Kinetic Monte Carlo Simulations of the Effect of the Exchange Control Layer Thickness in CoPtCrB/CoPtCrSiO Granular Media

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A hybrid kMC/LLG algorithm is used to simulate experimental MH hysteresis loops for dual layer ECC media. The calculation of the rate coefficients and difficulties arising from low energy barriers, a fundamental problem of the kMC method, are discussed and the methodology used to treat them in the present work is described. The results from simulations are compared with experimental data on dual layer ECC CoPtCrB/CoPtCrSiO media. A quantitative relationship between the thickness of the exchange control layer and the effective exchange constant between the layers is demonstrated.

The modeling of MH hysteresis loops of highly anisotropic materials at experimentally relevant temperatures and sweep rates based on standard micromagnetic models represents a significant challenge. Such materials typically show a strong sweep rate dependence as the grain reversal process is dominated by thermal activation involving large energy barriers ($\Delta E \gg k_B T$). As a consequence, the usual stochastic Landau-Lifshitz-Gilbert (sLLG) method [1, 2], that is widely used in micromagnetics to simulate magnetic materials at finite temperature, is simply not feasible because of the long time scales involved. Perpendicular recording media (PRM) used in hard disc drives (HDD) represent an important class of such materials. By characterizing the relaxation process as a sequence of quasi-equilibrium states separated by thermally assisted grain reversals, kinetic Monte Carlo (kMC) provides an alternative approach to sLLG that can be applied to study such materials [3–11].

This work presents results based on a hybrid kMC/LLG formalism, that has been applied to single layer PRM [12], to simulate MH loops of dual layer exchange coupled composite (ECC) media [13]. As shown in earlier work the parameters obtained from fitting experimental MH loops for ECC media from simulations using the kMC/LLG formalism at experimental sweep rates differ significantly from those obtained using stochastic LLG that are limited to sweep rates several orders of magnitude greater than the experimental sweep rates [14]. The simulation results presented here are compared with published experimental VSM studies that examine the effect of the thickness of the exchange control layer (ECL) in CoPtCrB/CoPtCrSiO ECC media [15]. Such measurements and the associated simulation studies represent an important tool in determining the material parameters in order to optimize the competing demands of the areal bit density, writability and stability of ECC media.

The model is based on grains represented by two exchange-coupled Stoner-Wohlfarth particles, which we label as $a$ (cap layer) and $b$ (oxide layer). The energy used in the formalism contains the usual intra-layer exchange, magnetostatic interactions, uniaxial anisotropy, as well as the exchange interactions between the layers within a single grain, characterized by $A$, the cross sectional area of the ECL, and $I$, the interlayer coupling constant.

The simulation of MH loops using the hybrid kMC/LLG approach is described in some detail for both single and dual layer materials in Refs. 12 and 13 which we summarize here. The simulation begins with the system in a fully saturated state with an applied field $H_0$ and is then input into an LLG ($T = 0$) simulation and relaxed to a local minimum energy state, and the interaction field is calculated for each grain. For grains with more than a single minimum energy state we compute the rate constants $r^k_{i \rightarrow j}$ between each pair of minimum energy states based on the Arrhenius-Néel expression

$$r^k_{i \rightarrow j} = f^k_{ij} \exp\left(-\frac{\Delta E^k_{ij}}{k_B T}\right)$$

where the ordered pairs $\{ij\}$ label the minimum energy states in the $k$th grain connected by a minimum energy path (MEP). $\Delta E^k_{ij}$ and $f^k_{ij}$ denote the energy barrier and attempt frequency separating the initial minimum energy state $i$ from the final state $j$. From the rate constant, the set of wait times $t^k_{i \rightarrow j} \log x$, where $x$ is a uniformly distributed random number between 0 and 1, is calculated for each of the grains and the grain with the minimum wait time $t_R = \min[t^k_{i \rightarrow f}]$ is determined. If $t_R$ is less than some user specified time interval $\Delta t$ then a new state at time $t_1 = t_R$ is constructed in which the grain at $k = k_R$, initially in state $i$, is replaced with the grain in state $f$ and the system is allowed to relax to some new local equilibrium with $H = H_1 = H_0 - R t_R$, where $R = |dH/dt|$ denotes the sweep rate. If, on the other hand, $t_R \geq \Delta t$, then the $k$th grain remains in the state $i$ and the system is allowed to relax to some new local equilibrium with $H = H_1 = H_0 - R \Delta t$. This process is repeated generating a sequence of states until the normalized magnetization $M < -M_s$, where $M_s < 1$ is some nominal value used to define saturation. The application of kMC to the case of single layer PRM is relatively straightforward [12].
TABLE I. Parameters used in modelling the cap layer ($M_a$, $K_a$ and $A_a$) and the oxide layer ($M_b$, $K_b$ and $A_b$), where $M$, $K$, and $A$ represent the magnetization, anisotropy and exchange stiffness. Experimental values were extracted from Ref. [15].

<table>
<thead>
<tr>
<th>Layer</th>
<th>$M$</th>
<th>$K$</th>
<th>$A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cap Layer</td>
<td>$M_a$</td>
<td>$K_a$</td>
<td>$A_a$</td>
</tr>
<tr>
<td>Experimental</td>
<td>425</td>
<td>2.20 $\times 10^6$</td>
<td>—</td>
</tr>
<tr>
<td>Simulation</td>
<td>450</td>
<td>2.10 $\times 10^6$</td>
<td>2.0 $\times 10^{-6}$</td>
</tr>
<tr>
<td>Oxide layer</td>
<td>$M_b$</td>
<td>$K_b$</td>
<td>$A_b$</td>
</tr>
<tr>
<td>Experimental</td>
<td>385</td>
<td>3.10 $\times 10^6$</td>
<td>—</td>
</tr>
<tr>
<td>Simulation</td>
<td>385</td>
<td>3.05 $\times 10^6$</td>
<td>0.018 $\times 10^{-6}$</td>
</tr>
</tbody>
</table>

Units (emu/cc) (erg/cc) (erg/cm)

The dual layer case on the other hand presents a number of challenges as described in our earlier study [13] and below.

In the present work, we discretize the unit sphere that describes the state-space of a single spin by triangulating the surfaces of an octahedron inscribed by the unit sphere and projecting the vertices onto the surface of the sphere resulting in a 3-polytope type polyhedron. The location of minimum energy states of the ECC grains are obtained from a deepest descent algorithm. Points that coincide with a certain tolerance are then merged to give the minimum energy states of the grain. All the paths between any two minimum energy states can then be constructed from the edges of the polyhedron and the minimum energy path on the lattice determined using a modified Bellman-Ford algorithm [16]. This provides an initial estimate of the location of the saddle points that can be further refined by fitting the energy surface to a quartic. From this the energy barrier separating the two states and the attempt frequency may be calculated [13].

In addition to the complexity of the energy landscape of dual layer ECC grains, the variation in the energy barriers can give rise to a range of rate constants that span several orders of magnitude. Transitions between states separated by low energy barriers do not contribute significantly to the hysteresis loops at experimental sweep rates as the rapid fluctuations between these transient states mean that they quickly equilibrate, an outstanding problem with the kMC algorithm [17]. The kMC/LLG code used here is programmed to detect the onset of high frequency fluctuations by identifying grains that return to their initial state after $N$ kMC steps (in the present code $N$ is set to 32). When these high frequency fluctuations are detected, minimum energy states that are connected by an energy barrier less than some predetermined threshold are combined into clusters. The kMC is then reformulated in terms of a combination of minimum energy states and clusters [13]. If the fluctuations persist, then the threshold is increased by a factor of 2 until such time as the high frequency fluctuations are suppressed and the time between successive kMC steps is appropriate. The threshold is then gradually reduced until the high frequency fluctuations reappear [13].

In the present model, grains are arranged on a $L \times L$ square lattice with periodic boundary conditions (where $L = 32$). The anisotropy constant, anisotropy axis and the magnetization are assigned grain-to-grain Gaussian distributions of values. Oxide and cap layers were 14 nm and 4 nm thick, respectively, as used in the experimental study [15]. Lateral grain dimensions were 7 nm $\times$ 7 nm. There was no spacer layer in the model. A sweep rate of $R = 7.5\, \text{kOe/s}$ at temperature $T = 300\, \text{K}$ was used in both the simulation and experimental studies. The material parameters used in the simulations that reproduced well the experimental data are shown in Table I and were determined as follows. Assumed values for the intra-layer exchange stiffness parameter, denoted as $A_a$ and $A_b$, were guided by previous modeling results on generic ECC media for the cap and oxide layers, with moderate and weak coupling, respectively [14]. Experimental values for $M_a$, $M_b$, $K_a$ and $K_b$ (see Table I) served as a starting point for these parameters in the MH loop fitting procedure. To simplify fitting the MH loops for the dual layer media, we first fit the kMC loop to the experimental results for only the oxide layer. Best results were achieved using the magnetization and anisotropy values indicated in Table I, along with a 10% variance in $K_b$ and $M_b$ as well as a $4^\circ$ variance in anisotropy axis direction about $z$. The outcome of this procedure is shown in Fig. 1 and illustrates excellent agreement between simulation and experimental results.

![FIG. 1. Normalized magnetization as a function of applied field for the 14 nm oxide layer, CoPtCrSiO, at a sweep rate $R = 7.5\, \text{kOe/s}$ from experimental data (blue) and kMC simulations (red).](image-url)
The MH loops obtained from the simulations shown in Fig. 2 give good quantitative agreement with the experimental data. The discrepancy between the experimental values of $H_s$ and those determined from the simulations is due in part to the shape of the tail of the MH curve in the region $H ≈ H_s$. Fig. 2 also shows that the simulation results underestimate the drop in the magnetization observed at $H ≈ 2$ kOe for $d = 0.05$ nm case.

The distribution of energy barriers for the case of a system allowed to relax to equilibrium from the fully saturated state for $H = 0$ has also been calculated for both the dual and single layer media. This is of particular interest as this distribution is often taken as a measure of thermal stability. We have calculated the average energy barrier $\Delta E = \langle \Delta E_{ik} \rangle$ over an extended range of the interlayer coupling constant $0 \leq I \leq 3.0 \text{erg/cm}^2$, where $\Delta E_{ik}$ denotes the minimum energy barrier separating the initial state $i$ from all possible final states $f$ of the $k^{th}$ grain, with the average $\langle \ldots \rangle$ denoting the average over all grains. The $\Delta E$ values, normalized with respect to the corresponding average calculated for the single layer case, are plotted in Fig. 5. The data show the average relative energy barrier increasing with increasing interlayer coupling constant $I$ thereby increasing stability of
the grains to thermally activated reversal. We note that \( \Delta E \) does not appear to have reached its saturation value corresponding to a completely coherent rotation of the grains \([13]\). Combining the results presented in Figs. 4 and 5 we see that up to \( I = 1.8 \text{ erg/cm}^2 \) \((d = 0 \text{ nm})\), the values of \( H_s \) obtained from the simulations decrease with increasing \( I \) (decreasing \( d \)) while the average energy barrier \( \Delta E \) increases. This is shown explicitly in Fig. 6 showing \( H_s \) vs \( \Delta E/k_B T \) \((T = 300 \text{ K})\). The first six points \((32.5 \leq \Delta E/k_B T \leq 42.5)\), corresponding the range of \( I \) used to fit the experimental data shown in Fig. 2 and show \( H_s \) decreasing with increasing \( \Delta E/k_B T \). Interestingly, however, for higher values of \( I \) the simulations (not shown here) also show \( H_s \) increasing with increasing \( I \), indicating that the minimum in \( H_s \) observed in the experimental data at \( d \approx 1.0 \text{ nm} \) \((I \approx 1.2 \text{ erg/cm}^2)\) in Fig. 4 also appears in the simulations but at a somewhat higher value of \( I \approx 1.8 \text{ erg/cm}^2 \).

\[ \langle \Delta E \rangle_{\text{ECC}}/\langle \Delta E \rangle_{\text{SL}} \]

\[ I \text{ (erg/cm}^2) \]

\[ 0.0 \quad 0.5 \quad 1.0 \quad 1.5 \quad 2.0 \quad 2.5 \quad 3.0 \]

\[ 0.9 \quad 1.0 \quad 1.1 \quad 1.2 \quad 1.3 \quad 1.4 \quad 1.5 \]

\[ H_s (ECC)/H_s (SL) \]

\[ \Delta E/k_B T \]

\[ -20 \quad -15 \quad -10 \quad -5 \quad 0 \quad 5 \]

\[ H (kOe) \]

\[ -1.0 \quad -0.5 \quad 0.0 \quad 0.5 \quad 1.0 \]

\[ M/M_z \]

\[ -0.2 \quad -0.15 \quad -0.1 \quad -0.05 \quad 0 \quad 0.05 \quad 0.1 \]

\[ H (kOe) \]

\[ 30 \quad 35 \quad 40 \quad 45 \quad 50 \]

\[ M_s (ECC) \]

\[ 1.0 \quad 0.9 \quad 0.8 \quad 0.7 \]

\[ H_s (ECC)/H_s (SL) \]

\[ \Delta E/k_B T \]

\[ 0.7 \quad 0.8 \quad 0.9 \quad 1.0 \]

\[ H (kOe) \]

\[ 0.0 \quad 0.5 \quad 1.0 \quad 1.5 \quad 2.0 \quad 2.5 \quad 3.0 \]

\[ 0.9 \quad 1.0 \quad 1.1 \]

\[ \Delta E/k_B T \]

\[ 30 \quad 35 \quad 40 \quad 45 \quad 50 \]

MH loops measured using VSM involve time scales that are several orders of magnitude less than those relevant to the write process in HDD media. We have extended our studies by analyzing MH loops with \( R = 10^7 \text{ kOe/s} \) using sLLG \([18]\) for both the single and dual layer media. MH loops calculated for single layer of CoPtCrSiO for a sweep rate \( R = 7.5 \text{ kOe/s} \) and \( 10^7 \text{ kOe/s} \) are shown in Fig. 6 and show a significant increase in \( H_s \) for the higher sweep rate. Results for normalized values of \( H_s (ECC)/H_s (SL) \) are plotted in Fig. 6 as a function of \( \Delta E/k_B T \). While the value of \( H_s \) calculated for both dual and single layer media for \( R = 10^7 \text{ kOe/s} \) is significantly larger than the corresponding results for \( R = 7.5 \text{ kOe/s} \), a comparison of the results presented in Fig. 6 show that the normalized values of \( H_s (ECC)/H_s (SL) \) track each other reasonably closely for smaller values of \( \Delta E/k_B T \) but start to diverge at \( \Delta E/k_B T \approx 42 \) \((I \approx 1.8 \text{ erg/cm}^2)\) where \( H_s (7.5 \text{ kOe/s}) \) begins to increase while \( H_s (7.5 \text{ kOe/s}) \) drops sharply.

We have presented here a formulation of the kMC algorithm that can be successfully applied to simulate dual-layer recording media at the relatively long time scales relevant to experimental MH loops, that are inaccessible using standard LLG micromagnetic simulations. The results illustrate excellent agreement with a series of experimental measurements on single and dual layer CoPtCrB/CoPtCrSiO granular media. For the first time, a quantitative relation between strength of the interlayer exchange parameter \( I \) and spacer-layer thickness \( d \) is calculated. Extraction of the energy barriers relevant to the thermal stability of the recording layer as a function of the saturation field provides a useful figure of merit for ECC media. Such modeling efforts can serve as useful guidance toward the optimization of this important parameter.

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[18] J. I. Mercer, MagLua is in-house stochastic micromagnetic simulation software with Lua scripting interface. https://github.com/jasonimercer/maglua