Computational Materials Science 97 (2015) 42–47

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Micromagnetic simulation of an antiferromagnetic particle

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ARTICLE INFO

Article history:
Received 25 July 2014
Received in revised form 5 October 2014
Accepted 7 October 2014
Available online 29 October 2014

Keywords:
Micromagnetic simulation
Finite element method
Antiferromagnet

ABSTRACT

A continuum micromagnetic model is derived, describing an antiferromagnet. Using the finite element method, magnetization curves are calculated for a spherical uniaxial particle, varying the particle's size and the anisotropy field strength. Different magnetization processes appear by increasing the size of the particle. For large particles nucleation and expansion of a reversed domain is observed, separated by an almost 90° wall. An estimation of the single domain radius R_c is made.

1. Introduction

Antiferromagnetic nanoparticles are of great interest for new composite magnetic materials [1–6], which can be used in applications like spin valves [7,8] and random access memories (MRAM) [5,9], so examining the magnetic behavior of antiferromagnets is of great importance.

Micromagnetism is a widely used theoretical model, due to its capability of predicting the magnetic behavior of a continuous medium. According to this model, the magnetization vector is treated as a continuous function in space [10]. The Finite Difference Method (FDM) [11,12] and the Finite Element Method (FEM) [13–15], both with their drawbacks and advantages, are the two basic techniques in computational micromagnetism. FEM has the main advantage that it can handle easily large particles and complex geometries. Extensive work has been done, by means of FEM, on the coupling of an antiferromagnet with a ferromagnet [16–19], but not for the antiferromagnet itself.

This paper is organized as follows. First, a continuous micromagnetic model is presented for a magnetic system consisting of two sublattices. Then, in order to test the validity of the model, simulation, under the absence of dipole interactions, of a spherical uniaxial antiferromagnetic particle by FEM is curried out, in order to be compared with known analytical calculations. After the validation, magnetization curves are simulated, under dipole field interactions, while varying the size and the anisotropy constant of the particle.

2. The simulation model

An antiferromagnet is composed of two sublattices (A and B) of equal magnetization norm, M_s and is characterized by a negative exchange integral between them. In an atomistic model, for each atom a unique magnetic moment is defined. In a continuous approximation, as the micromagnetic model, the magnetization vector is considered a continuous function in space, so the magnetization of each sublattice, $\vec{M}^A$ and $\vec{M}^B$ must be defined at every point in space.

The evolution of the magnetization vectors is governed by the damped Partial Differential Equations (PDE) [20]

$$\tau\frac{\partial\vec{M}^A}{\partial t}=\frac{1}{M_s^2}\left(\vec{M}^A\times\vec{H}^A_{\text{eff}}\right)\times\vec{M}^A \text{ and } \tau\frac{\partial\vec{M}^B}{\partial t}=\frac{1}{M_s^2}\left(\vec{M}^B\times\vec{H}^B_{\text{eff}}\right)\times\vec{M}^B,$$

where $\vec{H}^I_{\text{eff}}$ is the effective field acting on sublattice $I=\{A,B\}$ and can be found from the variational derivative of the micromagnetic energy with respect to the magnetic polarization [10]. The main contributions are the exchange, magnetocrystalline, dipole, and Zeeman energies. Summing up for all the above contributions, an effective field $\vec{H}^I_{\text{eff}}$ can be defined at every point in space as

$$\vec{H}^I_{\text{eff}}=\vec{H}^I_{\text{ex}}+\vec{H}^I_k+\vec{H}_d+\vec{H}.$$

$\vec{H}^I_{\text{ex}}$ is the exchange field acting on sublattice I. The exchange energy is described by a Heisenberg Hamiltonian

$$E_x=-\frac{1}{2}\sum_{i,j}J_{ij}\left(\vec{S}_i\cdot\vec{S}_j\right),$$

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http://dx.doi.org/10.1016/j.commatsci.2014.10.010
0927-0256/

where i runs for all atoms in the particle and j for the first neighbors of each atom. In the micromagnetic model discrete atoms cannot be defined. As already mentioned, at each position $\vec{r}_i$ inside the particle the magnetization of each sublattice is defined, and in the neighborhood $\vec{r}_j$ around this position, each magnetization component can be approximated by a Taylor expansion as

$$M_k^l(\vec{r}_j) = M_k^l(\vec{r}_i) + (\vec{r}_j - \vec{r}_i)\cdot\nabla M_k^l(\vec{r}_i) + \frac{|\vec{r}_j - \vec{r}_i|^2}{2}\left\{\nabla^2 M_k^l(\vec{r}_i)\right\},$$
$$k = \{x, y, z\}.$$

For a symmetric distribution of neighborhood atoms the first order terms vanish. For an isotropic one, the off diagonal second order terms vanish too. Under these assumptions, the exchange energy takes the form:

$$E_{ex} = -\frac{z}{2M_s^2 v}\int \begin{bmatrix} J_{AA}\vec{M}^A\left(\vec{M}^A + \frac{a^2}{2}\left\{\nabla^2\vec{M}^A\right\}\right) + J_{BB}\vec{M}^B\left(\vec{M}^B + \frac{a^2}{2}\left\{\nabla^2\vec{M}^B\right\}\right) + \\ + J_{AB}\vec{M}^A\left(\vec{M}^B + \frac{a^2}{2}\left\{\nabla^2\vec{M}^B\right\}\right) + J_{BA}\vec{M}^B\left(\vec{M}^A + \frac{a^2}{2}\left\{\nabla^2\vec{M}^A\right\}\right) \end{bmatrix} dV,$$

where the integration takes place in the particle's volume, v is the atomic volume, z is the number of the first neighbors and a is the first neighbors distance. $J_{AB} = J_{BA}$ are the antiferromagnetic exchange integrals and $J_{AA} = J_{BB}$ are the ferromagnetic ones. The latter interactions must be considered seriously and cannot be omitted, because in a continuum approximation there is no validation of the magnetization norm conservation rule. The terms of the form $\vec{M}^l\cdot\vec{M}^l$ can be omitted, because they contribute as constants in the energy expression.

The exchange field for the two sublattices is

$$\vec{H}_{ex}^A = \lambda\vec{M}^B + \ell_{AA}^2\left\{\nabla^2\vec{M}^A\right\} - \ell_{AB}^2\left\{\nabla^2\vec{M}^B\right\} \text{ and}$$
$$\vec{H}_{ex}^B = \lambda\vec{M}^A + \ell_{BB}^2\left\{\nabla^2\vec{M}^B\right\} - \ell_{BA}^2\left\{\nabla^2\vec{M}^A\right\},$$

where $\lambda = zJ_{AB}\Big/\left(2\mu_o M_s^2 v\right)$ is a negative dimensionless mean field constant, $\ell_{AA} = \ell_{BB} = a\sqrt{zJ_{AA}/\left(4\mu_o M_s^2 v\right)}$ is a ferromagnetic exchange length and $\ell_{AB} = \ell_{BA} = a\sqrt{z|J_{AB}|/\left(4\mu_o M_s^2 v\right)}$ is an antiferromagnetic exchange length. In order for the antiferromagnetic order to exist, the two sublattices must be ferromagnetically stable, so the antiferromagnetic exchange length cannot be larger than the ferromagnetic one. In the limiting case, which was used in the following simulation results, the two lengths have the same value ℓ_x.

Assuming a uniaxial anisotropy for each sublattice, with different strength and orientation, the magnetocrystalline energy can be written as

$$E_k = \int\left[K_1^A\left(\hat{u}^A\cdot\frac{\vec{M}^A}{M_s}\right)^2 + K_2^B\left(\hat{u}^B\cdot\frac{\vec{M}^B}{M_s}\right)^2\right]dV$$

where K_1^l is the first order anisotropy constant and $\hat{u}^l$ is the direction of easy axis. The anisotropy field for each sublattice is

$$\vec{H}_k^l = \frac{2K_1^l}{\mu_o M_s}\left(\hat{u}^l\cdot\hat{M}^l\right)\cdot\hat{u}^l.$$

For the simulations presented in this work, both the anisotropy constants and easy axis directions were assumed to be the same for the two lattices.

For the dipole interactions the energy takes the form:

$$E_d = -\frac{\mu_o}{2}\int\vec{H}_d\cdot(\vec{M}^A + \vec{M}^B)dV$$

where $\vec{H}_d$ is the demagnetizing field and is equal to the gradient of the magnetic scalar potential for which the Poisson equation holds [21]

$$\nabla^2\phi = -\nabla\cdot(\vec{M}^A + \vec{M}^B).$$

The Zeeman energy is written as

$$E_z = -\mu_o\int\vec{H}\cdot(\vec{M}^A + \vec{M}^B)dV$$

where $\vec{H}$ is the external applied field.

The governing equations are supplemented by the boundary conditions $\partial\vec{M}^A/\partial\hat{n} = 0$ and $\partial\vec{M}^B/\partial\hat{n} = 0$, where $\hat{n}$ represents the normal unit vector on the surface of the particle.

The six PDE for the magnetization components and the one for the magnetic scalar potential are solved simultaneously through the FEM by directly applying the weak form, which is derived by the Galerkin method. The Poisson equation is solved by applying a mapped infinite element scheme [22,23], thus an outer domain surrounding the particle is used. Magnetization is interpolated using 3rd order Lagrange elements in the domain of a magnetic particle. For the magnetic potential, 2nd order Lagrange elements have been used, both on the magnetic particle domain and on the surrounding outer domain. The time integration was performed by a variable step size and order BDF method [24] and the algebraic system of linear equations was solved with PARDISO [25]. More information about the method used can been found in [20].

3. Simulation results

Magnetization curves were calculated for a spherical uniaxial antiferromagnetic particle with the above-mentioned magnetic parameters for variable radius and anisotropy constant. The external field was set parallel to the easy axis direction $\hat{u}$, which coincides with x-axis, and was varied from zero to the maximum value in $10^6\tau$. As initial condition at all simulations the magnetization of the two sublattices was set to $\vec{M}_A = M_s\hat{u}$ and $\vec{M}_B = -M_s\hat{u}$, resulting in a zero net magnetic moment.

In order to check the validity of the model, simulations were made under the absence of dipole field interactions. In this context, analytic atomistic models describe magnetization process by spin flip and spin flop transitions [26,27]. Fig. 1 shows calculated magnetization curves for spin flop (Fig. 1(left)) and spin flip (Fig. 1(right)) regions. In the first case at spin flop field, H_{sf}, the magnetization vectors of the two lattices jump coherently to opposite angles (sharp increment in Fig. 1(left)) with respect to the external field axis. This state is shown in Fig. 2. Then both lattices gradually rotate towards

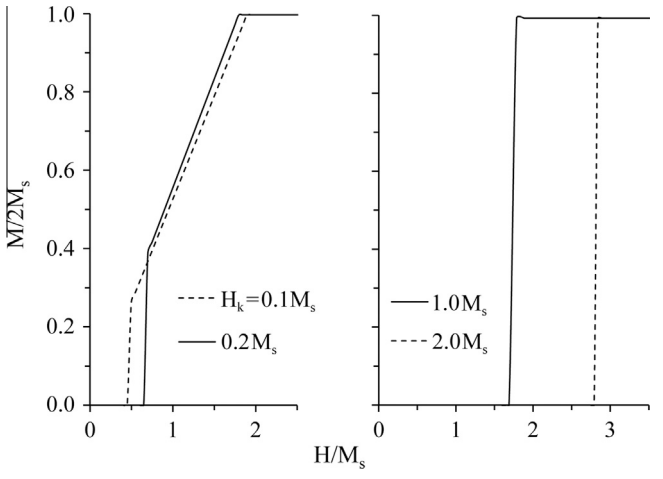

Fig. 1. Magnetization curves for a spherical uniaxial antiferromagnetic particle with $\lambda = -1$ and $R/\ell_x = 1$ without dipole interactions. On the left are spin flop cases and on the right spin flip cases.