Applied and
Computational
Mathematics
Division

NISTIR 90-4427

Center for Computing and Applied Mathematics

Micromagnetic Calculations of 180° Surface Domain Wall Magnetization Profiles with Comparison to Measurements

James L. Blue and M. R. Scheinfein

September 1990

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
Gaithersburg, MD 20899

DATE DUE

NISTIR 4427

MICROMAGNETIC CALCULATIONS OF 180° SURFACE DOMAIN WALL MAGNETIZATION PROFILES WITH COMPARISON TO MEASUREMENTS

James L. Blue
M. R. Scheinfein

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
Center for Computing and Applied Mathematics
Applied and Computational Mathematics Division
Gaithersburg, MD 20899

U.S. DEPARTMENT OF COMMERCE
Robert A. Mosbacher, Secretary
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
John W. Lyons, Director

Micromagnetic Calculations of 180° Surface Domain Wall Magnetization Profiles with Comparison to Measurements

James L. Blue and M. R. Scheinfein*
National Institute of Standards and Technology
Gaithersburg, MD 20899

ABSTRACT

We compare measurements of magnetization profiles across 180° surface domain walls in a permalloy ferromagnet with calculations from micromagnetic models. The models were solved both by relaxation and by a time-evolution calculation. The measurements were made using scanning electron microscopy with polarization analysis (SEMPA). We obtain good agreement without postulating any surface anisotropy effect. This is the first successful comparison between experiment and a time-evolution calculation of domain walls.

*Current Address: Physics Dept., Arizona State University, Tempe, AZ 85287

The surface of a ferromagnetic material has a large effect on equilibrium magnetic microstructure, such as domains and domain walls. Surface magnetic microstructure is important to the understanding of the fundamental properties of magnetic materials as well as the limitations on the density of information stored on magnetic media. Additionally, the observation of surface magnetic microstructure provides us with important clues that assist in the determination of the underlying bulk magnetic microstructure.

In this paper, we use the usual nonlinear micromagnetic equations to simulate 180° domain walls [1,2,3,4,5,6,7,8], and compare two separate approaches for calculating the magnetization distribution. We then compare the results of the micromagnetic calculation with the experimental measurements.

The first method for solving the micromagnetic equations, which we call the relaxation method, utilizes an iterative scheme [1,2,3,4,5] to minimize the total system energy by systematically varying the magnetization within a discretized region of the domain wall. The second method directly integrates the Landau-Lifshitz-Gilbert (LLG) equations in time [6,7,8]. We call this the time method.

The energy of a ferromagnetic system is composed of 1) the mean field exchange energy between nearest neighbors; 2) the magnetocrystalline anisotropy energy, which reflects the interaction of the magnetic moments with the crystal field; 3) the magnetostatic self-energy, which arises from the interaction of the magnetic moments with the magnetic fields created by discontinuous magnetization distributions both in the bulk and at the surface; 4) the surface magnetocrystalline anisotropy energy, which corrects for broken symmetry near surfaces in the interaction of the magnetic moments with the crystal field; 5) the external magnetostatic field energy, which arises from the interaction of the magnetic moments with any externally applied magnetic fields; and 6) the magnetostrictive energy, which arises when mechanical stress is applied to a ferromagnetic material, introducing effective anisotropy into the system. In this study we do not consider surface anisotropy, nor do we consider effects due to thermal fluctuations. We use only bulk values for all parameters.

We solve for the magnetization distribution in a domain wall by considering a boundary value problem in two spatial dimensions with the constraint of constant magnetization M_s throughout the sample. We approximate the continuous magnetization distribution of a ferromagnet by a discrete distribution; the magnetization is discretized in the x-z plane of the cross section, but is uniform in y. There is one column of boundary cells at either side of the discretized region, which impose Dirichlet boundary conditions. Neumann boundary conditions apply at the top and bottom surface of the film. In the absence of surface anisotropy, the normal derivative of the magnetization at the surface is zero [2,9]; with surface anisotropy, we would use the Rado-Weertman boundary conditions [9,10].

Fundamental to our solution of the micromagnetic equations is that the saturation magnetization M_s is constant microscopically throughout the ferromagnet, that is, the magnetization distribution, $\mathbf{M}$, obeys $|\mathbf{M}| = M_s$.

For the time method of calculating domain wall microstructure in ferromagnets, we solve the Landau-Lifshitz-Gilbert (LLG) equation [6,7,8]. This equation has the following form [8, e.g.].

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma'(\mathbf{M} \times \mathbf{H}_{\text{eff}}) - \alpha' \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}) \tag{1}$$

The parameters are given by $\gamma' = \gamma/(1+\alpha^2)$ and $\alpha' = \gamma\alpha/(1+\alpha^2)$. Here the gyromagnetic ratio $\gamma = \gamma_e g/2$ is determined from the free electron value of γ_e and the spectroscopic splitting factor, $g = 2$. The gyromagnetic ratio γ, the damping parameter α, and the magnitude of the effective fields ($|\mathbf{H}_{\text{eff}}|$) determine the time scales of interest. For our time method simulations, we use the free electron gyromagnetic value of $\gamma, 1.78 \times 10^7$ Oe/sec. The damping parameter α is not well known and hence we bracket its value between 0.005 and 2.0.

The effective magnetic field on each magnetic moment, a function of the magnetic moments themselves, is determined from the total system energy $\mathcal{E}_{\text{tot}}$ as

$$\mathbf{H}_{\text{eff}} = -\partial \mathcal{E}_{\text{tot}} / \partial \mathbf{M} \tag{2}$$

(Together, Eqs. (1) and (2) guarantee $\partial \mathcal{E}_{\text{tot}}/\partial t <= 0$.) The effective magnetic field incorporates all the effects of exchange, anisotropy, external fields and demagnetizing fields. We integrate equation (1) directly in time using a robust integration routine, SDRIVE [11]. SDRIVE uses a form of Gear's method [12] to insure highly accurate solutions for systems of stiff differential equations. As an indication of the accuracy, $\mathcal{E}_{\text{tot}}$ decreases steadily as the evolution progresses, until the limiting accuracy is reached. This behavior is to be compared to that shown in Fig. 10 of [13], in which $\mathcal{E}_{\text{tot}}$ fluctuates.

Alternatively, we notice from the LLG equation that an equilibrium magnetization distribution, $\partial \mathbf{M}/\partial \mathbf{t} = \mathbf{0}$, requires the effective magnetic field to be parallel to the magnetization [2]. We relax the magnetization configuration iteratively, in turn rotating each magnetization vector to lie along the local effective magnetic field vector. We call this the relaxation method; it provides only the equilibrium distribution. When the largest residual of a single value of $|\mathbf{M} \times \mathbf{H}_{\text{eff}}|/|\mathbf{M}||\mathbf{H}_{\text{eff}}|$ decreases below a convergence minimum, we stop the iteration process [2].

The technique of scanning electron microscopy with polarization analysis (SEMPA) has been developed as a means of obtaining high resolution quantitative maps of the surface magnetization of ferromagnets [14,15, e.g.]. From such measurements one can obtain the profile of the magnetization across a domain wall at its intersection with the surface [1,16]. In SEMPA, a finely focused beam of medium energy (5-30 keV) electrons is rastered across a sample's surface. Secondary electrons are excited near the surface by the focused electron beam; emitted electrons maintain their spin orientation. The net polarization of the emitted electrons is characteristic of the net spin density in the solid for a variety of ferromagnetic materials. Surface magnetization maps with high spatial resolution can be generated by analyzing the spins of the secondary electrons emitted at each beam position on the sample surface.

SEMPA images of the surface magnetization from a region near a 180° surface domain wall in a 0.24 μm thick permalloy ($Ni_{81}Fe_{19}$) film are shown in Fig. 1a and 1b. These images are 4 μm across. Each SEMPA image shows positive magnetization as white and negative as black. In Fig. 1a, showing M_x, the x-component of the magnetization, positive means to the right; in Fig. 1b, showing M_y, positive means upward. Both M_x and M_y are in the plane of the page. We measured no out-of-plane component of the magnetization M_z for this surface domain wall structure; the magnetization lies completely in the plane of the surface. Figs. 1a and 1b are characteristic of the SEMPA images from which we extract surface domain wall magnetization profiles.

The experimental surface domain wall profiles extracted from SEMPA data (solid points) for a 0.24 μm thick permalloy film are compared to the results of the relaxation method calculation (solid line), in Fig. 2a. The experimental data is the result of averaging several line scans across the wall. The error bars give the standard deviation about the mean for the averaged line scans. The parameters used in the simulations are $A = 1.05\times10^{-6}$ erg/cm [17,18,19], $M_s = 813$ emu/cm^3 [20] and $K = 1743$ erg/cm^3 [20]. For the calculation, a region of the film 1.2 μm wide was discretized with 50 $\times$ 10 square cells. The initial condition had $M_y = M_s$ on the right, $M_y = -M_s$ on the left, and interpolated linearly across the wall. The other two components were equal and positive, and such that $|\mathbf{M}|$ $= M_s$. The wall energy for this simulation was 1.124 erg/cm^2. The wall energy was divided among the exchange energy, 74.9%, the magnetostatic energy, 23.0%

and the anisotropy energy, 2.1%. The root-mean-square deviation between the experiment and the theory is 0.086 for M_x and 0.106 for M_y, approximately equal to one standard deviation of the measurements. From this result, we conclude that the micromagnetic model is verified by SEMPA measurements [1], with no surface anisotropy effect needed.

We now compare the results of the time method with the relaxation method in Fig. 2b for the identical domain wall simulated with identical parameters and initial conditions. The solid line is the relaxation method result as in Fig. 2a. The solid points in Fig. 2b are the time method results. For the time method simulation, we used $\gamma = 1.78 \times 10^7$ Oe/sec and $\alpha = 2.0$. The agreement between the two results is striking. The RMS deviation between the relaxation method and the time method is 0.016 for M_x and 0.007 for M_y. The total wall energy for the time method is 1.126 erg/cm^2, divided among exchange energy, 74.5%, magnetostatic energy, 23.3% and anisotropy energy, 2.2%. We show the complete magnetization distribution of this domain wall in Fig. 3. The asymmetric Bloch wall vortex structure is clearly visible.

For other values of the damping parameter α between 0.005 and 2.0, we found negligible change in the wall energy or in the surface domain wall magnetization distribution, so long as metastable states are avoided [21]. With this proviso, we conclude that the relaxation method and the time method yield equivalent results for the micromagnetic structure of domain walls in thin films. This conclusion is supported by the results of Victora [17] in investigating hysteresis in CoNi thin films. In contrast, Zhu and Bertram [22], found a weak dependence of the coercivity on the damping parameter, α, for a hard thin-film medium. The equivalence of the relaxation method and the time method is significant in that the time method is guaranteed to converge to a physical solution of the LLG equation, while the relaxation method is not. The relaxation method takes less computer time, but the time method gives additional information about the evolution of the solution. Detailed comparisons will be given for a wide variety of materials, including bulk-like Fe, and a variety of initial conditions in a subsequent publication [21].

We would like to acknowledge support from the Office of Naval Research. We would like to acknowledge Dr. J. Unguris, Dr. D.T. Pierce and Dr. R.J. Celotta for useful discussions, and Dr. M.H. Kelley and R. Freemire for image processing.

References

[1] M.R. Scheinfein, J. Unguris, R.J. Celotta, D.T. Pierce, Phys. Rev. Lett. **63**(6), 668 (1989).

[2] A.E. LaBonte, J. Appl. Phys. **40**(6), 2450 (1969).

[3] A. Hubert, phys. stat. sol. **32**, 519 (1969).

[4] A. Aharoni, J. Appl. Phys. **46**(2), 908 (1975).

[5] M.R. Scheinfein, J. Unguris, J.L.Blue, K.J. Coakley, D.T. Pierce, R.J. Celotta, unpublished.

[6] L. Landau, E. Lifshitz, Phys. Z. Sowjet **8**, 153 (1935).

[7] C.C. Shir, J. Appl. Phys. **49**(6), 3413 (1978).

[8] R. Victora, Phys. Rev. Lett. **58**(17), 1788 (1987).

[9] G.T. Rado, J.R. Weertman, J. Phys. Chem. Solids **11**, 315 (1959).

[10] G.T. Rado, Phys. Rev. **B40**(1), 407 (1989).

[11] D. K. Kahaner and C. D. Sutherland, private communication.

[12] C.W. Gear, *Numerical Initial Value Problems In Ordinary Differential Equations*, (Prentice Hall Inc, Englewood Cliffs, NJ, 1971).

[13] M. Mansuripur and R. Giles, Computers in Phys. **4**(3), 291 (1990).

[14] M.R. Scheinfein, J. Unguris, M.H. Kelley, D.T. Pierce, R.J. Celotta, Rev. Sci. Instrum. (in press, October 1990).

[15] G.G. Hembree, J. Unguris, R.J. Celotta, D.T. Pierce, Scanning Micro. Intern., Supp. 1, 229 (1987).

[16] H.P. Oepen, J. Kirschner, Phys. Rev. Lett. **62**(7), 819 (1989).

[17] R. Victora, J. Appl. Phys. **62**(10), 4220 (1987).

[18] G. Shirane, V.J. Minkiewicz, R. Nathans, J. Appl. Phys. **39**(2), 383 (1968).

[19] N. Smith, D. Markham, D. LaTourette, J. Appl. Phys. **65**(11), 4362 (1989).

[20] P. Ryan, private communication.

[21] J.L. Blue and M.R. Scheinfein, unpublished.

[22] J.-G. Zhu and H.N. Bertram, J. Appl. Phys **63**(8), 3248 (1988).

Fig. 1: SEMPA images from a 0.24 μm thick permalloy sample. The images are 4 μm across and white (black) indicates positive (negative) magnetization in the (a) horizontal and (b) vertical direction in the plane of the page.

Fig. 2: (left) A comparison between experimental wall profiles in a 0.24 μm thick permalloy film (solid points) with results using the relaxation method (solid line). (right) A comparison between the results using the relaxation method (solid line) and the time method (solid points) for the same film.

Fig. 3: Contour plots for the calculated magnetization distribution in the domain wall. Each contour plot extends 1.2 μm horizontally and 0.24 μm vertically. The panels show, from top to bottom, the x-, y-, and z-components of the magnetization. Contours are at 0.1 M_s increments from -0.95 M_s to +0.95 M_s. Dashed lines are negative contours, and solid lines are positive.

NIST-114A
(REV. 3-90)

U.S. DEPARTMENT OF COMMERCE
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

BIBLIOGRAPHIC DATA SHEET

1. PUBLICATION OR REPORT NUMBER
NISTIR 4427

2. PERFORMING ORGANIZATION REPORT NUMBER

3. PUBLICATION DATE
SEPTEMBER 1990

4. TITLE AND SUBTITLE
Micromagnetic Calculations of 180° Surface Domain Wall Magnetization Profiles with Comparison to Measurements

5. AUTHOR(S)
James L. Blue and M. R. Scheinfein

6. PERFORMING ORGANIZATION (IF JOINT OR OTHER THAN NIST, SEE INSTRUCTIONS)
U.S. DEPARTMENT OF COMMERCE
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
GAITHERSBURG, MD 20899

7. CONTRACT/GRANT NUMBER

8. TYPE OF REPORT AND PERIOD COVERED

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (STREET, CITY, STATE, ZIP)

10. SUPPLEMENTARY NOTES

11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)
We compare measurements of magnetization profiles across 180° surface domain walls in a permalloy ferromagnet with calculations from micromagnetic models. The models were solved both by relaxation and by a time-evolution calculation. The measurements were made using scanning electron microscopy with polarization analysis (SEMPA). We obtain good agreement without postulating any surface anisotropy effect. This is the first successful comparison between experiment and a time-evloution calculation.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)
domain wall; ferromagnetism, Landau-Lifshitz-Gilbert equation; mathematical modeling; micromagnetics; SEMPA, surfaces

13. AVAILABILITY
- [X] UNLIMITED
- [ ] FOR OFFICIAL DISTRIBUTION. DO NOT RELEASE TO NATIONAL TECHNICAL INFORMATION SERVICE (NTIS).
- [ ] ORDER FROM SUPERINTENDENT OF DOCUMENTS, U.S. GOVERNMENT PRINTING OFFICE, WASHINGTON, DC 20402.
- [X] ORDER FROM NATIONAL TECHNICAL INFORMATION SERVICE (NTIS), SPRINGFIELD, VA 22161.

14. NUMBER OF PRINTED PAGES
11

15. PRICE
A02

ELECTRONIC FORM