Scaling Properties of Spin-Reorientation Transitions in Magnetic Thin Films with Surface Anisotropy

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Journal: Physical Review. B
Volume: 54
Number: 1
Page Range: 65-67
Year: 1996
URL: http://hdl.handle.net/10097/53315
doi: 10.1103/PhysRevB.54.65
Scaling properties of spin-reorientation transitions in magnetic thin films with surface anisotropy

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(Received 24 January 1995; revised manuscript received 5 February 1996)

Spin-reorientation transitions in ultrathin magnetic films sandwiched by nonmagnetic films are clarified by means of the variational calculation on a micromagnetic discrete model. Scaling relations among the film thickness, exchange coupling, and magnetic anisotropies are revealed. It is shown numerically that the scaling behaviors should be observed experimentally in magnetic materials. The phase diagram with scaled variables for spin reorientation coincides with the one derived analytically by the continuum model. This coincidence implies the sufficiency of continuum modeling in the study of ultrathin magnetic films of several atomic layers.

Spin-reorientation transitions in thin films of transition metals have been the object of many experimental and theoretical works. In this study, we explore the spin-reorientation transitions by means of a discrete model. The comparison of the present results with those obtained by the continuum approach is important for checking the sufficiency of the continuum approximation.

The continuum approach introduced by Thiaville and Fert has revealed analytically several important aspects of the spin-reorientation transitions. The following question is then natural and important, whether the continuum approximation describes appropriately the systems investigated experimentally, since the spin-reorientation transitions occur at thicknesses of several atomic layers. In order to clarify this point, it is necessary to investigate the spin-reorientation transition in terms of the discrete model and to compare the results with those obtained by the continuum approach. This investigation is also of general importance for the study of thin films, superlattices, and small clusters where surface effects are essential and the discreteness of the systems is important since the relevant dimension is very small. If it is verified that the continuum model can give an overall acceptable picture, the understanding of the systems will be promoted more deeply, since a continuum model allows it to be approached analytically, as in the present case.

The discrete model for the energy per unit area of an ultrathin magnetic film is

\[
\gamma = -Jm^2 \sum_{i=1}^{N-1} \cos(\varphi_i - \varphi_{i+1}) + K_v^s \sum_{i=2}^{N-1} \cos^2 \varphi_i + K_v^p \cos^2 \varphi_N,
\]

where the orientation angle \( \varphi \) is measured from the normal of the film. The first term on the right-hand side of the above expression covers the exchange coupling energy between the classical spin vectors on the nearest-neighbor atomic layers. The second term is for the in-plane shape anisotropy, and the third term is for the surface anisotropy. The perpendicular surface anisotropy is confined exclusively to the single surface layer, since it is known that the perpendicular component in the anisotropy constant on other layers are about 100 times smaller. One has the following relations between the quantities in the present discrete model and the continuum model: \( Jm^2 \hat{a} = A \quad K_v^s \hat{a} = K_v^s \quad K_v^p \hat{a} = K_v^p \), where \( \hat{a} \) is the lattice constant.

It is noticed that in the continuum model, the surface anisotropy contribution to the total energy is taken into account as an additional term to the bulk integral of shape anisotropy energy. Mathematically, this surface term determines the derivative boundary conditions for the Euler equation. This treatment is not necessarily sufficient and should be checked by comparison between its results and that of the discrete model (1).

The stable spin configuration is determined by minimizing the energy functional (1). In the present discrete model, no analytic results can be expected. For numerical calculation, we take \( Jm^2 = 1 \) and \( \hat{a} = 1 \). Fixing the magnetic constants, we have found a spin-reorientation transition from the perpendicular uniform configuration to a nonuniform configuration, as the number of layers is increased from \( N = 2 \). A further transition is observed, where the nonuniform configuration is switched into the in-plane uniform configuration. The phase diagram with the number of atomic layers and the surface anisotropy as variables is depicted in Fig. 1, for two different values of volume anisotropy. The phase boundaries consist of steps, as the result of the discrete variance of the thickness, namely the number of atomic layers. The locations of the phase boundaries depend sensitively on the value of volume anisotropy.

The spin-reorientation transition is the result of the competition between the perpendicular surface anisotropy and the in-plane volume anisotropy. The increase in the number of atomic layers enhances the effect of volume anisotropy in an extensive way and triggers the transitions observed above. The effect of the volume anisotropy can be amplified intensively, as a theoretical treatment, by increasing the value of anisotropy \( K_v^p \) itself. This consideration helps us significantly in the understanding of the spin-reorientation transitions, as will be revealed in the following. The results thus obtained are presented in Fig. 2, where the anisotropies are variables and the number of atomic layers is a parameter. We have found three phases: a perpendicular uniform phase around the \( K_v^s \) axis, an in-plane uniform phase around \( K_v^p \) axis, and a
nonuniform phase between these two uniform phases. The phase boundaries depend on the number of atomic layers significantly.

It is physically reasonable to believe and is shown numerically in Figs. 1 and 2 that the increments in the number of layers and in the value of the volume anisotropy have the similar effects in determining the spin configuration. This property is not only qualitative but can further be expressed quantitatively. To this end, we have calculated the magnetic configuration in systems of $N = 2$ to 20 and various values of $K_s$ and $K_v$, and tried to rearrange the data into a single diagram. We then arrive at the conclusion that if one takes the variables as $(N - \Delta N) \sqrt{K_v}$, $K'_v/\sqrt{K_v}$, and $K'_v/(Jm_z)$, and tried to rearrange the data into a single diagram. We then arrive at the conclusion that if one takes the variables as $(N - \Delta N) \sqrt{K_v}$, and $K'_v/\sqrt{K_v}$ as in Fig. 3, where $\Delta N = 2.2$ is selected to obtain the best plotting, all the phase boundaries, such as those shown in Figs. 1 and 2, fall into two smooth curves. This fact implies the presence of the following scaling relations among the film thickness, the anisotropies and the exchange coupling in the spin-reorientation transitions: $(N - \Delta N) \sqrt{K'_v/(Jm_z^2)}$ and $K'_v/\sqrt{K_v}Jm_z^2$.

It should be noticed that the scaling relations mentioned above are satisfied sufficiently in the whole region of $K'_v/(K_vJm_z^2)$, while adequately only by small volume anisotropies $K'_v/(Jm_z^2) \leq 0.05$, as shown in Fig. 3. For the data given in the preceding section for the typical transition metal Fe, one has

$$K'_v/(K_vJm_z^2) = \frac{K_v}{2A} = 0.003,$$

with the bulk value of lattice constant $\hat{a} = 2.87 \, \text{Å}$. Similar estimations are obtained for other magnetic materials. Therefore, the scaling relations derived in the present study are expected to be observed experimentally in real magnetic materials.

One must find the coincidence between the phase diagram in Fig. 3 using scaling variables and that in Fig. 4 based on the results of the continuum approach.23,24 This coincidence establishes the sufficiency of the continuum approach in the study of spin-reorientation transitions occurring in ultrathin magnetic films of several atomic layers. This point can be understood from another way: The continuum approximation is sufficient if the lattice constant $\hat{a}$ is much smaller than the...
domain-wall width $\sqrt{A/K_p}$, whatever the surface anisotropy is. This condition turns out to be well satisfied by various materials as shown in (2).

From Figs. 3 and 4, the film thickness in the continuum model should be evaluated from the number of atomic layers in the relevant metallic lattice as $2a = (N-2)\hat{a}$. The physics meaning of the value $\Delta N=2$ is clear, comparing the energy expression (1) and those in Refs. 23 and 24. One also finds that the treatment of surface anisotropy in the continuum model is correct provided the film thickness is taken in the above way.

The temperature effect has not been studied explicitly in the present study and in Refs. 23 and 24. Nevertheless, if one takes the exchange stiffness and the anisotropies as functions of the temperature, the effect of thermal fluctuation can be taken into account partially. For nonzero temperature, the energy expressions should be considered as free-energy functionals.

To summarize, spin-reorientation transitions are observed as the film thickness and/or the magnetic constants are varied. Scaling relations among the relevant quantities in these transitions are derived. It is shown that experimental data for spin-reorientation transitions in real magnetic materials should fall into the scaling region. Therefore, these scaling relations provide a systematic way of data analysis for experiments conducted in real magnetic materials, which are of lattice structures and discrete, and thus are important for understanding observed spin-reorientation transitions in various ultrathin magnetic films in a unified way. It is expected that systematic experimental investigations will be performed to verify the present predictions.

The results derived from the continuum and the discrete models for ultrathin magnetic films are compared with each other quantitatively. From the comparison we have found that the continuum approximation is sufficient for the study of the spin-reorientation transitions in ultrathin magnetic films of several atomic layers. The continuum approach is more reliable than expected generally for studies of surface effects in systems of small relevant scales, such as small particles and thin films. The continuum approach makes mathematical analyses possible and can reveal many important properties, such as scaling relations among the various physical quantities, more directly than numerical calculations based on the discrete model, and thus should be used more extensively.

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