Magnetic microstructure of the spin reorientation transition

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The scenario of the magnetization reorientation in second-order perpendicular anisotropy approximation is theoretically studied by means of Monte–Carlo simulations. The microstructure is investigated as a function of the difference between first-order anisotropy and demagnetizing energy $K_{\mathrm{eff}}=K_1-E_D$ and the second-order anisotropy K_2. An influence of the second-order perpendicular anisotropy on the spin reorientation transition is found when K_{eff} vanishes. The broadening and coalescing of domain walls found earlier for $K_2=0$ is prevented by positive K_2. The domain wall width and energy are determined by K_2. For $K_2>0$ the transition via a canted vortex-like structure is found which yields the smooth, continuous connection between the vertical domain structure and the vortex structure with in-plane magnetization.
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Experiments on spin reorientation transition in ultrathin films have revealed that the magnetic microstructure determines to a large extent the magnetic behavior of the system.[1–5] Theoretically, the microstructure of the spin reorientation transition (SRT) has been investigated in first-order approximation of perpendicular magnetic anisotropy.[6–8] In recent years, the importance of higher-order anisotropy contributions for SRT in ultrathin magnets has been pointed out.[9–13] Phase diagrams were put forward.[11,12,13] In continuum approximation,[11] the reorientation either through the canted phase or through the phase with coexistence of in-plane and vertical magnetization has been postulated. The evolution of the magnetic microstructure caused by higher-order perpendicular anisotropies, however, was not studied.

In this article, we present a spatially resolved description of the magnetization reorientation in the framework of competing dipolar, first- and second-order perpendicular anisotropy energies for a given exchange coupling. For this purpose, Monte–Carlo (MC) simulations have been performed to find the equilibrium spin configuration at a given temperature. The approach is more general than the models[6,12] as neither a restriction to one dimension is made nor a particular domain structure and wall profile is assumed. The Hamiltonian of the problem includes exchange, dipolar interactions, and perpendicular anisotropy of the first and the second order

$$H=-J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+D\sum_{i,j}\left(\frac{\mathbf{S}_i\cdot\mathbf{S}_j}{r_{ij}^3}-3\,\frac{(\mathbf{S}_i\cdot\mathbf{r}_{ij})(\mathbf{S}_j\cdot\mathbf{r}_{ij})}{r_{ij}^5}\right)$$
$$+K_1\sum_i \sin^2\theta\pm K_2\sum_i \sin^4\theta, \tag{1}$$

where J is the exchange coupling constant which is nonzero only for nearest-neighbor spins, D the dipolar coupling parameter and r_{ij} the vector between sites i and j. The coefficients K_1 and K_2 are correspondingly the first- and the second-order anisotropy constants. Via scaling arguments the realistic effective values for the ratio of dipolar to exchange interactions can be achieved by considering spin blocks of appropriate size.[14] For the extended MC computations, we take a monolayer of classical magnetic moments on a regular, triangular lattice of about 10 000 effective magnetic sites. This corresponds to a surface orthogonal to the c axis of a hexagonal-close-packed lattice or to the (111) surface of a face-centered-cubic structure. The magnetic moment is described by a three-dimensional vector S of unit length. The MC procedure is the same as in Ref. 8. To avoid artificial periodic patterns, we use open boundary conditions.

We have studied the magnetic microstructure in the anisotropy space of the system. The latter is represented by the difference between first-order anisotropy and demagnetizing energy $K_{\mathrm{eff}}=K_1-E_D$ and the second-order anisotropy K_2 (Fig. 1). Positive K_{eff} and K_2 favor vertical magnetization while the negative energies impose an in-plane state [see Eq.

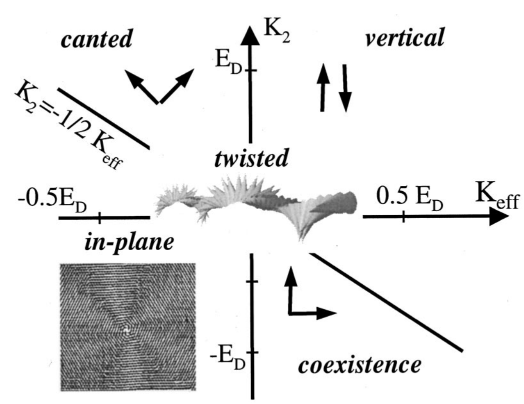

FIG. 1. Micromagnetic phases of a monolayer of classical magnetic moments as a function of the difference between first-order anisotropy and demagnetizing *energy* $K_{\mathrm{eff}}=K_1-E_D$ and the second-order anisotropy K_2. The lines $K_2=-1/2K_{\mathrm{eff}}$ and $K_{\mathrm{eff}}=0$ separate vertical, canted, in-plane, and coexistence phases (see the text). The reorientation transition is characterized by the evolution of magnetic microstructure between vertical and in-plane phases.

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(1)]. In the region of ''vertical'' magnetization (Fig. 1), we find the following microstructure. Macroscopic domains with vertical magnetization appear for $K_2 > -1/2K_{\mathrm{eff}}$. The results are the same as found before for $K_2=0$.[6,8] In the interval $0.2E_D < K_{\mathrm{eff}} < 0.5E_D$ more and more vertically magnetized domains appear and become smaller with decreasing K_{eff}. The domain walls, on the other hand, become broader with decreasing K_{eff} (similar to Ref. 8). In the close vicinity of $K_{\mathrm{eff}}=0$ $(0 < K_{\mathrm{eff}} < 0.2E_D)$ the width of the domain walls is determined mainly by K_2. This width is finite in contrast to the first-order anisotropy approximation. The stronger the second-order anisotropy the narrower are the walls. This means that K_2 substitutes K_1 in the definition of wall width and energy.[15] At $K_{\mathrm{eff}}=0$ and $K_2=0$, adjacent walls touch and no vertical domain persists anymore. The microstructure consists of moments of spatially varying orientation. The arrangement of the magnetic moments is illustrated in the central inset of Fig. 1. The magnetization rotates in a helicoidal form along all three principal axes. The structure formed is called the twisted phase. At this particular point, the magnetic moments are evenly oriented in all directions which is characteristic of the twisted configuration.[8]

For negative K_{eff} and $K_2 < -1/2K_{\mathrm{eff}}$ (Fig. 1), the vertical magnetization vanishes revealing a complete in-plane orientation of the magnetic moments. Minimization of the magnetostatic energy causes vortex structures to form as the magnetic anisotropy in-plane is zero. With $K_2=0$ the three-dimensional twisted configuration transforms continuously into the planar vortex structure between $K_{\mathrm{eff}}=0$ and $K_{\mathrm{eff}}=-0.2E_D$. A continuous reorientation transition occurs from an out-of-plane magnetization to a vortex structure via the origin of the anisotropy space.

In the region between $K_{\mathrm{eff}}=0$ and $K_2=-1/2K_{\mathrm{eff}}$ (Fig. 1) the negative K_{eff} competes with the positive K_2. The energy minimization causes the canted phase to appear.[11–13] The canting angle depends on the balance between K_{eff} and K_2. As we do not have any anisotropy in the film plane, the moments are canted with respect to the normal but are free to have any orientation in the film plane. On the other hand, the demagnetizing energy in finite-size samples supports the charge-free vortex structure. Due to the cooperation of these energies, a canted vortex structure forms (Fig. 2). The canted vortices transform continuously into their planar counterparts with decreasing K_2 and K_{eff}. A reorientation transition through continuous canting of the magnetization occurs.

In conclusion, an influence of the second-order perpendicular anisotropy on the spin reorientation transition is found when K_{eff} vanishes. The broadening of domain walls, found for $K_2=0$[6,8] is eliminated by positive K_2. The domain wall width and energy are determined by K_2. For $K_2>0$, the transition via a canted vortex-like structure is found which yields the smooth, continuous connection between the vertical domain structure and the vortex structure with in-plane magnetization. The investigation of the magnetic microstructure for negative K_2 is under progress.

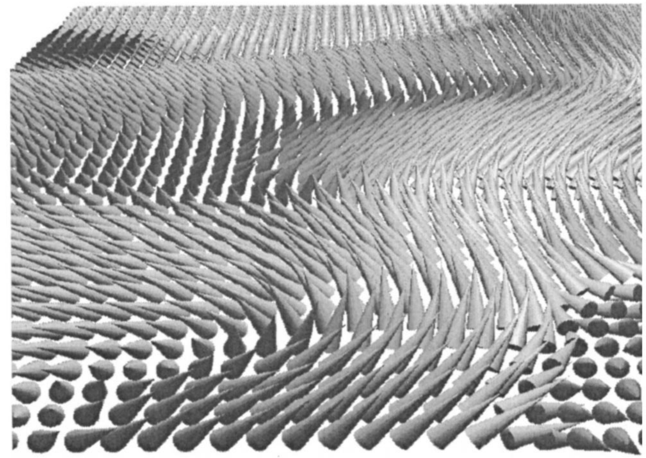

FIG. 2. Canted spin structure for $K_{\mathrm{eff}}=-0.4E_D$, $K_2=0.75E_D$, and $k_BT/J=0.05$. Perspective view of an enlarged part of the sample. For clarity, only one row out of two and one moment out of two in the row are drawn as cones.

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