Micromagnetic simulation of structure-property relations in hard and soft magnets

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ABSTRACT

Finite element micromagnetics describes the influence of the microstructure on the magnetic properties of thin film nano-elements and permanent magnets. The particle shape and the grain structure influence both the coercive field and the reversal time of NiFe and Co nano-elements. The performence of a Runge-Kutta method and a semi-implicit backward difference method for the time integration of the Gilbert equation of motion are compared. In an array of closely packed patterned elements, the magnetostatic interactions lead to a spread in the switching field depending on the magnetic state of the neighbors. The effect of the magnetostatic interaction on magnetization reversal can be effectively treated using a hybrid finite element / boundary element method. The very same method is applied to simulate magnetostatic interactions between the particles of a bonded magnet. The magnetostatic interaction field decreases both the remanence and the coercive field of nanocomposite magnets. In hard magnets, domain walls may be pinned at grain boundaries between misoriented grains. The simulation of domain wall motion requires adaptive refinement and coarsening of the mesh, in order to keep the number of degrees of freedom reasonable low.

1 Introduction

The physical structure determines the magnetic properties in such different materials like magnetic nano-elements for patterned media or MRAM applications and permanent magnets. Microstructural features such as particle shape and grain structure influence both static and dynamic properties. The static hysteresis properties comprise the domain structure of the remanent state, the coercive field, and the coercive squareness. Dynamic properties include the waiting time required to initiate the formation of vortices, the transient magnetic states during irreversible switching and the total reversal time. Finite element and boundary element methods provide the means to solve the underlying partial differential equations. A priori or adaptive refinement of the finite element mesh adjusts the computational grid to the physical and the magnetic structure. Examples of the structure-property relationship are given for magnetization reversal in NiFe and Co nano-elements, magnetostatic interactions in bonded permanent magnets, and domain wall motion in hard magnetic thin specimens.

2 Magnetization reversal in magnetic nano-elements

2.1 Static properties

Magnetic nano-elements may be the basic structural units of future patterned media or magneto-electronic devices. The switching properties of acicular nano-elements significantly depend on the shape of the ends. Pointed ends suppress the formation of end domains in the remanent magnetic state of NiFe nano-elements. As a consequence the switching field decreases by a factor of 1/2 as compared to non-elements with blunt ends. A hybrid finite element / boundary element method [3] effectively treats the magnetostatic interactions between distinct elements, as no mesh is required outside the magnetic elements. Different magnetization reversal mechanisms occur depending on the strength and direction of the magnetostatic interaction field. The simulations predict a spread in the switching field due to magnetostatic interactions in the order of 8 kA/m for 200 nm wide, 3500 nm long and 26 nm thick NiFe Elements with a center-to-center spacing of 250 nm. An interaction field in the range of 8 kA/m to 20 kA/m was found in granular Co elements with an extension of 40x200x25 nm and a center-to center spacing of 80 nm. Finite element simulation of magnetization reversal show that the random crystalline anisotropy of granular Co elements favors the formation of vortices. Thus the coercive field decreases to 95 kA/m as compared to calculations assuming zero anisotropy which show a coercive field of 140 kA/m. Once vortices are formed they easily break away from the edges causing the reversal of the entire element.

2.2 Dynamic properties

In addition to the quasi-static properties, the switching dynamics depends on the shape of the NiFe elements and on the polycrystalline microstructure of Co elements. The time integration of the Gilbert equation of motion provides the transient magnetic states during irreversible switching. The numerical integration requires to take into account the stiffness of the equations. A Runge-Kutta method optimized for mildly stiff systems [6] proved to be effective for the time integration of the Gilbert equation, when zero anisotropy is assumed. Including random magnetocrystalline anisotropy enhances the stiffness of the equations, leading to a time step smaller than 10 fs. Then a reasonable progress in time is only possible using a semi-implicit scheme for time integration [5]. Submicron NiFe elements with an extension of 200x100x10 nm switch well below 1 ns for an applied field of 80 kA/m, assuming a Gilbert damping constant of 0.1. The elements reverse by nonuniform rotation. Under the influence of an applied field, the magnetization starts to rotate near the ends, followed by the reversal of the center. This process only requires about 0.1 ns. In what follows, the magnetization component parallel to the field direction shows oscillations which decay within a time of 0.4 ns. The excitation of spin waves originates from the gyromagnetic precession of the magnetization around the local effective field. A much faster decay of the oscillations occurs in elements with slanted ends, where surface charges cause in transverse magnetostatic field. In elements with zero magnetocrystalline anisotropy and in elements with random magneto-crystalline anisotropy magnetization reversal occurs by the formation and motion of vortices. However, in granular Co elements with random magneto-crystalline anisotropy, vortices form immediately after the application of a reversed field. For zero magnetocrystalline anisotropy a vortex breaks away from the edge only after a waiting time of about 0.8 ns.

3 Permanent magnets

3.1 Magnetostatic interactions in bonded magnets

Bonded permanent magnets are an important part of many consumer electronic and computer peripherial devices. With the advance of the miniaturization of the products, nanocomposite magnets may be used because of their higher magnetizability as compared to conventional melt-spun magnets [1]. An important question for practical applications is the influence of the magnetostatic interactions between the particles of the bonded magnet on the magnetic properties. A hybrid finite element / boundary element method was used to calculate the influence of the magnetostatic interaction field on the demagnetization curve for different particle arrangements. The magnetostatic interaction field decreases rapidly with distance. For a gap of 2.5 nm between the particles, the region where the magnetostatic interaction field exceeds 150 kA/m penetrates only 10 nm into the neighboring particle. Under the influence of the magnetostatic interaction field of its neighbor, the coercive field of an elongated particle decreases by about 50 kA/m. The decrease in the remanence magnetization was 5 % as compared to the remanence of an isolated particle.

3.2 Domain wall motion in hard magnets

In hard magnets domain walls may be pinned at grain boundaries between misoriented grains. The magnetization is uniform within the domains whereas it is highly non-uniform in the domain walls. In order to describe domain wall motion in permanent magnets, an adaptive finite element method was developed [4] that adjust the finite element mesh to the current wall position. Combined refinement and coarsening of the mesh leads to a fine mesh that moves together with the domain wall. This examples clearly demonstrates the benefits of the finite element method for the simulation of the structure-property realationship in magnetic materials.

The numerical results obtained for a thin Nd-Fe-B specimen show that domain walls going through small misoriented grains are unstable for zero applied field. The wall move towards the boundary of the misoriented grain, where it remains pinned owing to a reduction of the exchange and anisotropy energy. The pinning fields greater than 200 kA/m where calculated for an misorientation angle of 45 degrees.

Without refinement a so-called domain wall collapse [2] will occur within large elements: The magnetization becomes aligned antiparallel at neighboring nodes and the torque on the magnetization vanishes. To simulate wall motion the mesh has to be adjusted accordingly. Adaptive meshing keeps the space discretization error below a certain threshold and avoids the collapse of the domain wall. A reliable refinement indicator is based on the constraint condition for the norm of the magnetization vector which successfully identifies the regions with non-uniform magnetization.

4 Summary

Finite element techniques for the simulation of the structure-property relationship in magnetic nano-elements and nanocrystalline permanent magnets were presented. The microstructure of the magnets significantly influences the static properties like the remanence and the coercive field as well the dynamic properties like the total reversal time.

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