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Simulations of magnetic hysteresis loops at high temperatures

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The kinetic Monte-Carlo algorithm as well as standard micromagnetics are used to simulate MH loops of high anisotropy magnetic recording media at both short and long time scales over a wide range of temperatures relevant to heat-assisted magnetic recording. Microscopic parameters, common to both methods, were determined by fitting to experimental data on single-layer FePt-based media that uses the Magneto-Optic Kerr effect with a slow sweep rate of 700 Oe/s. Saturation moment, uniaxial anisotropy, and exchange constants are given an intrinsic temperature dependence based on published atomistic simulations of FePt grains with an effective Curie temperature of 680 K. Our results show good agreement between micromagnetics and kinetic Monte Carlo results over a wide range of sweep rates. Loops at the slow experimental sweep rates are found to become more square-shaped, with an increasing slope, as temperature increases from 300 K. These effects also occur at higher sweep rates, typical of recording speeds, but are much less pronounced. These results demonstrate the need for accurate determination of intrinsic thermal properties of future recording media as input to micromagnetic models as well as the sensitivity of the switching behavior of thin magnetic films to applied field sweep rates at higher temperatures. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4896582]

I. INTRODUCTION

The characterization of magnetic recording media through the study of *MH* loops continues to be an important tool for the evaluation of new designs that hold promise for future high density storage applications. Apart from the primary interest in the coercivity (H_c), other features such as the nucleation (H_n) and saturation (H_s) fields, as well as the slope near H_c are also used as predictors of recording quality. Models of the magnetic recording process often start with parameterizations of recording media *MH* loops through fits to experimental data. This allows for the estimation of fundamental model parameters such as the saturation moment, anisotropy, and various distributions that characterize the thin-film microstructure.[1] The relatively long time scales (minutes) involved in experimental loops are inaccessible through micromagnetic modeling using traditional Landau-Lifshitz-Gilbert (LLG) type dynamic equations for which the longest simulation times span only several μs. An alternative approach to study MH loops and other magnetic recording metrics is based on the kinetic Monte Carlo (KMC) algorithm. The KMC method provides a stochastic model of thermally activated grain reversal based on the Arrhenius-Neel law. This approach has the advantage that it can span much longer time scales than stochastic LLG while using the same microscopic parameters.[2–4] The KMC algorithm therefore complements the LLG method and it has been shown that in regimes where the two methods can be applied they give good agreement.[3]

Evaluation of high anisotropy heat-assisted magnetic recording (HAMR) media[5–8] is of current interest. The KMC approach was recently applied to study HAMR media (Ref. 9, hereafter referred to as I), where a model fit experimental data taken at room temperature using the magneto-optic Kerr effect (MOKE) with an effective sweep rate of $R = 700$ Oe/s yielded a significantly different parameterization than that obtained from LLG with $R = 10^{11}$ Oe/s. The sensitivity of H_c, H_n, and H_s to variations in various model parameters and their distributions was explored using KMC assuming $R = 700$ Oe/s at $T = 300$ K. LLG simulations at these slow sweep rates are simply not feasible.

In the present work, we extend the KMC and LLG simulations reported in I to high temperatures to examine the behavior of FePt-based HAMR recording media *MH* loops at both slow ($R = 700$ Oe/s) and fast ($R = 10^{12}$ Oe/s) sweep rates, corresponding to MOKE and near recording time scales, respectively. The same model parameters used to fit the experimental MOKE data at room temperature in I serve as the basis for this new study. For both KMC and LLG simulations, the magnetization *M*, axial anisotropy *K*, and exchange parameter *A* are assigned a temperature dependence intrinsic to FePt particles.[10,11] Our results show a pronounced dependence on sweep rate that increases as the temperature approaches the effective particle Curie temperature $T_c \simeq 680$ K. Unexpectedly, the slopes of the loops increase as *T* increases. In addition, the impact of distributions in M_s and *K* are also examined.

II. MODEL: KMC vs LLG

Standard LLG simulations give detailed information on the dynamics of grain magnetic moment reversal. The KMC method utilizes the fact that this information is not required for long-time scale equilibrium properties. It is based on the

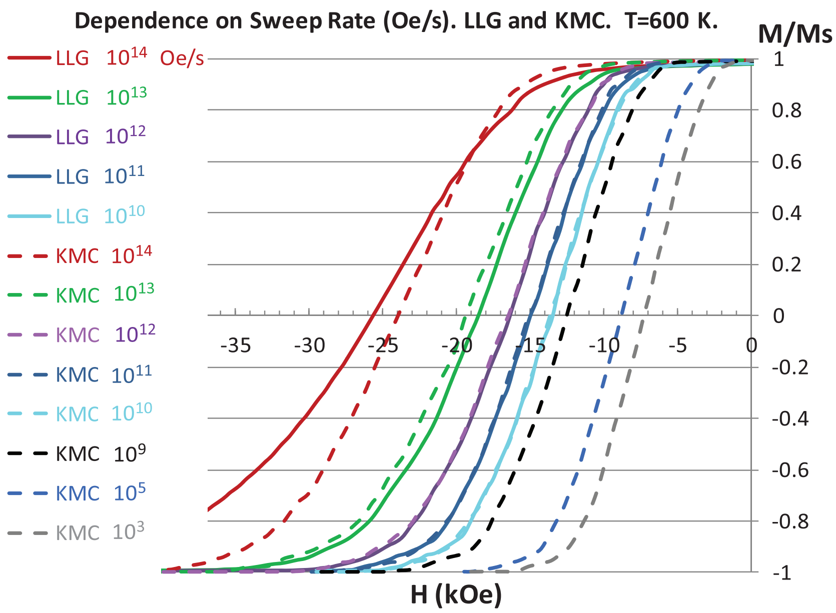

FIG. 1. Comparison of KMC and LLG results for *MH* loops at $T = 600$ K at various sweep rates *R* (in Oe/s).

determination of the time between grain reversal calculated by the Arrhenius-Neel law, which assigns a switching probability to individual grain magnetic moments under the influence of local anisotropy, and an effective field from the other grain moments and the external field.[3,4] Our implementation of KMC uses LLG to relax the system to equilibrium after an individual grain moment is reversed. The Arrhenius-Neel expression for the mean reversal time involves the attempt frequency f_0, which is both field and temperature dependent. Details can be found in Refs. 3 and 4.

As in I, the systems size was set to $32 \times 32 \times 1$ grains and a thickness of 8 nm. (A thickness of 11 nm was reported in I but the actual thickness used in those simulations was 8 nm.) Periodic boundary conditions were used and the full magnetostatic interaction was included. The results of the best fit, using the KMC method at $R = 700$ Oe/s, to the experimental data (with the field applied perpendicular to the film plane) at $T = 300$ K obtained in I were with a grain size having lateral dimensions of 11 nm $\times$ 11 nm, an exchange stiffness between grains of $A = 0.05\,\mu$erg/cm, uniaxial anisotropy $K = 1.67 \times 10^7$ erg/cm^3, saturation magnetization $M_s = 650$ emu/cm^3, Gaussian distributions in K and M_s are assumed to be the same, with a standard deviation of 15%. A Gaussian dispersion in the anisotropy direction with a standard deviation of 6.3° is also used. As noted in I, distributions in the magnetic properties are assumed to also mimic effects of variations in grain size. Intrinsic grain temperature dependence for $M_s(T)$ was based on atomistic simulations of 9 nm diameter FePt particles[12] having an effective Curie temperature of 680 K. Note that there is rounding of thermodynamic properties near T_c due to finite-size effects. The anisotropy[13,14] and the exchange parameter[11,15] were assumed to have a temperature dependence governed by $K(T) \sim M_s^2(T)$ and $A(T) \sim M_s^2(T)$. The magnetization $M_s(T)$, anisotropy $K(T)$, and exchange $A(T)$ values were scaled to the above fitted results at $T = 300$ K. Although a temperature dependence of the damping parameter α has been discussed,[11] we found that this had no impact on the *MH* loops calculated here. A constant value was thus adopted ($\alpha = 0.05$), as in our previous applications of KMC and LLG micromagnetic simulations.[3,4,9]

As a prelude to the examination of the temperature dependence of *MH* loops, we show first a comparison of LLG and KMC at 600 K over a range of values of sweep rate *R* in Fig. 1. The longest LLG run, $R = 10^{10}$ Oe/s took several hours. The next decade slower sweep rate would have taken 10 times longer. Each half-loop with the KMC method took about 2 min to complete (on a standard workstation). Coercivity, saturation, and nucleation fields estimated from these loops are shown in Fig. 2. As emphasized in our earlier work, the KMC approach does not include details of the dynamics of the magnetization switching process that are relevant at short time scales, accounted for by LLG simulations. This difference is responsible for the divergence between KMC and LLG for $R > 10^{13}$ Oe/s. The results show very good agreement between the two methods over the four decades of sweep rate 10^{10}–10^{13} Oe/s (also see Ref. 3) and

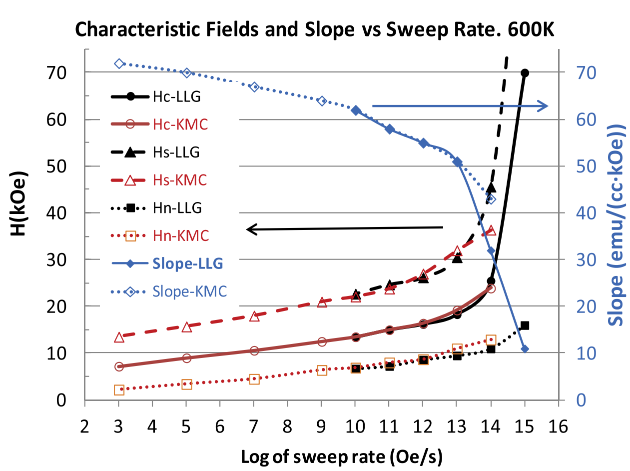

FIG. 2. Comparison of coercivity (H_c), saturation (H_s), and nucleation (H_n) field values as well as slopes near H_c, estimated from Fig. 1.

serves as a validation of our KMC algorithm at higher T. Note that for all three of the characteristic fields, Arrhenius-Néel like logarithmic rate dependence is observed over many decades at the slower sweep rates. Also shown in Fig. 2 are estimations of the slope of the MH loops near H_c, which exhibits a pronounced dependence on sweep rate at this high temperature.

III. TEMPERATURE DEPENDENCE OF *MH* LOOPS

In addition to using the KMC method to make predictions for MH loops at MOKE sweep rates and higher temperatures which are difficult to access with traditional experimental setups, we also examined high temperature loops at a fast sweep rate of $R = 10^{12}$ Oe/s (using LLG simulations) that mimics the changing write field impacting the media during recording. The evolution of loop shapes as T increases at such fast time scales may be a more relevant predictor of recording quality than those at slower sweep rates.

Simulated MH loops over a temperature range 300 K–680 K are shown in Fig. 3. Included are the experimental data from I and the result of the KMC model fit at 300 K. LLG results are shown over the full temperature range whereas the KMC method breaks down at temperature above 620 K. This is due to the fact that an underlying assumption of the KMC method is that the energy barriers $\Delta E/k_BT$ are significantly larger than unity. As T approaches T_c, the anisotropy is reduced and this criterion is no longer satisfied. Fig. 3 shows the same simulation results plotted three different ways that are popular in the literature, M vs H, M/M_s vs H, and M/M_s vs H/H_K (where $H_K = 2K(T)/M_s(T)$). Experimental data are usually represented as curves of M vs H, as in Fig. 3(a). Comparing micromagnetic simulation results for MH loops is usually shown as plots of M/M_s vs H. In the present case, care must be taken in comparing curves involving this normalized quantity since the slope is artificially enhanced with increasing T due to the decrease in $M_s(T)$. This large slope enhancement is seen in Fig. 3(b), but not in Figs. 3(a) and 3(c). The latter representation, M/M_s vs H/H_K, is also common in the presentation of simulation or analytic results based on the non-interacting Stoner-Wolfarth model. In this case, the temperature dependence of the anisotropy normalizes the field. The overall effect is that Fig. 3(c) illustrates the main impact of increasing temperature due to thermal fluctuations between grains. This leads to, for example, a much larger decrease in $H_c(T)/H_K(T)$ at the slow sweep rate compared to the fast sweep-rate results. Note that at the effective T_c, $M_s = 25$ emu/cm^3 was used (estimated from the 9 nm results of Ref. 12), and not zero, due to finite-size rounding. The scaled anisotropy value at T_c is then very small, $K = 2.41 \times 10^4$ erg/cm^3. The LLG loops at this temperature (680 K) seen in Fig. 3(a) appears distorted from the conventional shape.

As well as the coercivity $H_c(T)$, both H_s (defined by field value where $M/M_s = -0.95$) and H_n (defined by field value where $M/M_s = 0.95$) decrease as T increases as shown in Fig. 4. All three of these loop features tend to zero at T_c at the fast sweep rate but the KMC results strongly suggest that they diminish at a lower temperature at the slow sweep rate. This is consistent with thermally activated reversal mechanisms that evolve with time. Note that in contrast to the sketch depicted in Fig. 1 of Ref. 5, there is no flat shoulder region in $H_c(T)$ in near room temperature. Also notable is that the difference in $H_s - H_n$ decreases as T increases, suggesting that the loops become more square-shaped due to thermal fluctuations. Shown in Fig. 4 is the temperature dependence of M_s used in the present simulations.

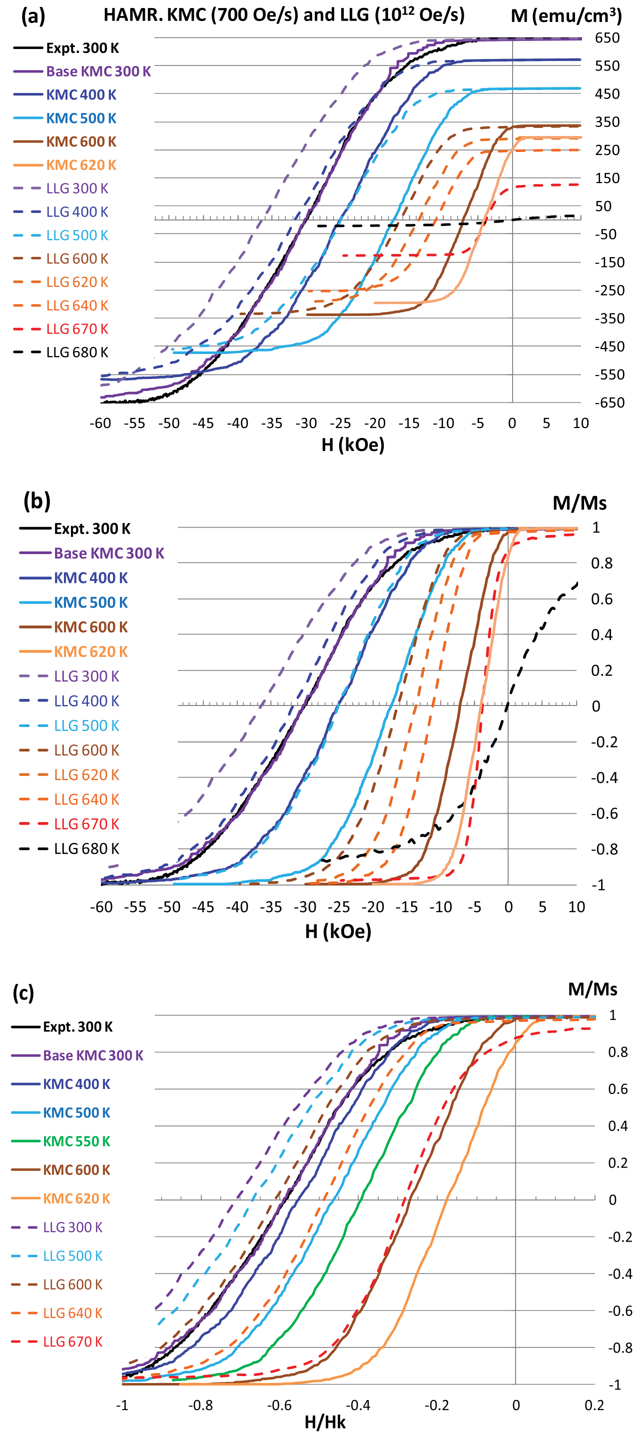

FIG. 3. Three representations of the same simulation results for MH loops at slow and fast sweep rates with increasing temperature: (a) M vs H, (b) M/M_s vs H, and (c) M/M_s vs H/H_K. Fewer loops are shown in (c) for clarity. Note that the similarity between some loops at the different sweep rates for different values T is accidental.

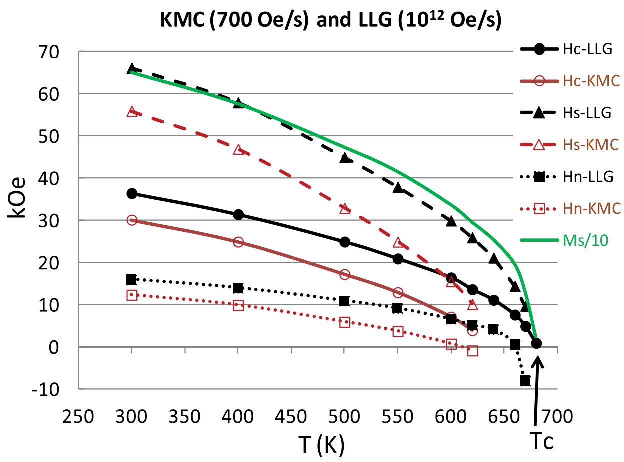

FIG. 4. Nucleation, coercivity, and saturation fields as a function of temperature estimated from Fig. 3. Also shown is $M(T)$ used in the simulations taken from the 9 nm results of Ref. 12.

The results of Fig. 3(a) also illustrate a surprising increase in the slope of the M vs H curves at both sweep rates as T increases. The slope, calculated at the coercivity values, shown in Fig. 5, indicates a dramatically more pronounced increase at the slower sweep rate. It is also known that increasing the Gaussian distribution sigma for M_s and K (always kept equal for both) increases the slope in MH loops (see, for example, I). In addition to the baseline 15% used in all the above simulations, MH loops were also calculated assuming both 10% and 20% sigmas. This effect on the slope vs T in the case of the fast (LLG) sweep rate is also shown in Fig. 5. Similar results were found at the slow sweep rate (not shown).

An increase in slope with temperature was not observed (at least below 350 K) in both the experimental data and KMC simulations of MH loops for Co-based dual-layer media.[4] The dependence of the shape of MH loops on temperature is sensitive to model assumptions. The present approach relies on input for $M_s(T)$ and $K(T)$ associated with the material and geometry of the grains in granular recording

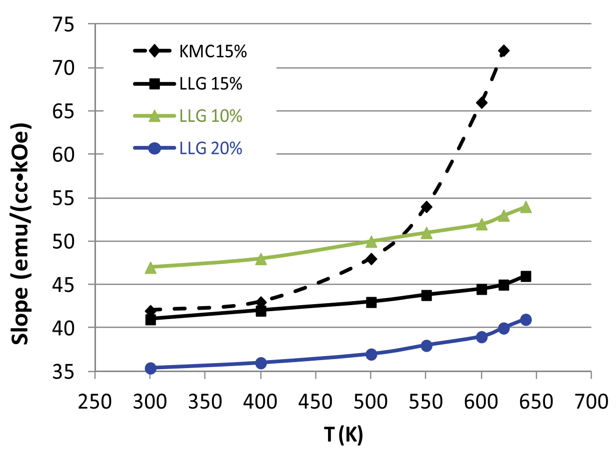

FIG. 5. Slope vs temperature for slow (KMC) and fast (LLG) sweep rates. Also shown is the effect of varying the distribution sigmas on M_s and K for the LLG simulations.

media, modeled as cells in this simulation. For FePt-based materials, these parameterizations are taken from numerous experimental and simulations studies that are all in reasonably good agreement. However, there has been little such characterization for Co-alloys used in recording media. Studies of longitudinal Co-based media are inconclusive on both the temperature dependence of $M_s(T)$ and $K(T)$ but suggest that the scaling relation $K \sim M_s$ might be justified[16] for at least the temperature range $300\,K < T < 450\,K$. If an assumption of scaling $K \sim M_s$ is used in the present KMC algorithm (with all other parameters identical), the slope at H_c is found to decrease with increasing T. These results indicate the importance of using realistic temperature dependences for input parameters when modeling thermal properties in magnetic recording based on HAMR technology.

The simulation techniques used in this work have omitted effects due to thermally induced fluctuations in the magnitude of the grain moments as have been modeled previously through an atomistic approach[7,17–19] or via the Landau-Lifshitz-Bloch (LLB) equations.[20,21] At the slower KMC time scales, it is unlikely the higher-energy fast dynamics associated with the strong inter-atomic exchange interactions will be important. For the faster sweep rates, such fluctuations can impact grain reversal distributions but it is not clear MH loops would be much affected. A previous study comparing atomistic and LLG simulations of HAMR recording write bubbles[7] showed little difference. That work also revealed inhomogeneous grain-reversal mechanisms since atoms near the surface of a grain show reversal before those in the bulk (an effect not captured by LLB). Although the average write bubbles were similar, there was more scatter in the atomistic simulation results. Some of this scatter would likely be captured by an LLB model and indeed relatively small differences between LLG and LLB HAMR recording simulation results for media signal-to-noise ratio have been reported.[22] Further, investigation of the effects of grain-magnitude fluctuations on MH loops at high temperatures close to T_c are desirable.

The grain size used in this work ($11 \times 11 \times 8\,nm^3$) was based on the experimental HAMR media used and is larger than that anticipated for eventual production in hard drives. Thermal fluctuation effects are expected to increase as the grain volume decreases. Preliminary simulations of MH loops using grains of size $7 \times 7 \times 8\,nm^3$, but otherwise identical parameters as used above, show a more pronounced temperature effect (the three field parameters all decrease faster as T_c is approached). Incorporating the faster decrease in the intrinsic grain moment temperature dependence, $M_s(T)$, as well as more rounding near T_c for smaller grains[12] will be of interest for future simulations.

IV. CONCLUSIONS

Increasing interest in HAMR recording technology has necessitated modifications to traditional experimental and modeling tools that will facilitate insight into recording properties at high temperatures. Measurements and simulations previously performed at or near room temperature may not be representative of how bits in the media are formed at temperatures close to 700 K. This includes the traditional manner in which recording media is evaluated, namely, *MH* loops. An additional factor is that the dependence on the rate at which data are recorded is enhanced as *T* increases due to thermally activated magnetic moment reversal. An essential ingredient for the present KMC modeling results is the ability to fit traditional micromagnetic modeling parameters to experimental data at experimental sweep rates. These parameters then provide the basis for simulations that predict *MH* loops at not only elevated temperatures but also at sweep rates relevant to recording data rates. For FePt-based media, our results show a surprising increase in the *M* vs *H* slope as *T* increases at the slow MOKE sweep rate, but much less so at the higher rate representative of recording data. This difference illustrates the importance of sweep rate in switching at high temperatures and the need to exercise caution when making a correlation between experimentally determined *MH* loop shapes (at low sweep rates) and recording (at high sweep rates) performance. A large slope in the recording media *MH* loop has been associated with higher quality bit formation,[23] a feature which may be observed in high-T *MH* loops but not realized under actual recording conditions.

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