Micromagnetic Studies of Finite Temperature M–H Loops for FePt-C Media *

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We have recently developed a new micromagnetic method at finite temperature, where the Hybrid Monte Carlo method is employed to realize the Boltzmann distribution with respect to the magnetic free energy. Hence, the hysteresis loops and domain structures at arbitrary temperature below the Curie point T_c can be simulated. The Hamilton equations are used to find the magnetization distributions instead of the Landau–Lifshitz (LL) equations. In our previous work, we applied this method on a simple uniaxial anisotropy nano-particle and compared it with the micromagnetic method using LL equations. In this work, we use this new method to simulate an L10 FePt-C granular thin film at finite temperatures. The polycrystalline Voronoi microstructure is included in the model, and the effects of the misorientation of FePt grains are also simulated.

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Finite-difference-method fast Fourier transform (FDM-FFT) micromagnetic simulations usually include two parts: first, based on a regular mesh, simulate the microstructure of ferromagnetic materials and set proper magnetic parameters for micromagnetic cells in different phases; secondly, solve the motion of magnetic moments using the Landau–Lifshitz–Gilbert (LLG) equation. Using this traditional micromagnetic method we can solve the M–H loops and domain structures at zero or low temperature compared with the Curie temperature, but it cannot give magnetic properties at finite temperature.

Recently we developed a new micromagnetic method based on the hybrid Monte Carlo (HMC) algorithm using the Hamilton equations,[1] which can simulate the hysteresis loops and domain structures at anarbitrary temperature below the Curie point. In Ref. [1] this new method was tested in a simple cube device with a uniaxial anisotropy. In this work, we use this method to simulate more realistic polycrystalline hard magnetic FePt-C HAMR recording media.[2]

The new micromagnetic method based on the HMC algorithm uses the Hamilton canonical equations to find configurations of magnetizations $\{\boldsymbol{M}_i\}$ in micromagnetic cells at certain temperature, following the Boltzmann principle $\exp(-\mathcal{F}/k_{\rm B}T)$, where $\mathcal{F}$ is the magnetic free energy of the material. The Hamiltonian and the Hamilton equations of motion are

$$\begin{aligned} H &= \frac{1}{2}\sum_i V_{\rm c}\boldsymbol{\Pi}_i^2 + \mathcal{F}[\{\boldsymbol{M}_i\}] \\ \frac{d\boldsymbol{M}_i}{d\tau} &= \boldsymbol{\Pi}_i \\ \frac{d\boldsymbol{\Pi}_i}{d\tau} &= -\frac{1}{V_{\rm c}}\frac{\partial\mathcal{F}}{\partial\boldsymbol{M}_i} = \boldsymbol{H}_{\rm eff}^i, \end{aligned} \tag{1}$$

where $V_{\rm c}$ is the cell volume, $\boldsymbol{M}_i$ is the magnetization, and $\boldsymbol{\Pi}_i$ is the conjugate momentum of the magnetization vector in the ith cell. In the HMC method, the conjugate momentum $\{\boldsymbol{\Pi}_i\}$ is generated following a Gaussian distribution or Boltzmann distribution for the kinetic energy $\exp(-V_{\rm c}\sum_i \boldsymbol{\Pi}_i^2/2k_{\rm B}T)$. After solving the Hamilton equations in Eq. (1) with certain steps of virtual time $\delta\tau$, a new set of $\{\boldsymbol{M}_i\}$ is generated, and it is accepted or rejected following the Monte Carlo method. Finally, the distribution of the magnetic moments in all micromagnetic cells will converge to the steady state following the Boltzmann principle $\exp(-\mathcal{F}/k_{\rm B}T)$ at a temperature, and the orbits solved by the LL equations are still the most probable configuration.

As a model, the mean field approximation is used such that the temperature dependent saturation $M_{\rm s}(T)$ equals the Brillouin function with $J = 1/2$. The Curie temperature of L10-FePt is 750 K. The temperature-dependent anisotropy is given by

$$K(T)/K(0) = [M_{\rm s}(T)/M_{\rm s}(0)]^{\eta}, \tag{2}$$

where we choose $\eta = 2$ for the L10-FePt media.[3]

The free energy $\mathcal{F}\{\boldsymbol{M}_i\}$ is almost the same as the conventional micromagnetic model using the LL equations, except that a double-well potential is added,

$$\frac{1}{V_{\rm c}}\mathcal{F} = \varepsilon_{\rm ext} + \varepsilon_{\rm ani} + \varepsilon_{\rm ex} + \varepsilon_{\rm m} + \varepsilon_{\rm W}, \tag{3}$$

where $\varepsilon_{\rm ext}$, $\varepsilon_{\rm ani}$, $\varepsilon_{\rm ex}$, $\varepsilon_{\rm m}$ and $\varepsilon_{\rm W}$ represent the Zeeman energy, anisotropy energy, exchange energy, magnetostatic energy and double-well potential, respectively. The double-well potential $\varepsilon_{\rm W} = \Sigma_i\varepsilon_{\rm W}^i$ will constrain the magnitude of a magnetization for the ith micro-

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magnetic cell $\boldsymbol{M}_i$ around the saturation $M_{\rm s}(i,T)$

$$\varepsilon^i_{\rm W} = [bK_1(i,T)/4M^4_{\rm s}(i,T)][\boldsymbol{M}^2_i - M^2_{\rm s}(i,T)]^2. \quad (4)$$

In the polycrystalline film, there are two values for the saturation $M_{\rm s}(i,T)$: in the crystalline phase inside a grain and in the disorder phase at the grain boundary. In Eq. (4), the parameter b is a dimensionless constant and $K_1(i,T)$ is the first order anisotropy energy constant in the anisotropy energy for tetragonal crystal[4]

$$\varepsilon^i_a = \iiint d^3\boldsymbol{r}\Big\{ -\frac{K_{\rm u1}}{M^2_{\rm s}}(\boldsymbol{M}_i\cdot\widehat{\boldsymbol{k}_c})^2 - \frac{K_{\rm u2}}{M^4_{\rm s}}[M^2_{\rm s} - (\boldsymbol{M}_i\cdot\widehat{\boldsymbol{k}_c})^2]^2 - \frac{K_{\rm c}}{M^4_{\rm s}}(\boldsymbol{M}_i\cdot\widehat{\boldsymbol{k}_a})^2(\boldsymbol{M}_i\cdot\widehat{\boldsymbol{k}_b})^2\Big\}, \quad (5)$$

where $\widehat{\boldsymbol{k}_a}$, $\widehat{\boldsymbol{k}_b}$ and $\widehat{\boldsymbol{k}_c}$ are the axes of the tetragonal unit cell. In the L10-FePt crystalline grain, the anisotropy mainly comes from the structure of Fe and Pt layers, $K_{\rm u1} = 6.6\times10^7\,{\rm erg/cm^3}$ is the first order parameter, and $K_{\rm u2}$ and $K_{\rm c}$ are small quantities compared with $K_{\rm u1}$, which are neglected as higher order parameters in this study.

In this work, we use the FDM-FFT method to simulate the polycrystalline thin film media at finite temperature. A square film of $64\times64\times10\,{\rm nm^3}$ is divided by a regular mesh with cells $(1\,{\rm nm})^3$ or $(1.25\,{\rm nm})^3$. The periodic boundary condition is applied in-plane. The L10 FePt-C granular film model with the Voronoi tessellation method[5] is shown in Fig. 1. The granular surface morphology is also taken into consideration. The grain boundary width is approximately the micromagnetic cell size.

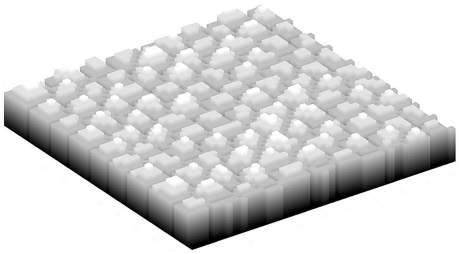

Fig. 1. A square film of $64\times64\times10\,{\rm nm^3}$ is divided by cells of $1\,{\rm nm^3}$. The average grain pitch is 7 nm, and the average grain boundary width is 1 nm.

The crystalline grains (FePt phase) in media are segregated by the disorder grain boundary (C-rich phase) to reduce the exchange among grains, thus the magnetic parameters in crystalline grains and at the disordered grain boundary are different. In crystalline grains, the saturation magnetization $M_{\rm s}$ at 0 K is 1138 emu/cc, the exchange constant A^* is $0.5\times10^{-6}\,{\rm erg/cm}$, and the first order anisotropy energy K at 0 K is $6.6\times10^7\,{\rm erg/cm^3}$. At the disorder grain boundary, the parameters are $0.1M_{\rm s}$, $0.9K$, $0.02A^*$, respectively. The axis of anisotropy should be perpendicular to the film plane for the recording media. However, in consideration of the substitutional disorder and other defects, we assume that the easy axis has a distribution in the form of $p(\theta) = C\exp(-\alpha\sin^2\theta)$, where θ is the angle between the easy axis and the normal vector of the film.

The hysteresis loops of FePt-C media are simulated at different temperatures. The physics behind the hysteresis loop simulation by the HMC micromagnetic method is that the complicated magnetic energy manifold of the magnetizations $\{\boldsymbol{M}_i\}$ will converge to the steady state following the Boltzmann principle $\exp(-\mathcal{F}/k_{\rm B}T)$ at a temperature, and this manifold will change with the external Zeeman energy. The double-well potential will constrain $\{\boldsymbol{M}_i\}$ near the sphere defined by $M_{\rm s}(T)$. With a large $H_{\rm ext}$ along the $+z$-axis, the 'north pole' will be the minimum energy state and more magnetizations $\{\boldsymbol{M}_i\}$ will distribute near here. When $\rm H_{ext}$ is decreased to zero and the simulation steps are not too large, $\{\boldsymbol{M}_i\}$ will still distribute near the 'north pole' (this is the cause of the nonlinear hysteresis effect) as the remnant state. When $H_{\rm ext}$ is decreased further to along the $-z$-axis, the 'south pole' will be the minimum energy state, and $\{\boldsymbol{M}_i\}$ will move following the Hamilton equations to distribute near the 'south pole', and thus a switch is achieved. The Boltzmann distribution $\exp(-\mathcal{F}/k_{\rm B}T)$ is related to T, thus the loops are temperature dependent.

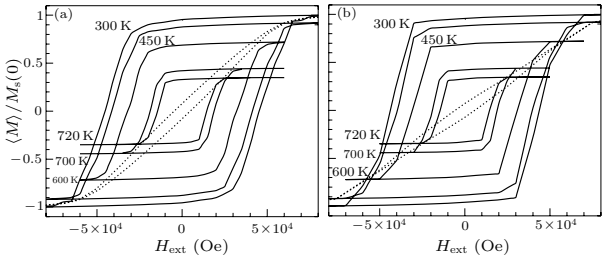

Fig. 2. Simulated M–H loops at different temperatures for the FePt film ($T_{\rm c} = 750\,{\rm K}$). (a) The M–H loops of grain boundary $A^*_{\rm gb} = 0.02A^*$, and (b) $A^*_{\rm gb} = 0.25A^*$. Solid lines are perpendicular loops while the dashed line is an in-plane loop at 300 K.

We find a set of parameters to simulate the M–H loop that are quite similar to the experimental results of Ref. [2], the average grain pitch is 7 nm, the grain boundary width is 1.25 nm, the orientation distribution coefficient α is 1.5 in grain and 0.3 at the grain boundary. The M–H loops at 300 K, 450 K, 600 K, 700 K and 720 K respectively, and the simulation results are plotted in Fig. 2(a). The simulated coercivity and the coercive squareness are plotted versus the temperature in Fig. 3. The coercive squareness S^* is defined by $\frac{dM}{dH}|_{M=0} = \frac{M_{\rm r}}{H_{\rm c}(1-S^*)}$,[9] where $M_{\rm r}$ is M at $H_{\rm ext} = 0\,{\rm Oe}$.

The exchange constant $A^*_{\rm gb}$ of the grain boundary is an important factor to affect the squareness and the coercive squareness. In the longitudinal recording me-

dia, A^*_{gb} should be as small as possible to isolate the grains and increase the stability and SNR. However, the simulation result of Zhao *et al.*[8] shows that a larger exchange constant A^*_{gb} around $0.25A^*$ will increase the SNR significantly in energy to assist recording, with only 10 grains in a bit. When A^*_{gb} is larger, the exchange field between grains is stronger, the grains are more likely to flip together. Thus the M–H loop has a higher coercive squareness in Fig. 2(b). This result is also confirmed with the former simulation by using the conventional micromagnetic method based on the LLG equation.[6]

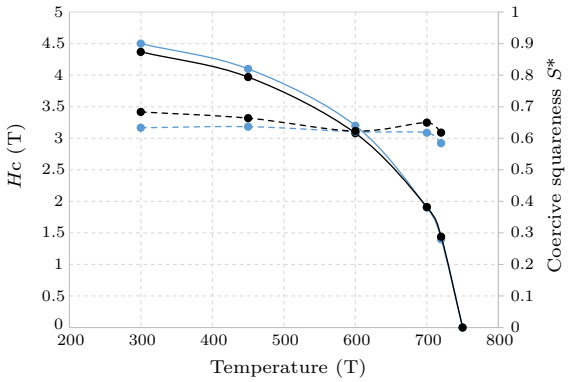

Fig. 3. Coercivity and coercive squareness versus temperature for loops in Fig. 2. The solid lines are coercivity while the dashed line is coercive squareness. The blue lines represent the result of $A^*_{gb} = 0.02A^*$ while the black lines represent $A^*_{gb} = 0.25A^*$. The coercivities in the blue line are 4.5 T, 4.1 T, 3.2 T, 1.9 T, 1.4 T, and the coercivity in the grey line is 4.4 T, 4.0 T, 3.1 T, 1.9 T, 1.4 T.

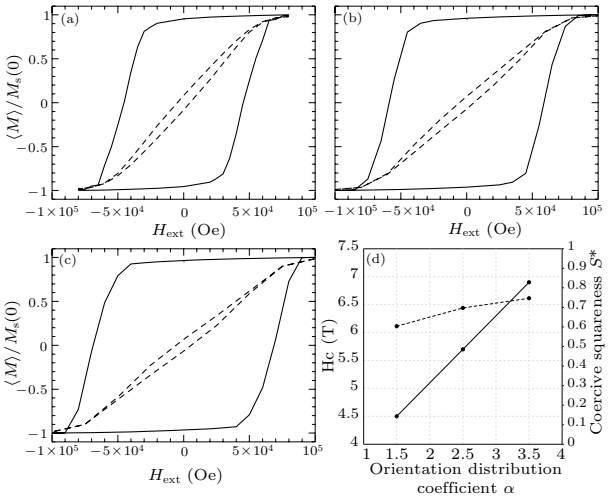

Fig. 4. Simulated perpendicular (solid lines) and in-plane (dotted lines) loops with the orientation distribution coefficient $\alpha = 1.5$ (a), 2.5 (b) and 3.5 (c), and the coercivities are 4.5 T, 5.7 T and 6.9 T, respectively. (d) The coercivities (solid line) and coercive squareness (dotted line).

The effect of orientation distribution is shown in Fig. 4, where the orientation distribution coefficients α are 1.5, 2.5 and 3.5 (K_{u1} is 6.6×10^7 erg/cm^3). The loops with different first order anisotropy constants are shown in Fig. 5, where K_{u1} are 4.0, 5.3 and 6.6×10^7 erg/cm^3 (the orientation distribution coefficient α is 2.5). The results show that reducing K_{u1} or α has a familiar effect on the perpendicular coercivity. The coercive squareness does not change much with K_{u1} while it increases with growing α.

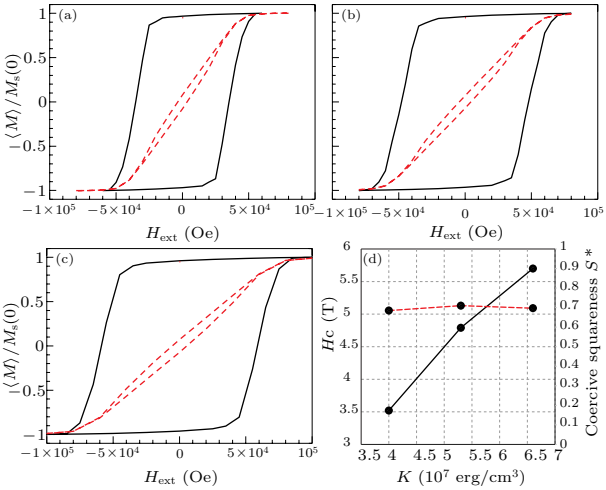

Fig. 5. Simulated perpendicular (solid lines) and in-plane (dotted lines) loops with anisotropy constant $K_{u1} = 4.0$ (a), 5.3 (b) and 6.6×10^7 erg/cm^3 (c), and the coercivities are 3.5 T, 4.8 T and 5.7 T, respectively. (d) The coercivities (solid line) and coercive squareness (dotted line).

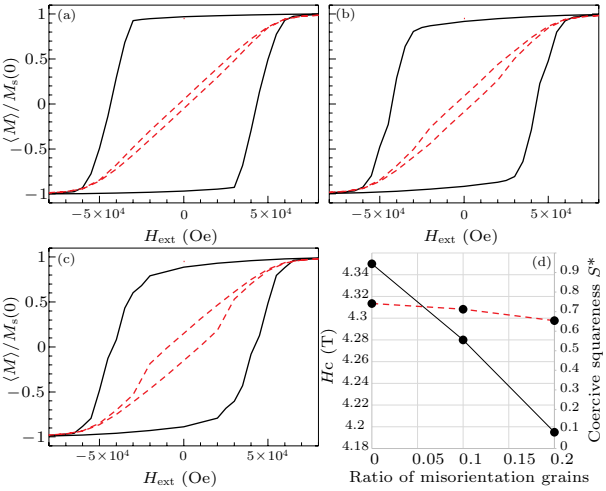

Fig. 6. The M–H loops of FePt films grown on the single crystal MgO underlayer and the polycrystalline MgO underlayer. There are 0% (a), 10% (b), and 20% (c) grains misoriented about 90°, respectively. (d) The coercivities (solid line) and coercive squareness (dotted line).

According to Ref. [2], the orientation maps of FePt-C granular films deposited on the single crystal and polycrystalline MgO underlayer are quite different. There are 10%–20% disorientation grains in the film grown on the polycrystalline MgO underlayer. The anisotropy axes in these grains are almost parallel to the film plane. This situation is also simulated in Fig. 6, the result is confirmed by the experiment. The average grain pitch is 10.22 nm, in Figs. 6(b) and 6(c) the axes of anisotropy of 10% and 20% grains miso-

rient about 90° (where the c-axis is rotated by 90° around the in-plane x-axis and rotated around the z-axis by a random angle ϕ) to simulate the film grown on the polycrystalline MgO substrate. In media with misoriented grains, the coercivity and slope reduce with the ratio of misoriented grains, the perpendicular loop is smoother and the in-plane loop becomes wider because the misoriented grains flip first.

The hybrid Monte-Carlo (HMC) micromagnetic algorithm makes progress in simulating hysteresis loops of the ferromagnetic device at arbitrary temperatures. In this work, we further apply the HMC MuMag method on the polycrystalline FePt-C media and the simulation result is confirmed with experiment.[2,7] At low temperature the result of simulations is also confirmed by using the LLG equations.[6] Further, we simulate the hysteresis loops with a higher inter-grain exchange $A^*_{\rm gb} = 0.25A^*$, and it is considered to be better for energy assist recording. It is confirmed in this study that this method works well for polycrystalline hard films.

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