6(f) than for the domain wall in Fig. 6(e).

In summary, the total energy minimum of a domain wall with the constraint of an anisotropic exchange was achieved with a domain wall oriented along the direction of stiffest exchange. The domain wall energy and domain wall width can be understood in the frame of the analytic solution of Landau [24]. The exchange constant had to be replaced by the exchange constant normal to the domain wall transition. Thus, domain wall energy and domain wall width became orientation dependent.

4 Conclusions

The influence of anisotropic exchange on the equilibrium distribution of the magnetization of submicron-sized magnetic structures was investigated. For this purpose, we included a generalized tensor representation for the exchange in a micromagnetic simulator. In case of isotropic exchange, the energy minimum
state is, as expected, characterized by a straight domain wall. For anisotropic exchange, the formation of a flux-closure domain structure in the easy plane governs the magnetization distribution, which now differs significantly from the domain structure apparent for isotropic exchange. It can be concluded that in this case the anisotropic exchange is responsible for their formation. The numerical results for the domain wall properties in presence of an anisotropic exchange are in agreement with the generalized domain transition scheme based on the Landau model. Now, in contrast to isotropic exchange, the energy and width of the domain wall is orientation-dependent. Thus, it can be concluded that anisotropic exchange may have profound effects on magnetic nanostructures.

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References

[18] It is still an open question whether β-MnAs is paramagnetic or antiferromagnetic.

Daniel M. Schaadt was born in St. Wendel, Germany, in 1973. He received his diploma degree in Physics from the Universität des Saarlandes, Germany, in 1997. He conducted his doctoral research on semiconductor and magnetic materials and devices at the University of California at San Diego, USA, where he received his Ph.D. in 2003. During the subsequent period as a postdoctoral researcher in San Diego, he started to work on micromagnetic simulations of various magnetic materials. In 2004, he joined the Paul-Drude-Institute in Berlin, Germany, to study the growth and characterization of III–V semiconductor and magnetic materials.