Patterned Films II Romel Gomez, Chairman

Nucleation in polycrystalline thin films using a preconditioned finite element method

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The dynamic response of a 80 nm×400 nm×25 nm Co film with and without polycrystalline grains is calculated. The numerical method combines a finite element scheme for space discretization with a preconditioned backward differentiation method for the time integration of the Landau–Lifshitz–Gilbert equation. The use of proper preconditioning techniques for the backward differentiation formulas increases its efficiency by a factor of 40. The speed up factor compared to the Adams method is more than three orders of magnitude. In the polycrystalline thin film the nucleation of reversed domains occurs throughout the sample at grain boundaries and sharp edges. For the single crystalline film reversal starts at particle ends. Surface roughness does not significantly change the reversal mode but reduces the switching time by 40%. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The precise understanding of the switching process of thin film nanomagnets is important for sensor and spin electronic applications. Surface irregularities and grain structure drastically change the reversal mechanism of thin film elements.[1,2] Taking into account surface roughness and grain structures requires an inhomogeneous computational grid which in turn causes very small time steps for time integration. Toussaint and co-workers[3] showed that the time step required to obtain a stable solution of the Landau–Lifshift–Gilbert (LLG) equation with an explicit time integration scheme has to be proportional to h.[2] Here h is the size of the spatial grid. Edge roughness and an irregular grain structure may cause small computational cells which leads to a small time step when an explicit time integration method is applied to solve the LLG equation.

In computational physics, the backward differentiation formula (BDF) methods are popular in order to solve the system of ordinary differential equations which results from the space discretization of partial differential equations.[4] Yang and Fredkin[5] originally applied a BDF method in dynamic micromagnetic simulations. They applied the Galerkin variant of the finite element method for space discretization and a generalized minimum residual method (GMRES) to solve the linear systems involved in the solution process. One linear system gives the magnetic scalar potential. It arises from the space discretization of the Poisson equation. The numerical solution of the LLG equation, which can generally be written in the form $\dot{y}=f(t,y)$, leads to discrete values y_n at time points t_n. For the BDF and Adam method the values y_n follow from the liner multistep formula:

$$\sum_{i=0}^{K_1} \alpha_{n,i} y_{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} f_{n-i} = 0, \tag{1}$$

where y_n are the computed approximations to the solution $y(t_n)$. The variable time step is denoted with h_n. $\alpha_{n,i}$ and $\beta_{n,i}$ are constants that depend on the integration formula. Depending on the values of K_1 and K_2, Eq. (1) describes the BDF or Adams formula. If $K_1=1$ and $K_2=q-1$ Eq. (1) leads to the Adams formula of order q. The BDF formula of order q is represented by Eq. (1) with $K_1=q$ and $K_2=0$. For the special case of $q=1$ the constants K_1 and K_2 are the same for the Adams and the BDF formula. For that case, Eq. (1) simplifies to

$$y_n - y_{n-1} = h_n f_n, \tag{2}$$

which represents the implicit Euler method. To solve Eq. (2) or generally Eq. (1) a nonlinear system of equations has to be solved at each time step which can be effectively solved using the Newton method. Thus a second linear system of equations arises at each Newton iteration. The linear iteration

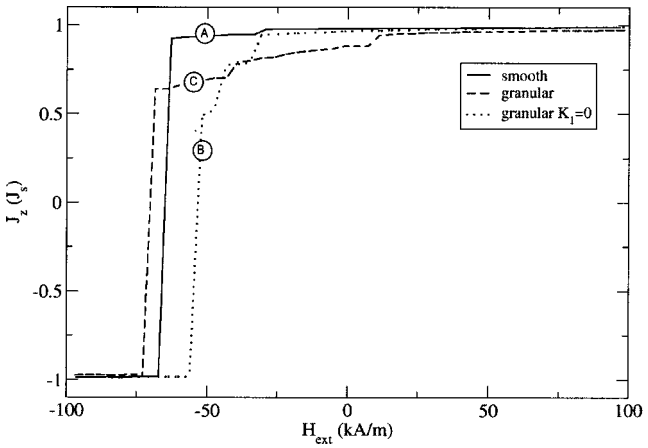

FIG. 1. Hysteresis loop of an element with (A) smooth surface and zero magnetocrystalline anisotropy, (B) surface roughness and zero magnetocrystalline anisotropy, and (C) granular structure with random anisotropy in every grain.

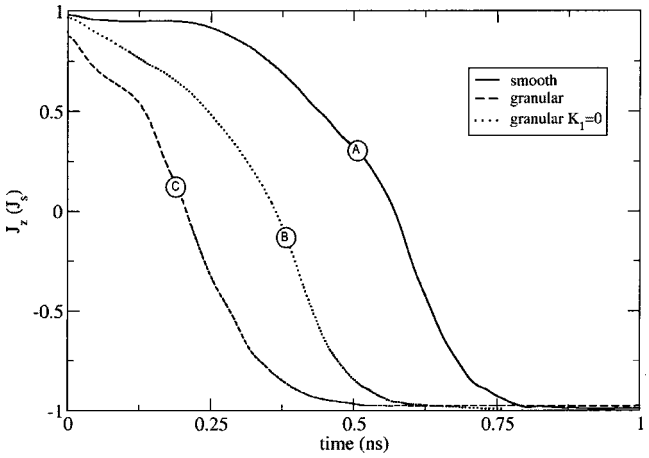

FIG. 2. Time evolution of the magnetic polarization after the application of a field of $H_{\text{ext}}=-100$ kA/m for the three different elements (A), (B), and (C).

is stopped when the desired accuracy is obtained or the linear iterations reaches the upper limit $l_{\max}$ called the maximum dimension of the Krylov subspace. The GMRES method is a matrix free iterative method to solve a linear system of equations. The number of iterations in the GMRES solver is very large when the linear system is ill-conditioned. However, even if the original system $A\boldsymbol{\Delta}\mathbf{y}=\mathbf{b}$ is ill-conditioned, an equivalent system $(AP^{-1})(P\boldsymbol{\Delta}\mathbf{y})=A'\mathbf{x}'=\mathbf{b}$ can be found, which is easy to solve. The equivalent system $A'\mathbf{x}'=\mathbf{b}$ can be solved with few iterations, if P is a good approximation to A, because then A' is close to the identity matrix. This procedure is called preconditioning. The crucial part is to find a good approximation to A. The problem is that usually the matrix A cannot be explicitly constructed or stored since it is a fully populated matrix. In micromagnetism the matrix A contains the second derivative of the Gibbs free energy. Due to the stray field energy, which describes a long term interaction, the matrix A is fully populated. With the GMRES method the system $A\boldsymbol{\Delta}\mathbf{y}=\mathbf{b}$ can be iteratively solved without explicit knowledge of the matrix A. For every iteration the GMRES solver has to calculate the product of the matrix A times a vector. That product is approximated using finite differences. We found that in micromagnetism a good approximation to A follows from the second derivative of the Gibbs free energy omitting the stray field interaction. As the short range interactions are the major source of stiffness in micromagnetic simulations, we obtain a significant speed up while keeping the system matrix sparse. For the investigated sample preconditioning speeds up the calculation by a factor of 40.

Preconditioning as described above allows the dynamic simulation of large realistic structures taking into account surface roughness and irregular grains within a reasonable CPU time. The numerical results show that both the quasistatic reversal process and the magnetization reversal dynamics significantly depend on the microstructure of thin film elements.

II. MICROMAGNETIC AND NUMERICAL BACKGROUND

The theoretical treatment of magnetization dynamics at zero temperature starts from the LLG equation.[6] The LLG equation preserves the norm of the magnetic polarization. Thus the deviation of $|\mathbf{J}|/J_s$ from unity may serve as a measure of the accuracy of the time integration scheme and the following time integration error can be defined:

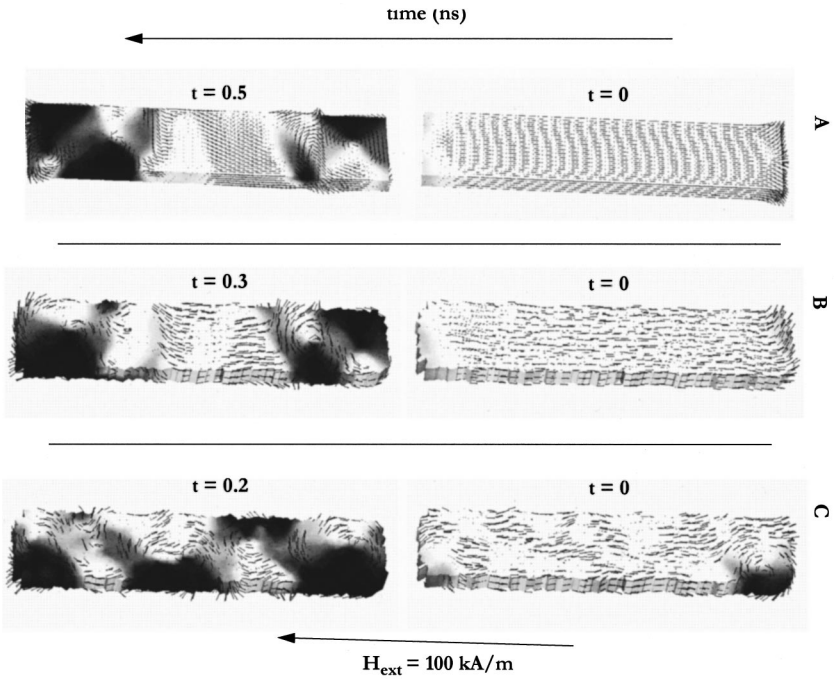

FIG. 3. Magnetization states after the application of a field of $H_{\text{ext}}=-100$ kA/m for elements (A), (B), and (C). The initial state is the remanent state. The component of the magnetic polarization is color coded ($J_z/J_s=1$=white, $J_z/J_s=-1$=black).

TABLE I. Compares statistical data for the Adams method, BDF method with and without preconditioning after 0.76 ns of simulated time. The Krylov subspace dimension $l_{max}=15$ in (BDF 15) and $l_{max}=600$ in (BDF 600) and (BDF Precond).

	Adams[a]	BDF 15	BDF 600	BDF precond
Total CPU time (s)	2×10^7	2×10^6	27.8×10^4	1.48×10^4
Average CPU per timestep (s)	1.6	26	69.4	9.69
Average number GMRES iterations per Newton step	⋯	14	64.3	1.18
Average timesteps (ps)	5×10^{-5}	6×10^{-3}	0.18	0.50
Number of renormalization steps *nrn* (error indicator)	1×10^4	21	216	6

[a]The data for the Adams method are extrapolated from a simulation of 0.02 ns simulated time.

$$e_{DN}=\max_i|1-(|\mathbf{J}_s|/J_s)|, \tag{4}$$

where i runs from 1 to the total number of nodal points.

The LLG equation is solved using a finite element method as described in Ref. 7.

III. RESULTS AND DISCUSSION

In order to investigate the influence of edge irregularities and a polycrystalline anisotropy on the reversal process we modeled different elements with the finite element method. All of the elements are 400 nm long, 80 nm wide, and 25 nm thick. The spontaneous polarization $J_s=1.76$ T and the exchange constant $A=1.3\times10^{-11}$ J/m. One element denoted by (A) consists of a perfect microstructure. The surface is flat, no grains are assumed within the particle, and the crystalline anisotropy is zero. Element (B) takes account of surface roughness. The notches average 8 nm. Element (C) consists of 500 columnar grains (diameter is 8 nm) with random distribution of the magnetocrystalline anisotropy directions. The anisotropy constant was $K_1=450$ kJ/m^3. The grain structure was calculated using a voronoi construction. Every grain consists of about 27 finite elements. In all simulations the angle between the external field and the long axis of the Co element is 1° to break the symmetry of the system. Figure 1 shows the hysteresis loop for elements (A), (B), and (C). The external field is decreased in steps of 4.2 kA/m, in order to calculate the hysteresis curve quasistatically. For each field value the LLG equation is integrated until equilibrium is reached. The granular element (C) has the largest coercive field, $H_c=72$ kA/m. The coercive field decreases by less than 10% for the perfect Co element without crystalline anisotropy. Surface roughness leads to a reduction of the coercive field by about 20%. Figure 2 shows the time evolution of the magnetic polarization for the three different elements. The initial state is the remanent state of the previously mentioned hysteresis loop calculation. The external field is applied instantaneously with a field strength of $H_{ext}=100$ kA/m. The Gilbert damping constant is assumed to be $\alpha=0.1$. The granular structure significantly influences the dynamics of the system. For perfect elements the high stray-field at the particle ends determines the reversal process. The stray field causes nucleation at the particle ends as shown in Fig. 3(a). In contrast, nucleations also occur within the particle for the granular element [Fig. 3(C)]. The particle ends become less important. The grain boundaries initiate the reversal process. Surface roughness does not significantly change the reversal mode. Also for rough surfaces vortices occur only at particle ends. However, the surface roughness reduces the switching time (time when J_z becomes smaller than 0) by about 40%.

To be able to integrate the LLG equation for granular elements, which leads to irregular finite element grids, sophisticated time integration scheme have to be used. We have varied a number of input parameters of the CVODE references package. Table I compares the Adams method with two BDF methods with different dimensions of the Krylov subspace (l_{max}) and one BDF method with preconditioning. The number of renormalized steps *nrn* acts as error indicator for the simulations. Usually the LLG equation conserves the norm of the magnetization, however, the numerical solution leads to a deviation of the norm. When the derivation norm exceeds 0.01 the magnetization is renormalized in our program. So a small number of *nrn* indicates an accurate solution. An increase of l_{max} in the BDF method without preconditioning decreases the CPU time but increases the error of the solution. Preconditioning drastically decreases both, the error of the solution and the CPU time.

IV. CONCLUSION

Numerical micromagnetics is an essential tool to optimize magnets in magnetic storage and sensors. The application of these devices requires a profound knowledge of the reversal mechanism. Using the LLG equation the time evolution of the magnetization can be calculated. The treatment of systems with realistic size leads to a system of ordinary differential equation with up to one million unknowns. State of the art time integration schemes provides an efficient numerical solution of the equation.

ACKNOWLEDGMENT

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