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# Simulation of $M$–$H$ Loops in FeCo Polycrystalline Thin Films at Finite Temperatures *

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*We apply the hybrid Monte Carlo (HMC) micromagnetic method to FeCo soft magnetic polycrystalline films and test the new method by comparing with the result worked out by micromagnetics using Landau–Lifshitz–Gilbert equations, and the magnetic properties of FeCo films are understood better by carefully considering the effects of polycrystalline microstructures. The hysteresis loops of the FeCo film from low temperature up to 1100 K are simulated by the new HMC micromagnetic method.*

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FeCo polycrystalline thin films are often used in hard disk write heads, TMR sensors, and magnetoresistive memory devices. FeCo alloy has highest intrinsic saturation magnetization and low anisotropy energy constant. The magneto-elastic effect related to the underlayer is also very significant in the FeCo film. Wang *et al.* have simulated the $M$–$H$ loops of FeCo films by conventional micromagnetics using the Landau–Lifshitz–Gilbert (LLG) equations,[1] where the magnetic parameters in micromagnetic cells inside the crystalline grain and at the disorder grain boundary are considered separately. Recently, in magnetic recording or magnetic memories, there are new requirements to understand the magnetic properties of FeCo films at finite temperatures. Wei *et al.* have brought up a new hybrid Monte Carlo (HMC) micromagnetic method based on the Hamilton equations to simulate the magnetic properties at finite temperatures,[2] and it has been applied in the hard magnetic L10-FePt polycrystalline thin films successfully. Here we would like to apply HMC micromagnetics in FeCo films.

First, we introduce the HMC micromagnetic method briefly. Like the conventional micromagnetic method using LLG equations, we build a model for magnetic materials on regular mesh divided by micromagnetic cells, but Hamilton canonical equations are used in the new method instead of LLG equations. The input parameters such as saturation magnetization $M_s$ and the anisotropy constant $K$ vary with temperature. In the $i$th cell, a pair of conjugate variables: the magnetization $\boldsymbol{M}_i$ and its momentum $\boldsymbol{\Pi}_i$ are iterated following the Hamilton equations. The conjugate momentum $\{\boldsymbol{\Pi}_i\}$ is generated following a Gaussian distribution at certain temperature. With Hamilton equations and the Monte Carlo method, the set of the magnetic moments $\{\boldsymbol{M}_i\}$ will converge to a metastable state at a given temperature, following the Boltzmann principle $\exp(-\mathscr{F}(\{\boldsymbol{M}_i\})/k_{\rm B}T)$.

The free energy $\mathscr{F}(\{\boldsymbol{M}_i\})$ is almost the same as the conventional micromagnetics using LL equations, except that a constraint potential is introduced for $\{\boldsymbol{M}_i\}$, because in HMC micromagnetics the amplitude of $\boldsymbol{M}_i$ is no longer fixed as $M_s$,[2]

$$\frac{1}{V_c}F = \varepsilon_{\rm ext} + \varepsilon_{\rm ani} + \varepsilon_{\rm ex} + \varepsilon_{\rm m} + \varepsilon_{\rm m.s.} + \varepsilon_{\rm W}, \quad (1)$$

$$\varepsilon_{\rm W}^i = [bK_1(i,T)/4M_s^4(i,T)][M_i^2 - M_s^2(i,T)]^2, \quad (2)$$

where $\varepsilon_{\rm ext}$, $\varepsilon_{\rm ani}$, $\varepsilon_{\rm ex}$, $\varepsilon_{\rm m}$, $\varepsilon_{\rm m.s.}$ and $\varepsilon_{\rm W}$ represent for the Zeeman energy, anisotropy energy, exchange energy, magnetostatic interaction energy, magnetoelastic energy and the constraint potential, respectively. The parameters in Eq. (2), the saturation magnetization $M_s(i,T)$ or the anisotropy $K_1(i,T)$ in the $i$th cell, can take two values either for the crystalline phase inside a grain or at the disorder grain boundary.

The FeCo crystal has a cubic symmetry, and the crystalline anisotropy energy is[3]

$$\begin{aligned}\varepsilon_{\rm a} = \iiint d^3\boldsymbol{r}\Big\{ & \frac{K_1}{M_s^4}[(M_i\cdot\hat{k}_1)^2(M_i\cdot\hat{k}_2)^2 \\ & + (M_i\cdot\hat{k}_2)^2(M_i\cdot\hat{k}_3)^2 + (M_i\cdot\hat{k}_1)^2(M_i\cdot\hat{k}_3)^2] \\ & + \frac{K_2}{M_s^6}(M_i\cdot\hat{k}_1)^2(M_i\cdot\hat{k}_2)^2(M_i\cdot\hat{k}_3)^2\Big\}, \end{aligned} \quad (3)$$

where $\hat{k}_1$, $\hat{k}_2$ and $\hat{k}_3$ are the axes of the cubic unit cell. The anisotropy constants $K_1$ and $K_2$ are found to vary with the composition and thermal treatment,[4,5] and the value varies in a large range even in the same composition.

The anisotropy energy constant is very sensitive to temperature. According to Akulov *et al.*[6] and studies since then, the empirical relation between $K_1$ and $T$ is

$$K_1(T)/K(0) = [M_s(T)/M_s(0)]^\eta, \quad (4)$$

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where $\eta = 10$ in cubic crystals. The anisotropy energy constant is also influenced by the order-disorder transition, which cannot be described by this formula. Bozorth[7] shows that both $K_1$ and $K_2$ vary with composition ratio and $K_2$ reaches 0 at about $Fe_{65}Co_{35}$, and in this work we will set $K_2$ to be zero.

The magnetostrictive effect of FeCo is the largest among all the $3d$ transition metals.[8] The strain in the FeCo film comes from the crystal lattice mismatch between FeCo and the substrate. In this model we set the magnetoelastic field in-plane in the layer of micromagnetic cells next to the underlayer, and the related energy is

$$\varepsilon_{\mathrm{m.s.}} = -\frac{1}{2}M_{\mathrm{s}}\iiint d^3\boldsymbol{r}\lambda\sigma_{ll}M_l^2$$
$$\lambda = \frac{\mu_0 M_{\mathrm{s}}}{3}\frac{\Delta H_k(1+\nu)}{\varepsilon Y_{\mathrm{m}}}, \qquad (5)$$

where $\lambda$ is the magnetostriction constant, $\sigma_{ll}$ is the normal stress element of strain matrix, $\Delta H_k/\varepsilon$ is the change in anisotropy when there is strain, $\nu$ is the Poisson ratio, and $Y_{\mathrm{m}}$ is the Young modulus. Notice that $M_{\mathrm{s}}\Delta H_k \propto \Delta\varepsilon_{\mathrm{a}}$, therefore in this work we assume that $\lambda$ has the same temperature dependence as $K_1$.

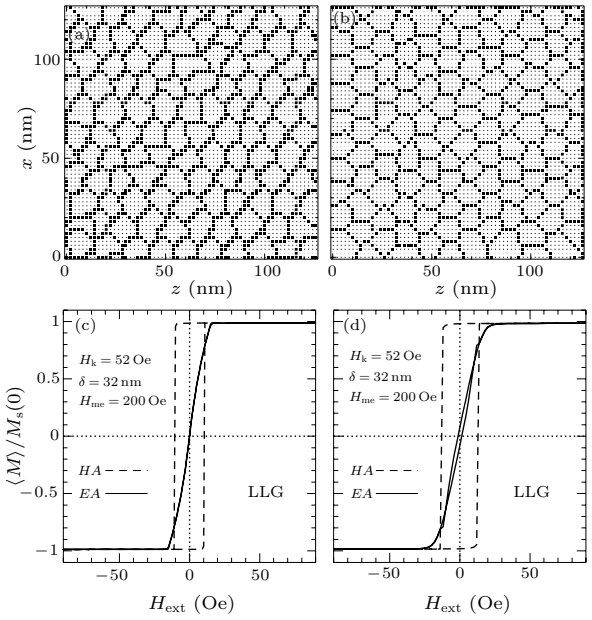



**Fig. 1.** The micromagnetic cells at grain boundary, generated by the random grain growth (a) or by the Voronoi tessellation method (b). Both (a) and (b) have (110) texture, and the ⟨001⟩ directions in different grains are random. The micromagnetic cell size is $(2\,\mathrm{nm})^3$, the film thickness is 16 nm, the grain pitch is 11 nm and the grain boundary width is 1.9 nm. The corresponding in-plane hysteresis loops along the easy (dashed line) and the hard (solid line) axes simulated by micromagnetics using LLG equations are shown in (c) and (d), corresponding to microstructures in (a) and (b).

At 0 K, in a crystal grain, the saturation $M_{\mathrm{s}}$ is 2.4 T, the anisotropy energy constant $K_1$ is chosen as $10^4$–$10^5\,\mathrm{erg/cm^3}$, and the exchange constant $A_1^* = 0.764\times10^{-6}\,\mathrm{erg/cm}$. At grain boundary, the saturation $M_{\mathrm{s}}' = 0.95M_{\mathrm{s}}$, the anisotropy constant $K_1' = 0.9K_1$, and the exchange constant $A_2^* = 0.1A_1^*$. The magneto-elastic field on the first layer is $H_{\mathrm{me}} = \lambda\sigma_{zz} = 200\,\mathrm{Oe}$ along the $z$-axis (easy axis). The influence of parameters on grain boundary have been discussed in a former work,[10] where the grain boundary saturation $M_{\mathrm{s}}'$ has to be greater than 0.9 Ms to reveal soft properties, and the hysteresis loops simulated by parameters chosen in this study agree with experiments.[11,12] At higher temperature, in this work we use a simplified model to assume that $M_{\mathrm{s}}(T)$ varies as the mean field Brillouin function, and $K_1(T)$ varies as Eq. (4).

In Ref. [1], the microstructure in FeCo films was generated by the random grain growth, as shown in Fig. 1(a). Wang *et al.* have developed another Voronoi tessellation method to simulate the polycrystalline microstructure,[9] as shown in Fig. 1(b). We find that the simulated FeCo loops in Figs. 1(c) and 1(d) are slightly different using the two microstructures, especially for the loop along the hard axis, because the magnetic parameters are different in the crystalline grain and at the disordered grain boundary, and the detail of the polycrystalline microstructure such as the arrangement of the grain boundary cells is important for the magnetic properties.

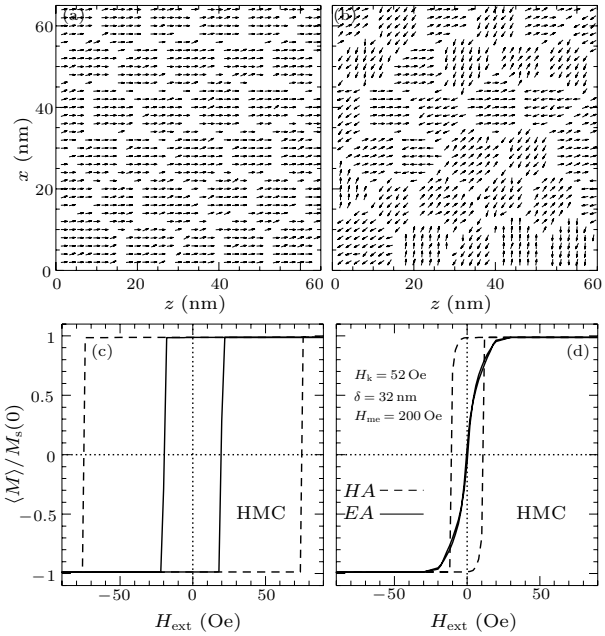



**Fig. 2.** Hysteresis loops of FeCo films at 300 K simulated by the HMC micromagnetic method. The polycrystalline microstructure is generated by the Voronoi tessellation. Here (a) and (b) only show a part of the microstructure in Fig. 1(b), and the arrows represent the in-plane ⟨001⟩ directions of the cubic unit cell, while the ⟨110⟩ direction is perpendicular to the film plane. The microstructure in (b) is for a typical polycrystalline film, and the magnetic structure in (a) is given as a comparison. The results in (d) are similar to the results in Fig. 1(d) using LLG equations.

The $M$–$H$ loops of FeCo films can also be simulated by the new HMC micromagnetic method. At

very low temperature, with the same polycrystalline micro-structure, the conventional micromagnetics using LL equations and the HMC micromagnetics give the same $M$–$H$ loops. A typical polycrystalline FeCo film with a {110} texture is shown in Fig. 2(b), while the cubic anisotropy axes in different grains are set in the same direction in Fig. 2(a) as a comparison. The easy axis and hard axis coercivities in Fig. 2(c) with respect to the microstructure in Fig. 2(a) are both much larger than the coercivities in the typical polycrystalline FeCo film in Fig. 2(d). This helps us to understand why the coercivity of the polycrystalline FeCo film is much smaller than the cubic anisotropy $H_k = 2K_1/M_s$. The easy axis coercivity of the entire film is the mean effect of the anisotropy of all the grains. If the anisotropy axes of the grains distribute randomly, the effect of cubic anisotropy is almost isotropic in plane, and the easy axis is determined by the magneto-elastic field between the FeCo layer and the underlayer. Since different cubic unit cell orientations in different grains make the cubic anisotropies cancel with one another, the coercivity of the FeCo film is more or less determined by the magneto-elastic field at the interface with the underlayer, as seen in Fig. 3. This is the same as our previous work by micromagnetics using LL equations,[1] which verifies that the new method is reliable at low temperature.

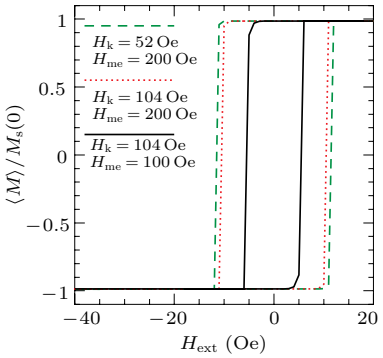



**Fig. 3.** At room temperature (300 K), the in-plane easy axis loops simulated by the HMC micromagnetic method with different cubic anisotropy fields $H_k = 2K_1/M_s$ and magnetoelastic field $H_{me}$ at interface. The grain structure is the same as in Fig. 2(b).

At higher temperatures up to the Curie point, the $M$–$H$ loops can only be simulated by the HMC micromagnetic method, but not the conventional micromagnetic method using the LLG equations. The simulated loops of the polycrystalline FeCo films with a microstructure in Fig. 2(b) are shown in Fig. 4. Here $T_c$ is 1250 K for FeCo. When the temperatures are 300 K, 700 K and 1100 K, and we assume that there is no phase transition up to 1100 K, $M_s(T)$ is given by the mean field Brillouin function, and the easy axis coercivity decreases from 10.5 Oe to 5.4 Oe and then to 0.6 Oe.

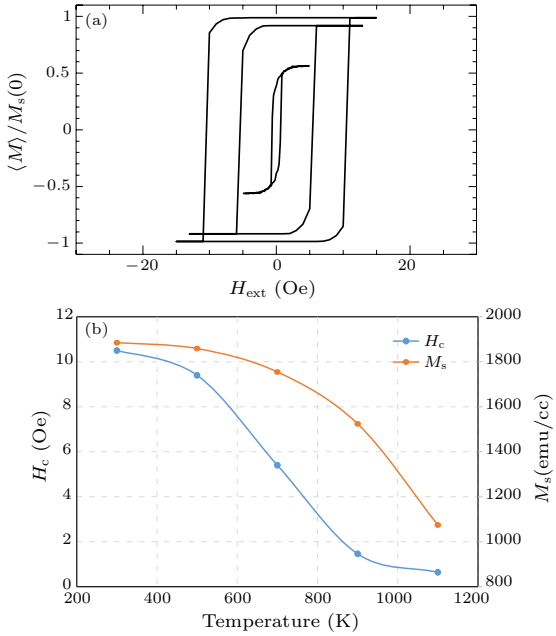



**Fig. 4.** Simulated in-plane easy axis loops by the HMC micromagnetic method at different temperatures for FeCo polycrystalline thin film ($T_c$ = 1250 K). In a mean field model, the saturation magnetization decreases from 1885 emu/cc to 1755 emu/cc and 1074 emu/cc when the temperature increases from 300 K to 900 K and to 1200 K, and the coercivity of FeCo thin films decreases from 10.5 Oe to 5.4 Oe and to 0.6 Oe, respectively. The grain structure is the same as that in Fig. 2(b).

In summary, the HMC micromagnetic method has been successfully applied in the soft magnetic polycrystalline FeCo film. We have verified that the new HMC micromagnetic method is suitable for polycrystalline hard or soft magnetic materials.

## References

[1] Wang S M, Wei D and Gao K Z 2010 *IEEE Trans. Magn.* **46** 1951
[2] Wei D, Song J J and Liu C 2016 *IEEE Trans. Magn.* **52** 7100808
[3] Landau L D and Lifshitz E M 1960 *Eletrodynamics of Continuous Media* (Oxford: Pergamon Press)
[4] Nesbitt E A 1950 *J. Appl. Phys.* **21** 879
[5] Hall R C 1960 *J. Appl. Phys.* **31** 157S
[6] Akulov V N et al 1936 *Z. Phys.* **100** 197
[7] Bozorth R M 1951 *Ferromagnetism* (Princeton: Van Nostrand)
[8] Cooke M D, Wang L C, Watts R, Zuberek R, Heydon G, Rainforth W M and Gehring G A 2000 *J. Phys.* D **33** 1450
[9] Wang L Z, Li J N, Zhao Z, Wei D and Gao K Z 2015 *IEEE Trans. Magn.* **51** 3202304
[10] Xie H L, Zhang K M, Li H J, Wang Y, Li Z H, Wang Y, Cao J W, Bai J M, Wei F L and Wei D 2012 *IEEE Trans. Magn.* **48** 2917
[11] Fu Y, Cheng X and Yang Z 2006 *Phys. Status Solidi* **203** 963
[12] Okada Y, Hoshiya H, Okada T and Fuyama M 2004 *IEEE Trans. Magn.* **40** 2368