Generalization of a Two-Dimensional Micromagnetic Model to Non-Uniform Thickness

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***Abstract*—A two-dimensional micromagnetic model is extended to support simulation of films with non-uniform thickness. Zeeman and crystalline anisotropy energies of each cell scale with the cell thickness, while the exchange energy of a pair of neighbor cells scales by a weight dependent on the thicknesses of both cells. The self-magnetostatic energy is computed by scaling the moment of each cell by its thickness, and adding a local correction to the out-of-plane field. The calculation of the magnetostatic field for a $10 \times 10 \times 1$ oblate spheroid is shown to be more accurate by the non-uniform thickness model than by a uniform thickness model. With the extended model a $530 \times 130 \times 10$ nm film in the shape of a truncated pyramid with tapering over the 15 nm nearest the edges is shown to have smaller switching field and different reversal mechanism compared with uniform thickness films of similar size and shape.**

I. Introduction

Micromagnetic simulation of thin-film devices frequently makes use of a two-dimensional micromagnetic model. A two-dimensional model requires less memory and less demanding calculations than a three-dimensional model. The magnetization patterns computed by a two-dimensional model can also be more easily visualized and interpreted. So long as the variation of magnetization through the thickness of a film can be neglected, two-dimensional models can represent the magnetic behavior of thin films acceptably well.

Any two-dimensional model is capable of solving only a limited set of micromagnetic problems that are consistent with the constraints of the model. More sophisticated models can expand the limits of those constraints while retaining the two-dimensional nature of the model. In previous work [1] we considered a more sophisticated calculation of the effective magnetostatic fields of a two-dimensional model. Rather than computing the magnetostatic field at a single sample point in the center of each computational cell, we computed the average magnetostatic field over the entire cell, using known formulas [2]. Using averaged values instead of sampled values of the magnetostatic field, we were able to use a two-dimensional model to reproduce the accuracy of a three-dimensional model [3] in the solution of μMAG standard problem 2 [4].

In this paper we consider another extension of a two-dimensional micromagnetic model as an alternative to three-dimensional modeling. All two-dimensional models neglect the variation of magnetization through the thickness of the film. Most two-dimensional models also assume the film has uniform thickness. In this paper we present a simple extension of a two-dimensional model to approximate the effects of non-uniform thickness of the film. This extension allows a two-dimensional model to be used to simulate a broader class of devices that otherwise might require a three-dimensional model. It can also be used to explore the impact that thickness variations may have on the properties of thin-film devices.

In Section II we describe the representation of variable thickness in each of the energy terms of our two dimensional model. Section III records the extended model's improved ability to represent the magnetostatic fields of an ellipsoid. Section IV presents some simulation results indicating that a film with a tapered edge has a significantly different reversal mechanism and switching field when compared with uniform thickness films of similar size and shape.

II. Energy Terms

We began with the two-dimensional model within the OOMMF public micromagnetic code [5] and extended the expressions of each of its energy terms to account for a variation in thickness from one cell to the next. In the original model, the cells lie on a regular rectangular mesh where each cell has dimensions $\Delta \times \Delta \times T$. In the modified model, each cell i has thickness T_i, or relative thickness $t_i = T_i/T_{\max}$.

Neither the applied field nor the crystalline anisotropy field are dependent on the magnitude of magnetic moment in the cell, so field calculations are unmodified. The Zeeman energy and the anisotropy energy in the cell are proportional to the volume of the film in that cell, so when calculating these energy terms, the energy of cell i is scaled by the relative thickness t_i. This is a simple adjustment to the calculation of these energy terms.

In our uniform thickness model, the total exchange energy is computed using an eight-neighbor cosine scheme [6]. In the variable thickness model, we weight the contribution to total exchange energy from each pair of neighbor cells i and k by the quantity $w(t_i, t_k)$,

$$\mathcal{E}_{\text{ex}} = \frac{A \cdot T_{\max}}{3} \sum_i \mathbf{m}_i^T \sum_{k \in \text{nn}_\text{i}} w(t_i, t_k)(\mathbf{m}_i - \mathbf{m}_k). \quad (1)$$

Here A is the exchange stiffness constant, and $\mathbf{m}_i = \mathbf{M}_i/M_s$ is the normalized magnetization of cell i. The weights reflect the lesser exchange energy contribution from cells of thickness less than $T_{\max}$. The corresponding expression for the exchange

energy density in cell i is

$$E_{\mathrm{ex},i} = \frac{A}{3\Delta^2}\,\mathbf{m}_i^T \sum_{k\in \mathrm{nn_i}} \frac{w(t_i,t_k)}{t_i}(\mathbf{m}_i - \mathbf{m}_k). \qquad (2)$$

The choice of weighting functions must satisfy the following properties:

$$w(t_1,t_2) \quad = \quad w(t_2,t_1) \qquad (3)$$

$$\min(t_1,t_2) \leq \quad w(t_1,t_2) \quad \leq \frac{2t_1t_2}{t_1+t_2} \qquad (4)$$

Our model's representation of exchange energy assumes the exchange energy contribution from cells i and k is the minimum exchange energy of any magnetization interpolation consistent with $\mathbf{m}_i$ and $\mathbf{m}_k$. The lower bound in (4) asserts that starting with two cells of equal thickness, increasing the thickness of one must increase the exchange energy. The upper bound in (4) is the minimum exchange energy among all magnetization interpolations meeting the constraint that $\mathbf{m}$ varies only along the direction from i to k. The minimum exchange energy over all unconstrained interpolations must be no greater.

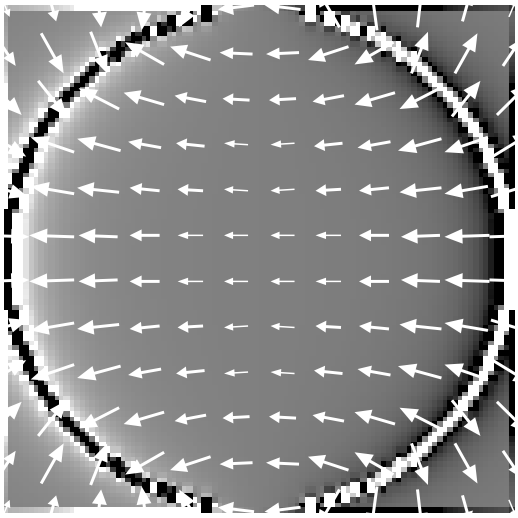
For simulations reported in this paper, the minimum weighting function $w(t_1,t_2) = \min(t_1,t_2)$ was used, but other weighting functions satisfying these constraints might also be considered.

Finally, we consider the self-magnetostatic energy of the film. The magnetization in each cell is assumed to be uniform, so magnetic charges on the cell boundaries are the sources of the magnetostatic field. The average magnetostatic field over each cell is computed [1]. Due to the regular mesh, the magnetostatic field convolution integral can be efficiently evaluated using FFT techniques.

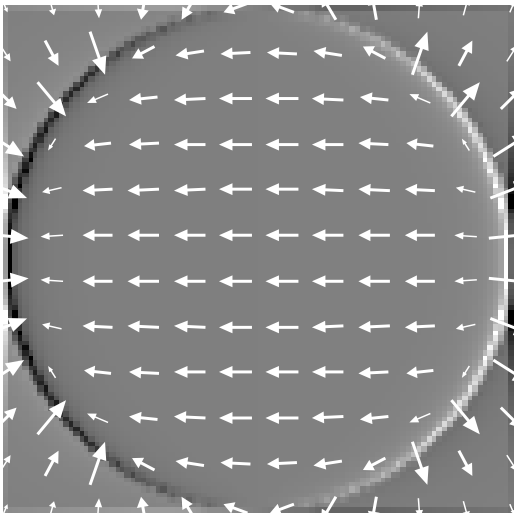
Adapting the model to properly include cells of variable thickness would destroy the regularity of the mesh, preventing the use of efficient FFT techniques. We consider instead a way to retain efficiency, yet reasonably approximate the effect of variable thickness on the magnetostatic energy.

The primary effect of a reduction in the thickness of a cell on the magnetostatic field is caused by the corresponding reduction in the magnetic moment of that cell. This suggests an adjustment to the magnetostatic field calculation that replaces $\mathbf{M}_i$ with $t_i\mathbf{M}_i$ as the source of magnetostatic field from cell i. In the far field, this approximation is reasonably accurate. However, errors in the near field produce incorrect results in an important limiting case and need correction.

Consider a uniformly magnetized thin film of infinite extent. The correct magnetostatic field is $\mathbf{H}_{\mathrm{d,z}} = -M_z\hat{\mathbf{z}}$ out-of-plane and $\mathbf{H}_{\mathrm{d,xy}} = 0$ in-plane. Assume our full thickness model properly calculates that field. When the thickness of the entire film is reduced to a fraction t of its original thickness, our variable thickness model will compute the out-of-plane magnetostatic field to be $\mathbf{H}_{\mathrm{d,z}} = -tM_z\hat{\mathbf{z}}$. This error can be corrected if at each cell i the quantity $-(1-t_i)\mathbf{M}_{i,z}$ is added to the out-of-plane component of the magnetostatic field. The in-plane field is computed correctly, so any single-cell correction to the in-plane field will increase errors. A single-cell local correction, added after FFT calculations, does not significantly hinder efficiency.



A.



B.

Fig. 1. Comparison of the in-plane magnetostatic field of a uniformly magnetized $10\times10\times1$ oblate spheroid as calculated by a uniform thickness model (A) and a variable thickness model (B). Grey scale indicates divergence of the magnetostatic field.

Note the effect of this correction on the demagnetization factors of a single calculation cell. Our original approximation represents a reshaping of the cell by a rescaling of its magnetization. Reshaping the cell should change its demagnetizing factors. By adding the out-of-plane correction, we do change the out-of-plane demagnetizing factor, and this change restores the property that the demagnetization factors sum to 1.

III. Magnetostatic Field Errors

As a measure of the improved ability of the extended model to represent films with non-uniform thickness, we computed the demagnetization factors of the best representation of a $10\times10\times1$ oblate spheroid using the original model (Fig. 1 A) and the extended model (Fig. 1 B). For this spheroid the correct demagnetization factors are 0.0696 in-plane and 0.8608 out-of-plane. The calculated values are respectively 0.1026 and 0.7947 using the uniform thickness model, and 0.0635

and 0.8730 using the extended model. In Fig. 1 A, the in-plane relative RMS error is 118%, compared to 29.1% in Fig. 1 B. In Fig. 1 A, the out-of-plane relative RMS error is 15%, compared to 3.6% in Fig. 1 B. In Fig. 1 B the errors are concentrated at the edge. Within the central region extending to a 90% radius, the in-plane RMS error is 12.7%.

We also compared our variable thickness model to a three-dimensional model. Our variable thickness model is limited in its ability to accurately compute magnetostatic fields due to approximations in the interest of efficiency. Our three-dimensional model is also limited in its ability to accurately compute magnetostatic fields due to its limited discretization through the thickness of the oblate spheroid. Our three-dimensional model requires a discretization of at least 10 layers to obtain magnetostatic field errors comparable to our variable thickness two-dimensional model, at a cost of 10 times the memory and more than 10 times the amount of computation.

IV. Simulation Results

To explore the effects of thickness variations at the edges of thin films, we computed magnetization reversal curves for two variations on μMAG standard problem 2 [4], [7]. Standard problem 2 considers magnetic reversal of a thin film with dimensions in ratio $5 \times 1 \times 0.1$ with applied fields along the $[1, 1, 1]$ axis. We specify the dimensions of the film as $500 \times 100 \times 10$ nm, and material parameters representing Permalloy. This yields a ratio of film width to exchange length $d/l_{\text{ex}} \approx 19$. All simulations used a cell size $\Delta = 2$ nm. From the standard problem 2 results, we know the long axis component of magnetization M_x switches when the applied field magnitude $\mu_0 H$ is about 54.5 mT.

For comparison, we also simulated the reversal of a Permalloy film with dimensions $530 \times 130 \times 10$ nm. We found for the larger film that M_x switches when $\mu_0 H$ is about 44 mT. The 20% drop in the switching field is due to the larger size and different aspect ratio of the second film

Finally, using the extended model, we simulated the reversal of a film in the shape of a truncated pyramid. The base dimensions of the film were 530×130 nm and the top dimensions of the film were 500×100 nm. The maximum thickness of the film was 10 nm with a linear tapering to zero thickness over the outer 15 nm of the film. Simulations of reversal in this film found that M_x switches when $\mu_0 H$ is about 37 mT. This drop of about 30% in the switching field compared to standard problem 2 exceeds that which can be explained by the change in film size and aspect ratio.

Examination of the reversal curves reveals clues about the difference. Fig. 2 A shows the reversal of M_x. Fig. 2 B shows the reversal of M_y. For both uniform thickness simulations, the reversal takes place in two stages, as we have observed before [7]. The end domains switch at a small reversed field magnitude, then at a larger applied field the end domains propagate inwards and annihilate, completing the reversal. The two-stage reversal is most apparent in Fig. 2 B, where M_y shows two discontinuities in opposite directions. The hysteresis loop for the film with a truncated pyramid shape

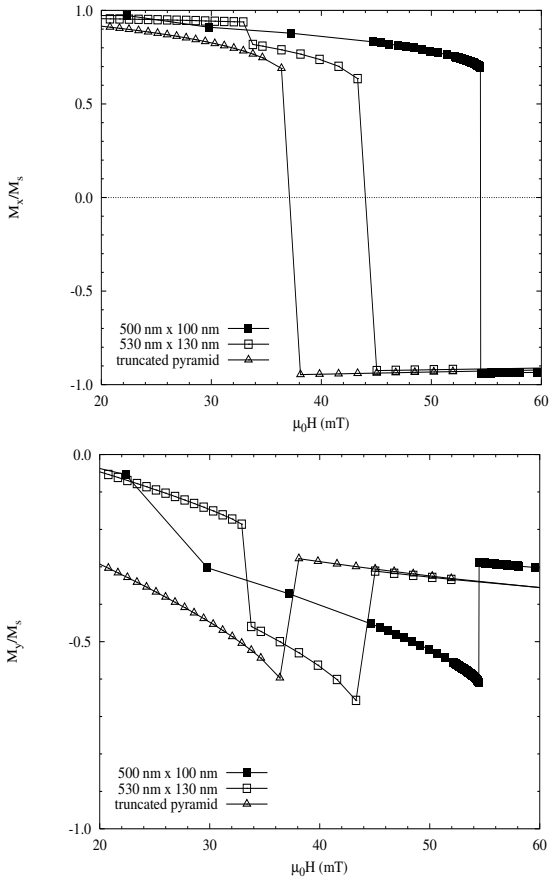


Fig. 2. Components of average magnetization along the long in-plane axis, M_x (A), and along the short in-plane axis, M_y (B), as a function of reverse applied field magnitude, for three simulated films. The films modeled with uniform thickness exhibit a two-stage reversal. The truncated pyramid film has only one switching event in its reversal.

shows no evidence of such a two-stage reversal. Simulation of the truncated pyramid with our three-dimensional model confirmed these results.

References

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