Magnetic Microstructure of the Spin Reorientation Transition: A Computer Experiment

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The scenario of the spin reorientation in two-dimensional films within first-order anisotropy approximation is theoretically studied by means of Monte Carlo simulations. The magnetic microstructure is investigated as a function of the ratio of the perpendicular anisotropy energy to the dipolar one. If the anisotropy dominates, out-of-plane domains will be found while in-plane vortices appear for a vanishing anisotropy. In the range of comparable anisotropy and dipolar energies a complex domain pattern evolves yielding a continuous transition between the two structures. The structure with equally distributed magnetic moment orientations is stable at the point where anisotropy and dipolar energies cancel each other.

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Over the last decade the investigation of the spin reorientation in ultrathin films has been a vivid field in basic research. Experimentally, the studies reveal that the magnetic microstructure at the spin reorientation determines the details of the switching of the magnetization and thus the macroscopic behavior of the ferromagnet [1–5]. Theoretically, Monte Carlo simulations and analytical studies have been performed in first-order approximation of perpendicular magnetic anisotropy. In those investigations emphasis was put on the change of the magnetization orientation as a result of competing anisotropy and dipolar energies with temperature or thickness as a driving parameter [6–15]. Phase diagrams were put forward and noncontinuous magnetization changes postulated [6,9]. The evolution of the magnetic microstructures was not studied in these numerical investigations.

An early analytical model of the spin reorientation, however, was mainly based on the microstructure that can evolve when perpendicular anisotropy becomes weak [13]. Based on the assumption of a stripe domain pattern [16] domain walls of finite width were introduced in the one-dimensional model as the microstructure. It was found that the existence of domain walls is crucial around the point where anisotropy and dipolar energies cancel. At that point the walls have microscopic dimensions, touch each other, and create a wavelike magnetic microstructure.

In summary, it is obvious from the experiments that microstructures are important in spin reorientation transition but from a theoretical point of view no general approach has been made up to now. The aim of our investigation is to achieve a general spatially resolved description of the magnetization reorientation in the framework of competing dipolar and anisotropy energies for a given exchange coupling. For this purpose, Monte Carlo (MC) simulations have been performed to find the equilibrium spin configuration of a monoatomic layer at a given temperature. The approach is more general than the model Ref. [13] 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

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_{ij} \left(\frac{\mathbf{S}_i \cdot \mathbf{S}_j}{r_{ij}^3} - 3 \frac{(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij})}{r_{ij}^5} \right) - K_1 \sum_i S_{i,z}^2 , \quad (1)$$

where J is the exchange coupling constant which is nonzero only for nearest-neighbor spins, D the dipolar coupling parameter, and $\mathbf{r}_{ij}$ the vector between sites i and j. The coefficient K_1 is the first-order anisotropy constant and a is the lattice parameter. In the calculations the ratio $D/(Ja^3) = 0.1$ was used. Via simple scaling arguments the realistic effective values for the ratio of dipolar to exchange interactions can be achieved by considering spin blocks of appropriate size [17,18]. We have performed MC simulations for three typical values of the ratio $R = J(a^3)/D$, namely $R = 10$, $R = 1$, and $R = 0$ (pure dipolar interactions with K finite). In all simulations continuous transitions were found. We focus on the results for $R = 10$ as the scales for Co/Au(111) (5 nm mesh width and 500 nm sample size) are best adopted to the microstructures that appear in the spin reorientation transition.

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 hcp lattice or to the (111) surface of a fcc structure. Assuming the parameters of Co/Au(111) for the interatomic distance, the exchange constant, and dipolar interaction constant, the MC calculations present sample sizes of about 500 nm. The magnetic moment is described by a three-dimensional vector $\mathbf{S}$ of unit length. The calculations have been performed for free boundaries. The commonly used periodic boundary conditions are dismissed, since they might

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induce artificial patterns commensurate with the size of the sample.

Because of the long-range character of the dipolar interaction, special attention was paid to the following problems: (i) As the demagnetizing field is depending on the shape of the sample we have to expect inhomogeneities at the sample edges. We have investigated the dependence of the microstructure on the sample geometry. The results for disc and square-shaped samples are identical for $f > 1.46$ (vertical regime). For the configurations with nearly in-plane moments the square-shaped samples have been avoided to obtain the "easy-axis" to "easy-plane" transition. (ii) Most of the computing time is spent on calculating the dipolar interaction between all magnetic moments. Computing time can be saved by calculating an effective dipolar field at one moment, which is created by moments in close vicinity. This is the main idea of the so-called cutoff in MC simulations. If the dipolar energy E_D is comparable to or larger than the anisotropy energy E_A any cutoff will affect strongly the MC spin configuration [17]. To prevent artificial effects due to the cutoff we have considered the dipolar interaction of each magnetic moment with all the other moments, i.e., we used no cutoff.

The MC simulations have been performed in the following way: (i) A random moment configuration is taken as the starting configuration representing the equilibrium at infinite temperature. (ii) The next step is to perform a MC relaxation at a finite temperature still above the Curie temperature. (iii) This high temperature MC equilibration is followed by a stepwise cooling until a low-temperature configuration is reached. At each temperature step a MC relaxation is performed and controlled by checking the total energy evolution. The relaxation is stopped when the energy does not show any remarkable drift over several hundred MC steps per magnetic moment.

We have investigated the magnetic microstructure for different ratios of the competing anisotropy and dipolar energies. In contradiction to previous studies [6,9] we find a continuous transition from vertical to in-plane orientation of magnetization. It is the magnetic microstructure we will discuss in the following that eliminates any discontinuity. Our MC study gives the complete transition from the vertical to the in-plane state of magnetization.

The results are presented as a low-temperature phase diagram in Fig. 1. We have plotted the averaged values of the vertical component S_z and the squared value S_z^2 of the magnetic moment versus f with $f = E_A/E_D$ as the ratio of perpendicular anisotropy energy E_A to the dipolar energy E_D. Usually the MC results are plotted as a function of K_1/D. As the behavior of the magnetic sample is governed by the total energy we find normalized energies more convenient. The magnetostatic energy is defined as the difference between the vertical single domain configuration and a stray field free vortex structure. This energy and the anisotropy energy is normalized with respect to the number of moments and used for calculating the f value

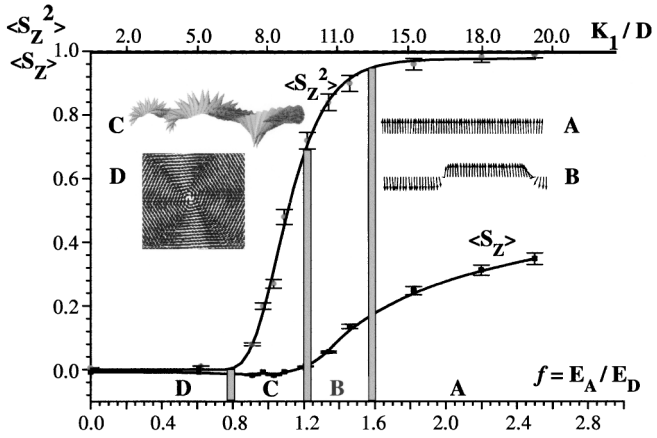

FIG. 1. Plot of $\langle S_z^2 \rangle$ and $\langle S_z \rangle$ versus f. $\langle S_z \rangle$ is the perpendicular component of magnetization and $f = E_A/E_D$ is the ratio of anisotropy energy to dipolar energy. The shaded areas separate the phases (A, B, C, D). The phases are characterized by the different microstructures, which are shown as insets in the diagram. The microstructures have been obtained for disk-shaped ($f \leq 1.46$) and rectangular samples ($f > 1.46$) of about 10 200 vector spins on a triangular lattice for $k_BT/J = 0.01$.

given in Fig. 1. By this we avoid major effects of shape and size on the graph and obtain a generalized behavior of the spin reorientation in thin films. $\langle S_z \rangle$ and $\langle S_z^2 \rangle$ have been obtained from the simulations. While $\langle S_z^2 \rangle$ is proportional to the total amount of the structure with out-of-plane magnetization orientation, $\langle S_z \rangle$ reveals information about the occupation of the two vertical states of magnetization.

As long as the perpendicular anisotropy E_A is dominant ($f > 1.5$), mesoscopic or even macroscopic domains with vertical magnetization appear. This phase corresponds to region A in Fig. 1 where $\langle S_z^2 \rangle$ is almost one and $\langle S_z \rangle$ is close to 0.4. Here the domain size is larger than the size of the sample (~500 nm). The anisotropy is very strong and within the mesh size the domain walls cannot be described accurately. The energy difference between the single domain state and the configuration with two domains is very small (<0.3%) as the wall energy is underestimated. The energy gain is so small that the sample will remain in a state with two domains if by chance two domains are created during cooling. For $\langle S_z \rangle = 0.4$ a large fraction (70%) of the domains is magnetized in one direction while only 30% are oppositely magnetized. In the interval $1.2 < f < 1.5$ more and more vertically magnetized domains show up and become smaller with decreasing f. For $f \sim 1.4$ a domain structure as shown in Fig. 2 is observed. The domain sizes in the range from 200 to 400 nm and the domain walls are small but broader than in region A. In Fig. 1 this region is denoted by B. Domains of that size have been experimentally observed close to the reorientation transition in annealed Co on Au (111) films [3]. When the domains get smaller the numbers of up and down domains become almost the same and $\langle S_z \rangle$ approaches zero. $\langle S_z^2 \rangle$ decreases to about 0.7 instead of

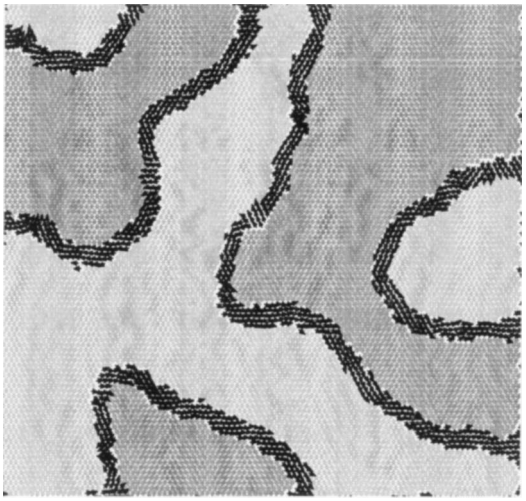

FIG. 2. Top view of the magnetic microstructure in a sample of finite size, i.e., ~500 nm for Co/Au(111) (for more details, see text). Dark and light-grey areas represent spin-up domains $S_z \geq 0.9|S|$ and spin-down domains $S_z \geq -0.9|S|$, respectively. The domains are separated by walls (black). The ratio of anisotropy energy to dipolar energy is $f = 1.4$; $T \sim 5$ K.

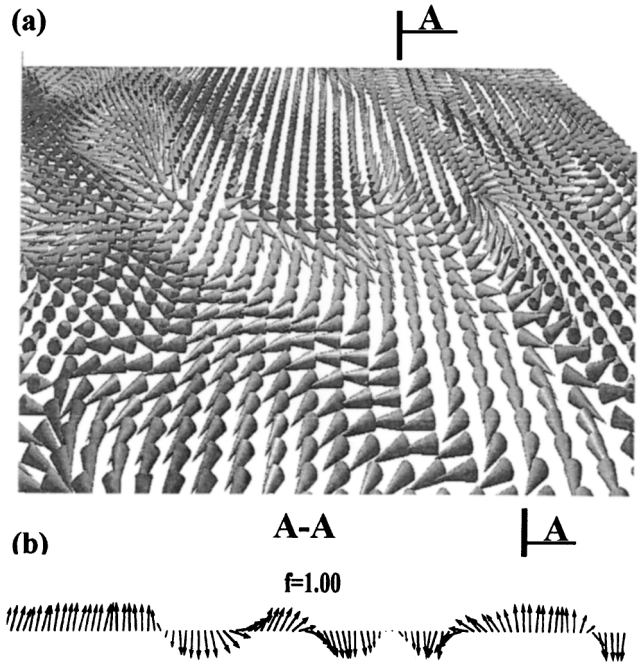

FIG. 3. Twisted spin structure for $f = E_A/E_D = 1$: (a) Perspective view of an enlarged part of the sample. For clarity, only one row out of two and one moment out of two in the row are drawn as cones. (b) Side view of the cross section *A-A*. $T \sim 5$ K. Same sample size as in Fig. 2.

being close to 1. The deviation is due to a slight tilting of the magnetization within the domains and a magnetization rotation within the domain walls. In the domains, however, the value of S_z is larger than $0.9|S|$. Further decreasing of f causes $\langle S_z^2 \rangle$ to approach zero continuously. For $\langle S_z^2 \rangle = 0$, all magnetic moments are lying in the film plane (D in Fig. 1). The region before that particular f ratio with $\langle S_z \rangle = 0$ and $\langle S_z^2 \rangle \neq 0$ is denoted by C. The walls get broader and broader and the wall width becomes comparable to the domain size. At $f = 1$, adjacent walls touch and no vertical domain persists any more. The microstructure consists of moments of spatially varying orientation. The arrangement of the magnetic moments is illustrated in Fig. 3(a) for $f = 1$. A side view is shown in Fig. 3(b). 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. This would yield $\langle S_z^2 \rangle = \langle S_y^2 \rangle = \langle S_x^2 \rangle = 1/3$ for a sample of infinite extension. In the simulation (see Fig. 1), however, the obtained value is smaller, which is due to the finite size of the sample. At the edges, the dipolar energy forces the moments into the film plane and parallel to the sample edges which gives a slightly lower occupation of the vertical component. The twisted phase corresponds to the two-dimensional wavelike profile of the Yafet and Gyorgy model [13]. The MC simulation, however, reveals a complete three-dimensional structure as no limitations to two dimensions were made. The twisted configuration is the starting point for the formation of vortices, as will be shown in the following.

Below $f = 0.8$ (region D in Fig. 1), both $\langle S_z^2 \rangle$ and $\langle S_z \rangle$ vanish revealing a complete in-plane orientation of the magnetic moments. Minimization of the magnetostatic energy causes vortex structures to form (Fig. 4). Details of this kind of configuration have been discussed in detail [17,19]. Between $f = 1$ and $f = 0.8$, the three-dimensional twisted configuration transforms continuously into the planar vortex structure.

Now we want to focus on some features of the magnetic microstructure within the reorientation transition. The first point is the stability of the twisted configuration. For $f = 1$ we have compared the energies for the twisted structure with several in-plane (vortex, single domain) and out-of-plane (with different periods of up and down domains) configurations. At that particular point of the phase diagram the twisted configuration remains the one with the lowest energy among all considered microstructures. The increase of the total energy per moment with respect to the twisted configuration is $2.5 \times 10^{-2} J$ for the ideal in-plane vortex, $3.5 \times 10^{-2} J$ for the in-plane single domain ferromagnetic state. The excess value varies between $2.58 \times 10^{-1} J$ and $1.7J$ for spin-up and spin-down striped domain configurations with periods from 1/2 to 1/10 of the sample size. These differences are comparable to the dipolar or anisotropy energies of that state. For the twisted phase the spin-spin correlation does not vanish on a large scale, which confirms the low-temperature long-range order of this structure [20].

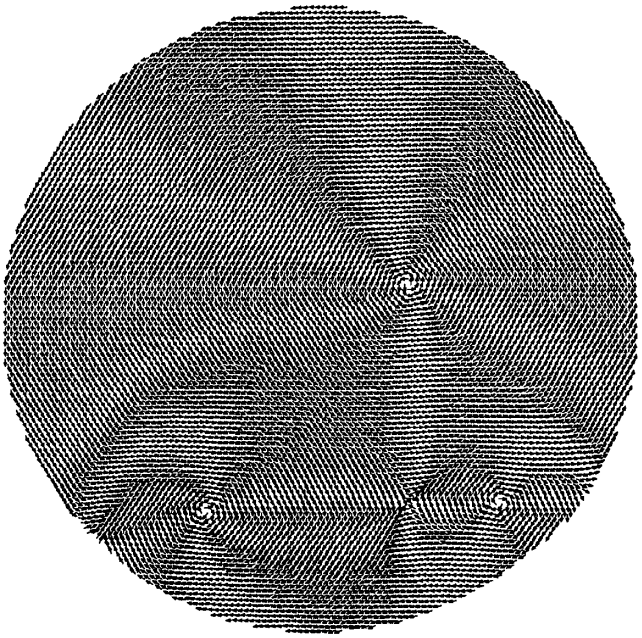

FIG. 4. Planar vortex spin configuration for the ratio $f = E_A/E_D = 0$; $T \sim 5$ K. Same sample size as in Fig. 2.

In conclusion, we have demonstrated that in first-order anisotropy approximation a continuous reorientation transition occurs from an out-of-plane magnetization to a vortex structure. A new phase, the twisted configuration, is found as an intermediate structure between these two states. At the point where the dipolar energy is equal to the perpendicular anisotropy energy the twisted configuration represents the minimum of the free energy.

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