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A finite element based real-space phase field model for domain evolution of ferromagnetic materials

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ABSTRACT

This paper proposes a real-space phase field model solved by finite element method for giant magnetostrictive materials. The model is based on the thermodynamic theory of ferromagnetic materials and employs the time-dependent Ginzburg-Laudau (TDGL) equation to predict the domain evolution process. We have derived the corresponding finite element formulation which takes the mechanical displacement, the magnetic potential, and the magnetization vector as the field variables, according to variational principle. A multi-field coupling finite element has been developed through the ABAQUS user element subroutine module to simulate the coupling between mechanical and magnetic characteristics for microstructures with arbitrary geometries and boundary conditions. The simulation results of a general magnetic nanoring coincide well with the reports in literature, which confirms the validity of the phase field method developed. The magnetization processes have also been investigated for nanorings with different geometries. The results suggest that the vortex chirality and multi-stable magnetization states can be controlled by changing both the symmetry of loading situation and the geometrical configuration. The phase field model solved by finite element method is expected to be a useful tool for the design of high density magnetic random access memories.

1. Introduction

Magnetic microstructures have attracted considerable interests since they are widely used in recording media, magnetic random access memories (MRAMs), magnetic actuators and sensors [1,2]. For the magnetic nanoring geometry, a flux closure vortex magnetic state with no demagnetizing field can be formed over a wide range of applied field, making it the ideal storage unit for MRAMs. Both experimental research and numerical simulation have been conducted for magnetic nanorings [3–5]. Due to the complex domain evolution process, numerical simulation has become an important and efficient tool for the investigation of ferromagnetic materials [6]. In the 1960s, Brown laid the basis of micromagnetics based on variational principle [7]. In traditional micromagnetics, the magnetization vector is employed as the field variable and has a constant magnitude when the temperature is fixed. The stable magnetization state is determined by the combined action of different energies including the magnetocrystalline anisotropy energy, exchange energy, magnetostatic energy and external field energy. By solving the Landau-Lifshitz-Gilbert (LLG) equation, we can acquire the temporal evolution of magnetization on microscale. Both the finite element method (FEM) and the finite difference method (FDM) have been employed to solve the nonlinear equation [8,9]. In order to increase the accuracy and efficiency of demagnetizing field calculation, some advanced numerical techniques have been employed, including the FDM with fast Fourier transform (FFT) method or Tensor grid (TG) method, and FEM with shell transformation or boundary element method (BEM) [10–12]. The micromagnetic simulation has been frequently applied in the prediction of magnetic properties for microstructures [13,14], the optimization and investigation of various magnetic devices [15–17].

For general ferromagnetic materials, the magnetostrictive strains are usually neglected in micromagnetic simulation. However, inhomogeneous magnetostriction induced strain and external strain, such as the mismatch strain of thin film and substrate [18], should be considered for the accuracy simulation and design of high density memory. In order to study the effect of stress on magnetic properties, the magnetoelastic energy term was introduced into the total Gibbs free energy in micromagnetic simulation [19,20]. However, this method can only be used for the case that the material is subjected to a uniaxial homogeneous stress, and cannot simulate the effect of magnetization on mechanical

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properties. By combining the micromagnetic model with the phase-field microelasticity theory [21], a phase field model for giant magnetostrictive materials was proposed [22]. The phase field model employs the magnetization vector as the order parameter and the LLG equation to simulate the dynamic magnetization behavior. The strain and magnetization under magnetic field and mechanical stress can be studied simultaneously. More phase field models for ferromagnetic materials and multiferroic composites can be found in literature [23–25]. However, the periodic boundary conditions need to be satisfied in most phase field models, thus the structure with irregular geometries or under complex load conditions cannot be simulated. Miehe presented a geometrically consistent rate-type incremental variational formulation for phase field models, where the geometric property of the magnetization director is exactly preserved pointwise by nonlinear rotational updates at the nodes [26]. Wang developed a real-space phase field model to study the domain evolution of ferromagnetic materials without considering free space [27].

In this paper, based on the phase field equations for micro-magneto-elastic model, a novel finite element formulation is established according to the variational principle. The TDGL equation is employed to simulate the temporal evolution of magnetization and the magnitude of magnetization is controlled by an additional constraint energy term in the total free energy. The magnetic potential is extended into the free space to calculate the magnetostatic energy. Through the ABAQUS user subroutine module, a multi-field coupling finite element for magnetostrictive materials has been developed, taking the mechanical displacement, magnetic potential and magnetization vector as the field variables. With the phase field model developed, we have investigated the geometrical regulation of magnetic properties for nanorings. It is shown that the vortex chirality and multi-stable magnetization states can be controlled by breaking the symmetry of loading condition and changing the geometrical configuration of nanorings reasonably.

2. Phase field model

According to the theory of micromagnetics, the total magnetic field can be decomposed into two parts, namely the applied magnetic field and the demagnetizing field, which can be written as

$$\mathbf{h} = \mathbf{h}_e + \mathbf{h}_d, \tag{1}$$

where $\mathbf{h}_e$ represents the applied magnetic field and $\mathbf{h}_d$ the demagnetizing field. The demagnetizing field is related to the magnetic potential as

$$h_{di} = -\phi_{,i}. \tag{2}$$

The magnetic field exists not only in the magnetic material body, but also in the free space. Since the demagnetizing field decays quickly in the air, a free space box containing the magnetic body

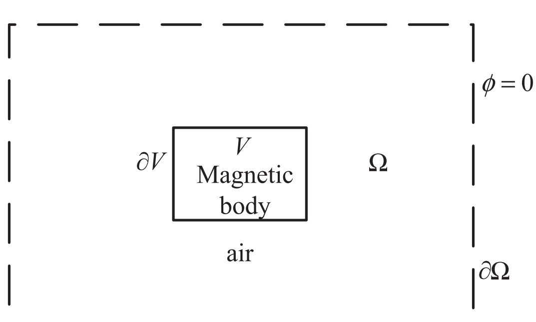

Fig. 1. The free space box including the magnetic body and the air.

is employed in the model, as shown in Fig. 1. In the surface of the free space, the magnetic potential is assumed to satisfy the Dirchlet condition

$$\phi = 0 \quad \text{on } \partial\Omega. \tag{3}$$

According to the Maxwell's equations, the magnetic induction vector **b** satisfies the condition

$$B_{i,i} = 0 \quad \text{in } \Omega. \tag{4}$$

The constitutive relationship between the magnetic induction vector, the magnetic field and the magnetization vector can be interpreted as follows

$$\mathbf{B} = \mu_0(\mathbf{h}_d + \mathbf{h}_e + \hat{m}_s\mathbf{m}) \quad \text{in } \Omega, \tag{5}$$

where μ_0 is the magnetic permeability of the vacuum and **m** the unit magnetization vector. $\hat{m}_s$ is the magnitude of the magnetization vector, the value of which can be written as

$$\hat{m}_s(\mathbf{x}) = \begin{cases} m_s & \text{for } \mathbf{x} \in V, \\ 0 & \text{for } \mathbf{x} \in \Omega/V, \end{cases} \tag{6}$$

where m_s is the magnitude of saturation magnetization of the magnetic material. The equation implies that the magnetization only exists inside the magnetic materials. Assuming that the applied magnetic field is constant in space, Eq. (4) can be rewritten as

$$h_{di,i} = -\hat{m}_s m_{i,i} \quad \text{in } \Omega. \tag{7}$$

The boundary conditions on the surface of magnetic body is given as

$$\phi^+ = \phi^- \quad \text{on } \partial V, \tag{8}$$

$$\frac{\partial\phi^+}{\partial n} - \frac{\partial\phi^-}{\partial n} = -m_s\mathbf{m}\cdot\mathbf{n} \quad \text{on } \partial V, \tag{9}$$

where the superscript + represents the value on the external surface and − on the internal surface. Eq. (8) suggests the magnetic potential is continuous across the surface of magnetic material. Eq. (9) requires that the magnetic flux coming into the interface is equal to that flowing out of the interface.

In order to predict the magnetic behavior of ferromagnetic materials, equations governing the evolution of magnetization vectors are still needed. In this model, the time dependent Ginzburg-Landau (TDGL) equation is employed to simulate the temporal evolution of magnetic domains:

$$\eta\frac{\partial\mathbf{m}(\mathbf{x},t)}{\partial t} = -\frac{\delta E}{\delta\mathbf{m}(\mathbf{x},t)}, \tag{10}$$

where η is the inverse mobility coefficient and E the total free energy density. Although the Landau-Lifshitz-Gilbert (LLG) is often used to describe magnetization evolution, it has been tested that when the applied magnetic field is of low frequency, as in the case simulated here, the TDGL equation gives the same simulation results with that obtained by the LLG equation [28]. In addition, the TDGL equation is much simpler in the numerical implementation than the LLG equation and has also been employed for the evolution of magnetic domains [29] and electric domains [30].

Since the surface anisotropy can be neglected in this model, the magnetization vector satisfies the following conditions on the surface of magnetic materials according to the theory of micromagnetics:

$$\frac{\partial\mathbf{m}}{\partial n} = \mathbf{0} \quad \text{on } \partial V. \tag{11}$$

According to the classical domain theory for ferromagnetic materials, the domain structures below Curie point are decided by the competition of free energies including the magnetocrystalline