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Model of advanced recording media: the angular dependence of the coercivity including the effect of exchange interaction

P. Chureemart,[1] J. Chureemart,[1, a)] and R. W. Chantrell[2]
[1)] *Computational and Experimental Magnetism Group, Department of Physics, Mahasarakham University, Mahasarakham, 44150, Thailand*
[2)] *Department of Physics, University of York, York, YO10 5DD, United Kingdom*

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We use a micromagnetic model based on the kinetic Monte Carlo (kMC) approach to investigate theoretically the magnetic properties of advanced recording media. The model is employed to examine the impact of the magnetostatic and exchange interaction between grains of realistic perpendicular recording media on the angular-dependent coercivity since the exchange field between grains is an important factor in recording performance. The micromagnetic model allows to take the easy axis distribution and the exchange interaction between grains into account. The results confirm the importance of exchange interaction since the variation of coercivity with angle between the applied field and the orientation of easy axis which is perpendicular to the film plane, (θ) is seen to broaden with decreasing exchange field. We show that a two-stage fitting procedure involving the separate determination of the exchange field and easy axis dispersion provides a useful tool for the characterization of media for perpendicular recording and heat assisted recording. We find excellent agreement between previous experimental results and the simulations including exchange interactions leading to estimates of the exchange coupling and easy axis dispersion.

I. INTRODUCTION

Granular perpendicular recording media (PRM) are currently used to store information in hard disk drives[1,2]. The PRM is commonly based on alloys of CoCrPt:SiO_2 where SiO_2 is introduced to create non-magnetic grain boundaries to achieve smaller grain size and to reduce the exchange field resulting in improved signal to noise ratios and increasing areal density[3]. However, complete exchange decoupling between grains would be detrimental since it counterbalances the demagnetizing field and promotes thermal stability. Hence, exchange and magnetostatic interactions may make an important contribution to the recording performance. One of the most critical factors to enhance the recording performance in PRM is the switching field distribution (SFD) which is the dispersion of the field required to reverse the direction of magnetization of each grain. It is crucial to understand the nature of the SFD in order to improve the performance of magnetic recording media. The SFD originates from several factors such as the distribution of the grain size as well as the distribution of composition, i.e., the anisotropy constant, K and saturation magnetization, M_s. However, a large contribution to the SFD comes from the angular dispersion of the easy axis orientation (σ_ϕ) as a small deviation from the perpendicular orientation leads to a large change in the switching field. This leads to a distribution of the intrinsic switching fields which can be described by

$$H_s = \frac{\alpha K}{M_s} \tag{1}$$

where H_s is the switching field of the grain and α is an alignment factor which describes the orientation of the grains. The value of α depends on the crystal structure. In the case of uniaxial structure, the value of α varies from 0.96 to 2.0 for random orientation of the grains and the perfect alignment respectively[4]. Because of the rapid reduction of switching field with angle the effect of easy axis distribution on the magnetic properties is clearly an important factor contributing to the SFD as shown theoretically by Hovorka *et al.* [5].

There have been several works proposing experimental[6,7] and theoretical[8–10] methods to investigate the easy axis distribution. Experimentally, the measurement of crystalline dispersion or *c*-axis dispersion characterized by the full-width half maximum (FWHM) of the X-ray rocking curve[6,7] is often-used. Although the effect of the intergranular magnetostatic and the exchange interaction are significant and complicated for the reversal processes, they are not evident in the crystalline dispersion measurement. Therefore, the measurement of hysteresis properties, for example M/H loops, which include both effects, is often used to investigate the easy axis dispersion. In the past, the variation of remanence technique was often used to investigate the easy axis distribution[6,7,11]. However, this method is highly complex in perpendicular recording media due to the presence of a large demagnetising field, $H_D = -4\pi M_s$ which is difficult to correct using an internal demagnetising field $H_i = H_a - H_D$ where H_a is the applied field and H_i is the internal field,[12–16] essentially because in practice the demagnetising field is not a constant; it varies with the magnetization.

Recently, the angular variation of coercivity technique[17–19] was proposed to measure the easy axis distribution of PRM via comparison with calculations based on the Stoner-Wohlfarth model[20] which is performed under the assumption that each grain reverses via coherent rotation. This is a promising technique due to the fact that the complicating effects of the demagnetizing field vanish at the coercivity. However, neither intergranular exchange nor dipolar coupling is included in this simple calculation which could not explain the behavior of the granular media with incomplete grain boundary segregation. Therefore, advanced micromagnetic modeling will be re-

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[a)] Electronic mail: jessada.c@msu.ac.th

quired to extract the easy axis distribution of the realistic PRM since the previous study[19] indicates the significant importance of the exchange coupling between grains on the variation of coercivity with angle.

In this paper, we develop an advanced micromagnetic model based on the kinetic Monte Carlo (kMC) approach to simulate media including a realistic approach to the introduction of interactions. This approach allows to investigate the effect of intergranular exchange interaction and dipolar interaction and to study the magnetic behavior for the long time scale associated with thermally assisted grain reversal based on the Arrhenius-Néel Law[8,10,21]. We perform simulations of PRM using the kMC model to investigate theoretically the angular dependence of the coercivity including the influence of exchange interaction. The paper is organized as follows. We first outline the basis of the computational model followed by an investigation of the effect of intergranular interactions and easy axis dispersion on the coercivity. Finally we compare the model calculations with previous experimental work in Ref. 19. Good agreement is found between theory and experiment and it is shown that a 2-stage fitting process leads to estimates of the exchange field and standard deviation of the easy axis dispersion.

II. MODEL DESCRIPTION

The microstructure of recording layer models a CoCrPt alloy in which the magnetic grains are separated by the segregation of non-magnetic grain boundaries such as SiO_2 to the grain boundaries. The grain size dispersion of the medium strongly depends on the grain boundaries and the incomplete grain boundary segregation also leads to the intergranular exchange coupling effect[22,23]. Previously, the grains of storage layer were modeled as having uniform grain size as shown in Fig. 1 (a)[24–26]. In order to model more realistic media with irregular shapes of grains separated by non-magnetic material, the Voronoi construction was employed to generate a series of microstructures with specified grain size and grain size distribution[25,27,28]. Grain structures were produced as follows. Starting with a regular hexagonal lattice, the grain centers are shifted randomly within a radius Δ following which the grain structures are produced using the randomized seed points. For large Δ the microstructures become non-physically distorted, but for small Δ the distribution of grain size is approximately lognormal and there is a functional dependence of the standard deviation on Δ, which we have determined numerically and inverted to determine the input Δ value for a required value of σ.

Typical structures of advanced PRM with non-uniform grains produced using a Voronoi construction are illustrated in Fig. 1 (b) and (c). High standard deviation of grain size dispersion results in more non-uniform grains in the recording layer. The magnetization within each grain is assumed to be uniform and a single magnetic moment is used to represent the magnetic moment for each grain, $\mu = M_s V$, where M_s is the saturation magnetization and V is the grain volume.

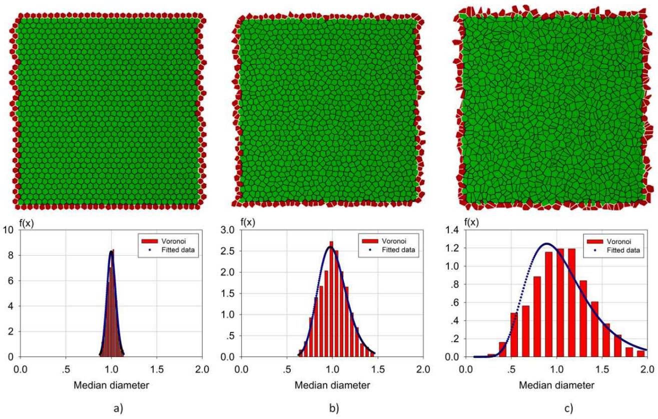
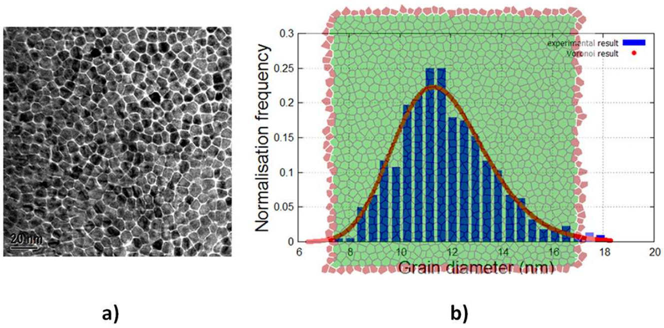


FIG. 1. (Color online) Voronoi construction of PRM with different grain size distributions: a) uniform structure, b) non-uniform case and c) more non-uniform case. Red grains indicate the first layer of translated grains from the imposition of periodic boundary conditions as a visual indication that the PBC are in place.



a)

b)

FIG. 2. (Color online) a) Bright field in-plane TEM image[19] and b)the comparison of grain size distribution between Voronoi and experimental results

To investigate the performance of the real PRM via simulation of the magnetic properties, we construct the recording layer of granular sample in Ref. 19 via the Voronoi construction which produces a physically realistic structure of the film and also provides the information of grain size and grain size distribution. The realistic model system is constructed by a statistical matching to the actual media in terms of grain size and the grain size distribution. Therefore, the granular media were characterized experimentally by in-plane TEM to determine the median diameter and the grain size distribution[19]. To ensure that the microstructure obtained from Voronoi construction modelled closely a realistic medium, we fitted the Voronoi grain size distribution to the actual grain size distribution obtained from in-plane TEM analysis. Fig. 2 b) shows the excellent agreement between the calculated value and the experimental result where the median diameter of the grains is 11.6 nm with the standard deviation of the lognormal distribution $\sigma_{\ln D} = 0.16$. Clearly, the Voronoi microstructure is a good approximation to the structure of a real PRM. Importantly, the Voronoi construction can also provide the configuration information, i.e., the positions, the volumes of the grains as well as the data of intergranular exchange interaction required for the kMC calculation.

In order to investigate the effect of the easy axis distribution of the grains on the angular dependence of the coercivity, we develop a model based on the kMC approach, which allows grain switching with a probability determined using the Arrhenius-Néel relaxation time. The influence of the intergranular exchange interaction and dipolar interaction are taken into account. The granular model consists of many grains whose position and structure are produced by the Voronoi construction. The easy axes of the grains are generated randomly from a Gaussian distribution with specified standard deviation. The behavior of the granular medium is simulated using a kinetic Monte-Carlo (kMC) based model[8], within which the grain dynamics are simulated via a rate equation based on the Arrhenius-Néel relaxation time. The energy barriers to switching are calculated using the free energy of the grain from Stoner-Wohlfarth theory:

$$E = KV(\mathbf{e}\cdot\mathbf{m})^2 - \boldsymbol{\mu}\cdot\mathbf{H}_\mathrm{T} \tag{2}$$

where K is the anisotropy constant, V is the volume of the grain, $\mathbf{e}$ and $\mathbf{m}$ are unit vector of the easy axis and the magnetization respectively and $\boldsymbol{\mu}$ is the magnetic moment of each grain. The total local field acting on each grain, $\mathbf{H}_\mathrm{T}$, is the contribution of the applied field ($\mathbf{H}_\mathrm{a}$), the dipolar field ($\mathbf{H}_\mathrm{dip}$) as well as the intergranular exchange field ($\mathbf{H}_\mathrm{e}$). Therefore, the total field acting on grain i is given by, $\mathbf{H}_\mathrm{T} = \mathbf{H}_\mathrm{a} + \mathbf{H}_\mathrm{dip} + \mathbf{H}_\mathrm{e}$, with

$$\mathbf{H}_{\mathrm{dip},i} = \sum_{i\neq j}\left[\frac{3(\hat{\mu}_j\cdot\hat{r}_{ij})\hat{r}_{ij} - \hat{\mu}_j}{|\vec{r}_{ij}|^3}\right] \tag{3}$$

where $\hat{\mu}_j$ is the unit vector of the magnetic moment of the grain number j, $|\vec{r}_{ij}|$ is the distance and $\hat{r}_{ij}$ is the corresponding unit vector between grains i and j.

The intergranular exchange interaction is formulated as in the work of Peng et.al.[29] under the assumption that the exchange energy is proportional to the contact area between neighbouring grains, taken to be proportional to the contact length L_{ij}. The approach also allows for a dispersion in the exchange J_{ij} due to variations in grain boundary thickness and composition. In terms of reduced parameters (relative to the median values L_m, A_m and J_m), with A_i the cross-sectional area of grain i which are set by the Voronoi construction,

$$\mathbf{H}_\mathrm{e}^{ij} = H_\mathrm{exch}\left(\frac{J_{ij}}{J_\mathrm{m}}\right)\left(\frac{L_{ij}}{L_\mathrm{m}}\right)\left(\frac{A_\mathrm{m}}{A_i}\right)\hat{\mu}_j, \tag{4}$$

where $H_\mathrm{exch} = J_\mathrm{m}L_\mathrm{m}/(a^2M_\mathrm{s}A_\mathrm{m})$ where L_{ij} is the contact length between grains i and j and a is the lattice constant. In practice H_exch is set by the requirement that the average exchange at saturation has a certain value $H_\mathrm{exch}^\mathrm{sat}$, that is;

$$H_\mathrm{exch}^\mathrm{sat} = H_\mathrm{exch}\sum_i^N\sum_{j\in n.n}\left(\frac{J_{ij}}{J_\mathrm{m}}\right)\left(\frac{L_{ij}}{L_\mathrm{m}}\right)\left(\frac{A_\mathrm{m}}{A_i}\right). \tag{5}$$

We note that a similar approach has been used by Miles et. al.[30], who use an intergranular exchange term which is also proportional to $\hat{\mu}_i\cdot\hat{\mu}_j$. However, in ref[30] the exchange is derived from a micromagnetic-like approach under the assumption of a linear variation of the magnetization across the grain boundary, whereas Peng et.al.[29] invoke the Heisenberg form directly. The dependence of the exchange coupling on the intergranular separation can be introduced via J_{ij} using experimental observations, for example Sokalski et al[31] or theoretically[23].

The time evolution of the magnetization is driven by thermal activation over the free energy barrier for a given grain under the influence of the total local field. Thermal activation is introduced into the model via the Arrhenius-Néel relaxation time expressed in terms of an energy barrier (E_b) and attempt frequency (f_0), $\tau^{-1} = f_0\,\exp(-E_\mathrm{b}/kT)$. The attempt frequency is explicitly assumed to be constant with a typical value of 1 GHz[32–34] leading to large energy barriers 25 kT for the slow dynamic magnetization processes typical of hysteresis measurements.

It is important to note that the magnetic moment of PRM with large energy barrier tends to be localized in one or other of the energy minima due to the small transition probabilities. Therefore, the two-state system will be employed[8,21]. To consider the direction of magnetic moment of each grain in PRM, the algorithm starts with calculating the transition probability as the following equation

$$P_\mathrm{t} = 1 - e^{-t_\mathrm{m}/\tau} \tag{6}$$

where t_m is the measuring time and τ is the Arrhenius-Neel relaxation time calculated from energy barrier. The model enables to take the contribution of easy axis distribution into account. Specifically, an approximate expression for the energy barrier with the inclusion of the angular dependence[35] is given by

$$E_\mathrm{b}(\mathbf{H}_\mathrm{T},\psi) = KV[1 - \mathbf{H}_\mathrm{T}/g(\psi)]^{\kappa(\psi)} \tag{7}$$

with $g(\psi) = [\cos^{2/3}\psi + \sin^{2/3}\psi]^{-3/2}$ and $\kappa(\psi) = 0.86 + 1.14g(\psi)$ where the angle ψ denotes the orientation of the easy axis with respect to the total local field ($\mathbf{H}_\mathrm{T}$) acting on the grain. The energy barrier in Eq. (7) is subsequently used to calculate the transition probability in Eq. (6). The magnetic moment of the grain has two states, and the total relaxation time can be obtained from the transition rate between the states, $\tau^{-1} = \tau_{12}^{-1} + \tau_{21}^{-1}$. The transition between states can be considered by comparing the probability P_t with the generated random number $x(0 < x < 1)$. If $P_\mathrm{t} > x$, the grain reversal is allowed. For a grain undergoing switching, the new direction of the magnetic moment with the minimum energy is determined. The kMC algorithm is applied to all grains of the PRM at each field step to investigate the magnetic behavior.

III. RESULTS AND DISCUSSION

To extract the easy axis distribution of real PRM, it is necessary to carry out a comprehensive study of the magnetic behavior of the system with the inclusion of the exchange interaction. We proceed by modeling the physical structure

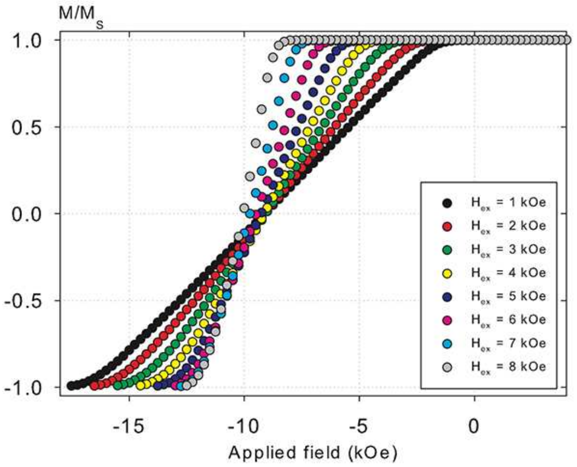


FIG. 3. (Color online) Schematic representation of the typical half hysteresis loop of the perfect alignment case with different exchange interaction fields

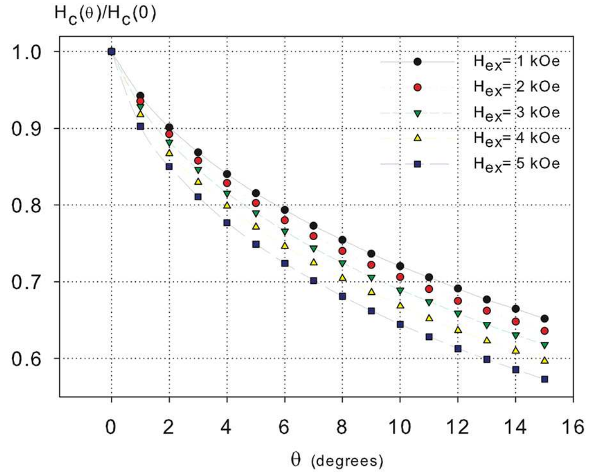


FIG. 4. (Color online) Variation of the normalised coercivity with varying of the exchange interaction and angle θ for the aligned case

of real PRM based on CoCrPt alloy via Voronoi construction with the lateral size of 300 × 300 grains and the thickness of 11.2 nm. In order to remove finite size effects the system size is extended using periodic boundary conditions. The importance of the angular variation of coercivity was pointed out by Miles et. al.[30] in the context of a model for parametric optimisation of perpendicular recording. Here we introduce the dispersion of easy axis dispersion and interactions use the model to develop a two-stage fitting procedure involving the separate determination of the exchange field and easy axis dispersion provides a useful tool for the characterization of media for perpendicular recording and heat assisted recording. We start by consideration of the case of a system with perfectly aligned interaction, which gives results in qualitative agreement with ref[30]

A. Perfect alignment case

In order to establish the intrinsic effect of the intergranular interactions on the variation of coercivity with angle, we consider first the perfect alignment case of $\sigma_\phi = 0^\circ$. The effect of the intergranular exchange interaction on the magnetization reversal process is studied by means of the kMC approach as mentioned previously. The following material parameters are used: the anisotropy constant is 5.1×10^6 erg/cc, the saturation magnetization is 600 emu/cc and the Curie temperature is 700 K. The exchange interaction can be calculated from Eq. (4) by using the exchange strength between grains provided by Voronoi microstructure. The effect of exchange interaction is investigated by varying the average exchange field from 1 kOe to 8 kOe with a field step of 1 kOe. The normalized hysteresis loops with different exchange fields are calculated using the kMC model by applying the external magnetic field in the direction of easy axis, i.e., $\theta = 0^\circ$. As illustrated in Fig. 3, the variation of magnetization with field strongly depends on the intergranular exchange interaction. For a strongly interacting case, it is clear that the slope of the normalized magnetization curve at the coercivity point (H_c) is steeper than that of weak exchange. This is due to the fact that the intergranular exchange interaction field tends to stabilise the magnetisation against the demagnetising field. Interestingly, it can be seen that the value of coercivity is non-monotonic for zero angle; an initial decrease is followed by an increase for strong exchange coupling. This non-monotonic behavior will be investigated shortly; first we illustrate the overall dependence of H_c on the angle with the exchange field H_{exch} as a parameter.

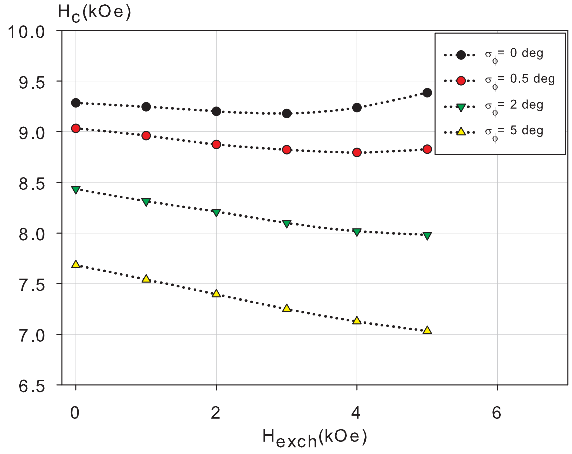


FIG. 5. (Color online) Variation of the normalised coercivity with the exchange interaction for the different easy axis distribution; 0, 0.5, 2 and 5 degrees.

There are a number of factors affecting the magnetic behavior of the system, such as ψ and θ which is the angle between the easy axis acting to the total local field and the external field respectively. Therefore, we have carried out an extensive investigation of the effect of intergranular exchange interaction on the variation of coercivity with angle θ ranging from 0° to 15°. Figure 4 shows the calculation of the coercivity versus the angle θ for various exchange interaction fields up to 5 kOe. The variation of H_c with the decreasing exchange field for the perfectly aligned case ($\sigma_\phi = 0°$) is seen to broaden. This confirms that the intergranular exchange interaction becomes an important factor for the variation of coercivity and cannot be ignored. The previous work in Ref. 19 calculated the variation of coercivity with different easy axis distribution by the approach based on the Stoner-Wohlfarth model in which the exchange interaction and dipolar interaction were not included. As a result, the model could not describe the behavior of real PRM although the easy axis distribution was taken into account.

The non-monotonic behavior referred to earlier is further investigated in Fig. 5 which shows the variation of H_c with exchange field for various values of the orientation of easy axis relative to the field. All orientations show an initial decrease of H_c with H_{exch}. However, the cases $\sigma_\phi = 0°, 0.5°$ show an increase of H_c with H_{exch} for large H_{exch}. The initial decrease is due to the tendency of the exchange to initiate a collective nucleation/propagation mechanism. The increase is probably due to an increase in the effective activation volume of reversal with increasing exchange, which mitigates against thermal activation of nucleation sites and compensates for the initial decrease. Interestingly, the exchange field corresponding to the minimum coercivity shifts to larger values with increasing angle. This suggests that the increase of activation volume with exchange is slower at large angles.

B. Determination of exchange field and easy axis distribution

We now proceed to investigate the coercivity of realistic PRM by including effects of easy axis distribution, intergranular exchange interaction and the dipolar field. To develop a realistic model of a granular medium, the exchange field of recording media is investigated. Subsequently, the effect of the easy axis distribution is introduced via a Gaussian distribution with a standard deviation σ_ϕ allowing its contribution to the magnetic behavior to be investigated. Figure 6 a) shows the kMC calculation of the typical half hysteresis loop at H_{exch} = 2 kOe and $\theta = 0°$. The effect of the easy axis dispersion is investigated by varying the standard deviation from 0° to 5°. It is found that the easy axis distribution affects only the value of coercivity but not the form of the hysteresis loop. The coercivity is decreased with increasing of the standard deviation σ_ϕ[30]. This allows to extract the exchange field and the angular dispersion of easy axes using the following 2-step procedure. Firstly, the intergranular exchange field of realistic PRM can be extracted by fitting the half hysteresis loop of the experiment with simulation results under the assumption of perfect alignment since the form of the loop is not strongly dependent on the easy axis dispersion. The gradient of the hysteresis loop at coercivity depends on the relative strength of the magnetostatic and intergranular exchange fields. The magnetostatic term is dependent on the saturation magnetization, which is accurately known, so the gradient is most sensitive to the exchange field, which can therefore be determined by comparison between simulations and experiment. As illustrated in Fig. 6 b), the half hysteresis loop of the real granular media is in excellent agreement with that of kMC simulation with an exchange field of 2 kOe.

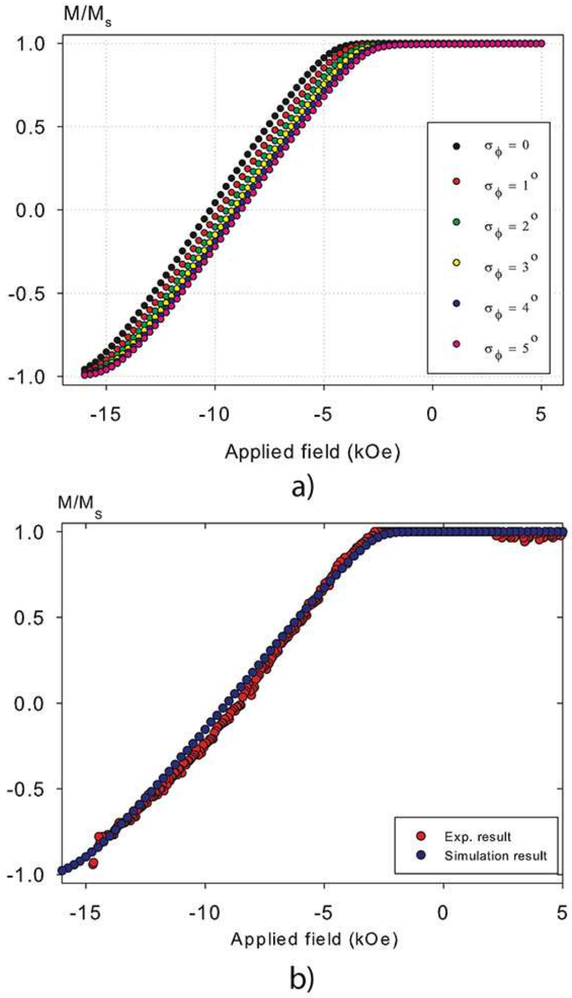


FIG. 6. (Color online) a) The typical half hysteresis loop of kMC calculation at H_{exch} = 2 kOe with the different easy axis dispersion from 0^o to 5^o. b)The comparison of half hysteresis loop between the experimental results and the kMC calculation at H_{exch} = 2 kOe

We now determine the easy axis distribution of the medium of Ref. 19 using the variation of the normalized coercivity with the angle, $H_c(\theta)$. This is achieved by comparing calculations using the kMC approach with the experimental results given in Ref. 19. The intergranular exchange field is taken as 2 kOe from the first stage of fitting, i.e. the determination of the exchange field from the slope of the hysteresis loop. The effect of easy axis distribution (σ_ϕ) is also included in the model by varying the angle σ_ϕ from 1° to 8° in order to compare with the experimental results. Figure 7 shows the kMC calculation of the coercivity as a function of the angle θ. For

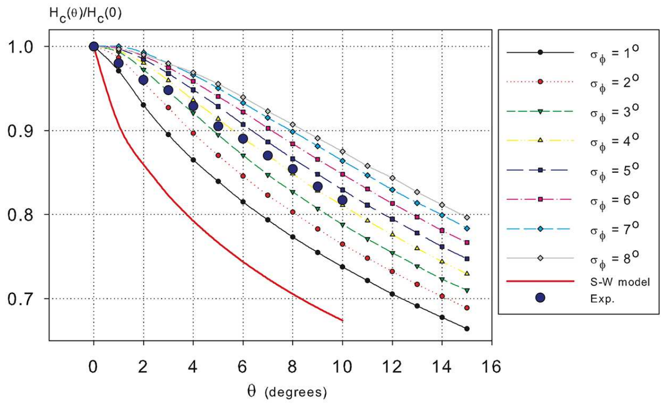


FIG. 7. (Color online) Variation of coercivity with angle θ from the experimental results[19], S-W model and kMC calculations

comparison we include the Stoner-Wohlfarth model prediction for granular medium with the narrow easy axis distribution and without the inclusion of intergranular exchange and dipolar interactions. As demonstrated, the variation of H_c is seen to broaden as the easy axis distribution increases which is due to the combined effect of the orientation distribution and exchange interaction. In practice, the easy axis distribution and the intergranular exchange interaction strongly affects the behavior of the real PRM. The experimental result is in excellent agreement with the kMC calculation with an easy axis distribution of $\sigma_\phi = 4^\circ$ and the exchange interaction field of 2 kOe, both of which are reasonable values. The results confirm that the exchange interaction effect is an important factor for the behavior of advanced recording media.

IV. CONCLUSION

We performed calculations using a kMC model including the intergranular exchange field and dipolar fields in order to extract the easy axis distribution of the real PRM since the Stoner-Wohlfarth model cannot adequately describe the magnetic behavior of real PRM due to the effect of the intergranular exchange interaction. The physical structure of the granular media in Ref. 19 is modeled via a Voronoi microstructure and the magnetic behavior of the media is then simulated by means of the kMC approach taking into account the intergranular magnetostatic and exchange interaction. The variation of coercivity with angle θ for different easy axis distribution was calculated. The result demonstrates a significant effect of the exchange interaction on the variation of the coercivity. The experimental result is compared with the simulated result to achieve the easy axis distribution.

The fitting approach is based on a 2-stage procedure. Firstly we use the dependence of the slope of the hysteresis loop at coercivity on the exchange coupling and its weak dependence on the easy axis dispersion to determine the exchange field. Simulations of the angular dependence of H_c, dependent on both exchange field and easy axis dispersion, are then used to determine the easy axis dispersion by fitting to experiment using the previously determined value of the exchange field. The experimental measurements on granular media in Ref. 19 are fitted well to the simulated results with an easy axis distribution of $\sigma_\phi = 4^\circ$ and an exchange interaction field of 2 kOe, both of which are reasonable for current recording media. Thus it is suggested that the fitting of the kMC model calculations to experimental data is potentially a useful characterisation tool for the determination of exchange fields and angular dispersion of practical media for perpendicular magnetic recording. Finally, although the method was developed specifically for perpendicular recording media, this is the geometry adopted for Heat Assisted Magnetic Recording (HAMR). Thus the current approach is likely also to provide an important characterisation tool for HAMR media.

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