Micromagnetic simulations of magnetization reversal of iron nanowire

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Abstract. Spontaneous magnetization and magnetization reversal of individual Fe nanowire with different diameter (d) and length (l) were simulated using a micromagnetic method. Results indicate that the coercivity of a Fe nanowire thinner than 20 nm approximately increases linearly with the increase of l/d ratio in the range of l/d ≤ 3, instead of 1/d² ratio as reported in a reference, and reaches a maximum at l/d ≥ 10. At d = 6 nm and l = 200 nm, the coercivity can be as large as 1294 mT. At l = 200 nm, the reversal mechanism significantly depends on the diameter of nanowire, in the subsequence of nucleation, vortex-like nucleation and vortex with the increase of d from 6 nm to 30 nm. At l/d ≥ 10, the rectangle degree of magnetization curve exceeds 0.95, fitting the prediction for the model of infinite cylinder. The rectangle degree decreases gradually with the decrease of l/d, consistent with the reported experimental behaviors of Fe nanowires deposited on AAO templates.

1. Introduction

Nanostructured materials have at least one relevant physical dimension ranging from one to tens of nanometers (e.g., the thickness of a film, the diameter of a wire, the radius of a particle, etc.). In recent years, regularly aligned arrays composed of one-dimensional soft-magnetic nanowires with high uniaxial shape anisotropy have been researched intensively [1-5], due to their potential application in the fields of magnetic storage and magnetic field sensing. By electrochemical deposition, nanowires with uniform diameter ranging from 4 nm to 200 nm can be fabricated into the packed columnar holes in self-assembled porous anodic aluminium oxide (AAO) templates, known as nanoporous alumite membranes [3, 6]. The magnetization reversal mechanisms of these soft-magnetic nanowires also have been investigated by various methods such as calculation, simulation and experiment to understand the interesting high coercivity and vertical magnetic anisotropy [7-9]. For the cylinders with an infinite length, it has been reported that the reversal mechanisms include curling, buckling, rotation in unison [10, 11], and various nucleations [3, 12] subsequently with the decrease of diameter. In this article, we simulate the spontaneous magnetization and magnetization reversal of individual Fe nanowire with finite length by solving Landau-Lifshitz-Gilbert (LLG) equation to investigate the effects of both length (l) and diameter (d) on the magnetic properties.

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2. Micromagnetic model
The micromagnetic simulation was performed by a public domain micromagnetics program developed at the American National Institute of Standards and Technology, known as the OOMMF (Object Oriented MicroMagnetics Framework) [13]. OOMMF is composed of a collection of application programs, each specializing in some task needed as part of the micromagnetic simulation system. The programs work together by providing services to one another. The user controls the launching of programs through the interface provided by a program named as mmLaunch, which is most closely connected to the account service directory. The extensible micromagnetic computation engine, Oxs (OOMMF eXtensible Solver), can solve problems defined on three-dimensional grids of rectangular cells holding three-dimensional spins. By loading a problem definition file written in the extensible format (MIF 2.1), the micromagnetic problem is communicated to the Oxssi (Interactive Interface to Oxs). Oxssi is a client of display/storage application programs for data table and vector field, and is the server of a solver control service for which the only client is mmLaunch. The user can save and display intermediate results, either interactively or via scheduling based on iteration and stage counts. A cylinder-shaped magnet can be specified in conjunction with the scalar field objects and vector field objects via either the Oxs extension object for geometric volume of space, Oxs ImageAtlas, or a user defined procedure for a dot with diameter of \( d \) and length of \( l \).

A finite element method is employed to simulate the spontaneous magnetization and magnetization reversal of individual Fe nanowire (including nanodot) with diameter in the range of \( d = [6, 50] \) nm and length in the range of \( l = [20, 1000] \) nm (but \( l \geq d \)). Wires are separated into uniform cubic meshes with a size of \( 0.2 \times 0.2 \times 0.2 \) nm\(^3\), in the magnitude order of an iron atom. The spontaneous magnetization is evolved from an initial configuration of randomly oriented spins, absence of any external field. The hysteresis loops in external fields along the longitude axis of wire (\( z \)) are subsequently simulated. The wires are assumed as geometrical symmetrical finite cylinders. The material parameters of Fe for simulation include [14]: \( K_1 = 4.8 \times 10^4 \) J/m\(^3\), \( M_s = 1.7 \times 10^6 \) A/m, and \( A = 2 \times 10^{-11} \) J/m\(^2\), where \( K_1 \) denotes the cubic magnetocrystalline anisotropy energy constant with the respective anisotropy directions along \( x, y \), and \( z \). \( M_s \) is the saturation magnetization, and \( A \) is the uniform exchange energy constant.

3. Results and discussion
Figure 1 shows the simulated spontaneous magnetization process of an individual Fe nanowire with \( l = 200 \) nm and \( d = 20 \) nm. Starting from the initial paramagnetic state (the vectors of spins in meshes are randomly aligned, absence of applied field) as shown in figure 1a, the configuration of spins in meshes firstly evolves into small magnetic clusters to minimize the free energy (see figure 1b), and finally becomes a single-domain structure containing precessions of spins (see figure 1c). In all range of chosen \( l \) and \( d \), the structure of spontaneous magnetization is the same single-domain type. The shape anisotropy and cubic magnetocrystalline anisotropy lead to the existence of two stable orientations of the magnetic moment, namely parallel or antiparallel to the wire axis. These orientations correspond to a symmetric potential with two energy minima separated by the barrier of anisotropy.

As the increase of magnetic field applied opposite to the spontaneous magnetization, the energy minima become asymmetric and the barrier decreases. The magnetization will switch irreversibly if the barrier vanishes. Figure 2 gives the \( x-z \) cross-section maps of spin vector at the instantaneity when the reversal is triggered by the respective switching field of Fe nanowires with \( l = 200 \) nm and \( d = 6, 10, 20, 30 \) nm, respectively. The simulation starts at the evolved final state of spontaneous magnetization as shown in figure 1c. At \( d = 6 \) and \( 10 \) nm (figures 2a and 2b), the reversal mechanism is nucleation. In the region of a nucleation, all the spins in an \( x-y \) plane rotate coherently, as the diameter of nanowire is less than the exchange length \( \lambda_x = \sqrt{A/\mu_B M_s^2} \approx 20 \) nm. The reversals nucleate in several regions cross the whole \( x-y \) section, and then the domain walls propagate quickly. With the increase of \( d \), the regions of nucleation move toward the ends of nanowire. Increasing \( d \) to \( 20 \) nm, as shown in figure 2c, the magnetization reversal mechanism transforms to vortex-like nucleation which
initiates only at two ends of nanowire. Different from the ideal nucleation as shown in figures 2a and 2b, the spins in the edges rotate at first, and in a plane of x-y cross section, the rotation angle is different at different position. At \( d = 30 \) nm (about a half of the domain wall thickness for Fe) as shown in figure 2d, the magnetization reversal is controlled by the buckling-like motion of larger vortices, similar to the situation in bulk material. Besides at the ends, the reversals also initiate in the middle sections. The vortices always initiate in the edge instead of the centre.

![Figure 1. Simulation of spontaneous magnetization of an individual Fe nanowire with \( l = 200 \) nm and \( d = 20 \) nm: initial state with randomly oriented spins (a), evolving forward ordered configuration (b) and final state (c, single domain).](image)

![Figure 2. Vector maps of spins at the instantaneity when reversal is triggered in Fe nanowires with \( l = 200 \) nm and \( d = 6 \) (a), 10 (b), 20 (c), 30(d) nm.](image)

Simulated hysteresis loops of Fe nanowires with typical sizes of \( l = 200 \) nm and \( d = [6, 50] \) nm are shown in figure 3. The rectangle degree of hysteresis loop is related to the ratio of length to diameter \( (l/d) \). At \( l/d > 10 \), the rectangle degree exceeds 0.95, consistent with the prediction of the model for an infinite cylinder (announcing that the hysteresis loop of a single wire always has a rectangular shape \([9, 10]\)). With the decrease of \( l/d \), the rectangle degree decreases gradually, agreeing with the experimental behaviors of Fe nanowires deposited on AAO templates \([3]\). At a given \( l \), the coercivity \( (B_c) \) decreases in a wide range with the increase of \( d \). The \( d \) dependence of \( B_c \) at \( l = 200 \) nm is shown as figure 4. At \( d = 6 \) nm and \( l = 200 \) nm, \( B_c = 1294 \) mT, greatly higher than the experimental coercivity \([3]\). This implies that the fabricated nanowires were not long enough, due to the defects. The inset in figure 4 is the replotted \( 1/d \) dependence of \( B_c \), which is approximately proportional to \( 1/d \), instead of \( 1/d^2 \) as reported in the reference \([15]\).

We should focus on discussing the properties of nanowires thinner than a half of the domain wall thickness (in the diameter range of \( d < 30 \) nm), as the magnetic behaviours are different from the behaviours of the bulk material. Figure 5 shows the hysteresis loops of Fe nanowires with \( d = 20 \) nm and \( l = [20, 1000] \) nm. The coercivity increases apparently in the range of \( l = [20, 200] \) nm, and reaches a maximum of 464 mT at \( l \geq 200 \) nm \((l/d \geq 10)\). The \( l \) dependence of \( B_c \) at \( d = 20 \) nm is shown in figure 6. \( B_c \) is approximately proportional to \( l \) in the range of \( l \leq 60 \) nm \((l/d \leq 3)\).
4. Conclusions
The spontaneous magnetization and magnetization reversal of individual Fe nanowire with finite length was simulated to investigate the effects of both length ($l$) and diameter ($d$) on the magnetic properties. The reversal mechanism significantly depends on the diameter. For the nanowires with $l = 200$ nm, the reversal mechanism is typical nucleation at $d = 6$ and $10$ nm with the spins in a plane of $x$-$y$ cross section rotating coherently, as the diameter of nanowire is less than the exchange length. With the increase of $d$, the regions of nucleation move toward the ends of nanowire. At $d = 20$ nm, the magnetization reversal mechanism transforms to vortex-like nucleation, initiating only at the ends of nanowire. At $d = 30$ nm, the magnetization reversal is vortex similar to the situation in bulk material. The vortices always initiate in the edge instead of the centre. The coercivity of Fe nanowire thinner than $20$ nm approximately increases linearly with the increase of $l/d$ ratio in the range of $l/d \leq 3$, and reaches a maximum at $l/d \geq 10$.

![Hysteresis loops of Fe nanowires with $l = 200$ nm and $d = [6, 50]$ nm.](image1)

![$d$ and $1/d$ (inset) dependences of $B_c$ for Fe nanowires with $l = 200$ nm and $d = [6, 50]$ nm.](image2)

![Hysteresis loops of Fe nanowires with $d = 20$ nm and $l = [20, 1000]$ nm.](image3)

![$l$ dependence of $B_c$ for Fe nanowires with $d = 20$ nm.](image4)
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