On The Single Domain Size of Ferromagnetic Cubic Particles By Micromagnetics Simulation

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Abstract The single domain size of ferromagnetic cubic particles are invesgated by micromagnetics simulation. The angular dependence of coercive forces and the angular dependence of hysteresis loops for particles of sizes 250Å, 350Å, 450Å, 500Å, 520Å, 530Å and 550Å are calculated and discussed. For a particle of size smaller than 450Å, it switches mostly in the coherent rotation, for a particle of size 500Å, its magnetization reversal resembles the incoherent fanning, while for a particle of size larger than 520Å, its magnetization reversal is due to the wall motion. The single domain size for cubic particle is about 510Å.

key words Micromagnetics Simulation, Ferromagnetic Particles, Single Domain Size
I. Introduction

The theory of micromagnetics using a continuous magnetization vector began with the wall calculation of Landau and Lifshitz\(^1\). The origin and principles of the theory were reviewed and discussed by Brown\(^2-3\). Micromagnetics is an important and challenging field for the computational physicist and is currently in a very high state of activity world-wide. The reasons for this are twofold. Firstly the arrival of large-scale computing facilities in the early 1990's made possible numerical solutions to the micromagnetics problem. This encouraged a number of groups to take on the problem of developing advanced theoretical and computational models for comparison with experimental data. Secondly, and contemporaneously, the technological evolution of a number of important magnetic materials reached a stage at which an increasing detailed understanding of their fundamental magnetic behaviour emerged as being of vital importance. Micromagnetics is essentially a theoretical formalism which enables the prediction of magnetization structures such as domain walls and the investigation of magnetization reversal mechanisms in bulk magnetic materials. As such it forms an important link between atomic scale magnetism and macroscopic phenomena. The technique has been used to the calculation of the magnetization reversal modes in isolated single-domain particles\(^4\), the study of closure domains in recording head materials\(^5\), the calculation of magnetoresistive elements\(^6\), and in simulating force interactions in magnetic force microscopy\(^7\). These efforts are far and wide, and the micromagnetics is currently in a very high state of world-wide activities.

In our previous papers, the effect of mesh size and convergence criterion on the equilibrium magnetization configuration and the switching behavior of ferromagnetic cubic particles are calculated and discussed\(^8-9\). In this paper, the single domain size of cubic particles are investigated by micromagnetics simulation. In the model calculations, the cubic particles are assumed to have uni-

\[axial\text{ crystalline anisotropy with an anisotropy constant of 18500 } \text{erg/cm}^3, \text{ a saturation magnetization of 370 } \text{emu/cm}^3, \text{ and an exchange constant of } 5 \times 10^{-7} \text{erg/cm. Several typical particle sizes such as 250\text{Å}, 350\text{Å}, 450\text{Å}, 500\text{Å}, 520\text{Å}, 530\text{Å}, 550\text{Å} are used in the simulation. } 7 \times 7 \times 7 \text{ mesh and convergence criterion } \epsilon = 10^{-5} \text{ are used in the calculations.} \]

The cubic discretization represents the ferromagnetic continuum by a simple cubic array of interacting closely packed cubic elements (Fig.1). The magnetization within each cubic element is constant but may vary in its direction from cube to cube. The total energy is minimized by successively rotating the magnetization of each cube, untill all of them have been adjusted. Then the process is repeated until no further minimization can be accomplished within experimental error.

![Fig.1 Cubic discretization procedure, D is the particle size, d is the cubic element size.](image)

II. The Model of Micromagnetics Simulation

Classical micromagnetics uses energy functionals for the description of the properties of ferromagnetic materials. The micromagnetic energy of a magnetic particle is written as the sum of
the Zeeman energy \(E_{\text{app}}\), the crystalline energy \(E_{\text{an}}\), the exchange energy \(E_{\text{ex}}\), and the magnetostatic interaction energy \(E_{\text{mag}}\):

\[
E_{\text{app}} = -M_s \int_V (\alpha \mathbf{t} + \beta \mathbf{j} + \gamma \mathbf{k}) \cdot \mathbf{H}_{\text{app}} dV
\]

\[
E_{\text{an}} = \int_V W_0 dV
\]

\[
E_{\text{ex}} = \int_V A[(\nabla \alpha)^2 + (\nabla \beta)^2 + (\nabla \gamma)^2] dV
\]

\[
E_{\text{mag}} = -\frac{1}{2} \int_V \mathbf{H}_d \cdot \mathbf{M} dV
\]

where \(\mathbf{M} = M_s(\alpha \mathbf{t} + \beta \mathbf{j} + \gamma \mathbf{k})\) is the magnetization vector, \(\mathbf{H}_{\text{app}}\) is the applied field, \(\alpha, \beta, \text{and}\ \gamma\) are the directional cosines of the magnetization \(\mathbf{M}\), \(W_0\) is an expression of the local crystalline energy density for the uniaxial case with easy axis along the z-direction, \(W_0 = K_1 \sin^2 \theta\), \(K_1\) are the anisotropy constants, \(\theta\) is the angle between z-direction and the direction of the magnetization, \(\mathbf{H}_d\) is the demagnetizing field from \(\mathbf{H}_d = -\nabla U\) and can be calculated from magnetostatic volume and surface charges. The magnetostatic volume charges are given by \(-\nabla \cdot \mathbf{M}\), and the magnetostatic surface charges are given by \(\mathbf{n} \cdot \mathbf{M}\), where \(\mathbf{n}\) is the unit vector normal to the surface.

The equilibrium state of a particle corresponds to a minimum of the free energy, expressed by \(\partial E_{\text{tot}}/\partial \phi = 0\), where \(\phi\) is the angular coordinate of the magnetization vector, or equivalently by the vanishing at all points of the forces \(\mathbf{T} = \mathbf{M} \times \mathbf{H}_{\text{eff}}\) exerted on the magnetization, where \(\mathbf{H}_{\text{eff}}\) is the effective field, which is defined as the negative functional derivative of the total free energy with respect to the magnetization vector

\[
\mathbf{H}_{\text{eff}} = -\partial E_{\text{tot}}/\partial \mathbf{M}
\]

The \(\mathbf{H}_{\text{eff}}\) can be written as

\[\mathbf{H}_{\text{eff}} = \mathbf{H}^A + \mathbf{H}^K + \mathbf{H}^D + \mathbf{H}^Z\]

\(\mathbf{H}^A\) and \(\mathbf{H}^K\) denote the effective exchange and anisotropy fields, respectively. \(\mathbf{H}^D\) denotes the demagnetizing field, and \(\mathbf{H}^Z\) denotes the applied field.

\[
\mathbf{H}^A = 2A/M_s^2 \nabla^2 \mathbf{M}
\]

\[
\mathbf{H}^K = \frac{2K}{M_s^2} (\mathbf{M} \cdot \mathbf{k})\mathbf{k}
\]

The most time-consuming term in \(\mathbf{H}_{\text{eff}}\) is the demagnetizing field. Several methods have been developed to solve \(\mathbf{H}^D\). As our previous papers, the local demagnetizing tensor is introduced to handle demagnetization field.

The algorithm for the energy minimization is based on the Landau-Lifshitz-Gilbert (LLG) equation without a precession term.

\[
\frac{d\mathbf{M}}{dt} = -\frac{\lambda}{M_s^2} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}})
\]

where \(\lambda\) is the damping constant. For each iterative step the effective field \(\mathbf{H}_{\text{eff}}\) is evaluated for all elements based on the current moment position \(\mathbf{M}_{\text{old}}\). Then for all moments simultaneously their new values are calculated as

\[
\mathbf{M}_{\text{new}} = \mathbf{M}_{\text{old}} - \lambda [\mathbf{M}_{\text{old}} \times (\mathbf{M}_{\text{old}} \times \mathbf{H}_{\text{eff}})]
\]

The criterion to termination the iterative process is based on the condition

\[
|
\mathbf{M} \times \mathbf{H}_{\text{eff}}\mid \leq \varepsilon
\]

where \(\varepsilon = 10^{-5}\) are used.

III. Results and Discussions

In application of small ferromagnetic particles for recording media, the angular dependence of the switching mechanism is of great importance. The equilibrium magnetization configurations are determined in a critical fashion by both the absolute value and the direction of the applied field. In this section, seven cubic particles are chosen to depict the behavior of small cubic ferromagnetic particles under the application of an applied field tilted with respect to the easy crystalline axis. Fig.2 shows the dependence of the coercive force on the angle \(\theta\) of the applied field for particle sizes 250Å, 350Å, 450Å, 500Å,
520Å, 530Å, 550Å. In order to obtain a reliable results, a large applied field is used in the calculations. The curves for 250Å, 350Å, 450Å resembles the corresponding one for a Stoner-Wohlfarth particle. The shape of the hysteresis loops for various angles is very much like the corresponding loop shape of a Stoner-Wohlfarth particle (Fig.3, Fig.4, Fig.5).

Fig.2 Angular dependence of the coercive force for seven particle sizes

Fig.3 Angular dependence of hysteresis loops for a particle of size D=250Å

![Graph](image1.png)

Fig.4 Angular dependence of hysteresis loops for a particle of size D=350Å

![Graph](image2.png)

Fig.5 Angular dependence of hysteresis loops for a particle of size D=450Å

Angular dependence of the coercive force for D=500Å resembles the incoherent chain-of-sphere fanning model(Fig.2), its angular dependence of hysteresis loops are shown in Fig.6, from which one can see the hysteresis exits even for \( \theta=90^\circ \).
Angular dependence of the coercive forces for D=520Å, 530Å, and 550Å show that for angles of the applied field from 0° to 90°, an increase in the coercive force are calculated, which means if a particle size large than 520Å, its magnetization reversal process is probably due to the wall motion instead of coherent or incoherent ratiations (Fig.2). Fig.7, Fig.8, Fig.9 show the angular dependence of hysteresis loops for D=520Å, 530Å, and 550Å, respectively. As the size of particle increases, the hysteresis increases for larger θ, and there exits rather complicated intermediate states.

From the above discussions, one can conclude that the single domain size of the particle is about 510Å.
IV. ACKNOWLEDGEMENTS

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References


