Anisotropic Spin Exchange Modeling and Curie Temperature Dispersion in L10-FePt Nanoparticles for HAMR Media

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We developed an anisotropic exchange spin model that accounts for magnetic anisotropy and evaluated the Curie temperature (T_c) dispersion due to finite size effects in $L1_0$-FePt nanoparticles. In heat-assisted magnetic recording (HAMR) media, a next-generation magnetic recording technology, high-density recording is achieved by locally heating $L1_0$-FePt nanoparticles near their T_c and rapidly cooling them. However, variations in T_c caused by differences in particle size and shape can compromise recording stability and areal density capacity, making the control of T_c dispersion critical. In this study, we constructed atomistic LLG models to explicitly incorporate the spin exchange anisotropy of L10-FePt, based on parameters determined by first-principles calculations. Using this model, we evaluated the impact of particle size on T_c dispersion. As a result, (1) the T_c dispersion critical to the performance of HAMR can be reproduced, whereas it was previously underestimated by isotropic models and (2) approximately 70% of the experimentally observed T_c dispersion can be attributed to particle size effects. This research highlights the role of exchange anisotropy in amplifying finite-size effects and underscores the importance of size control in HAMR media.

Index Terms— **Computer simulation, Heat-assisted magnetic recording, Magnetic materials, Nanostructured materials**

I. Introduction

With the rapid growth of cloud-based infrastructure, the global data volume is soaring, presenting challenges to overcome the fundamental limitations of recording density, known as the "Magnetic Trilemma." Heat-Assisted Magnetic Recording (HAMR) has emerged as a promising next-generation technology to tackle these challenges [1,2]. HAMR achieves high-density recording by heating the magnetic particles of the storage medium to near their Curie temperature (T_c) and quickly cooling them, all while maintaining high magnetic anisotropy.

Among the candidate materials, the L10-phase FePt (L10-FePt) stands out due to its exceptionally high magnetic anisotropy constant (Ku) [3]. However, its layered structure leads to strong anisotropic exchange interactions. This results in Curie temperature dispersion caused by variations in particle size, shape, and degree of order, posing critical challenges. Such T_c dispersion causes a mismatch between the writing temperature and the actual Curie temperature of particles, ultimately reducing recording stability and the signal-to-noise ratio (SNR)[4]. Moreover, its impact on areal density capability (ADC) is well-recognized, highlighting the importance of controlling T_c dispersion in HAMR media design.

To address these issues, this study presents an atomistic-scale spin model that incorporates the intrinsic anisotropic exchange interactions of L10-FePt and conducts numerical simulations to investigate T_c dispersion stemming from realistic particle size distributions.

II. Theories and Computational Methods

In $L1_0$-FePt, alternating monolayers of Fe and Pt are stacked along the (001) axis [5]. The in-plane exchange coupling within Fe layers ($J_{//}$) is strong due to direct Fe–Fe interactions, whereas the out-of-plane exchange coupling between adjacent Fe layers ($J_\perp$) is comparatively weaker as it is mediated through Fe-Pt-Fe pathways. This pronounced exchange anisotropy is a key factor in determining magnetization reversal mechanisms and thermal spin fluctuations.

To investigate these properties, we developed an anisotropic spin model [6]. This model approximates their layered crystal structure by employing a modified simple cubic lattice that incorporates only Fe degrees of freedom. It explicitly integrates the exchange interaction anisotropy derived from first-principles calculations (DFT), particularly the anisotropy induced by the layered structure (Figure 1).

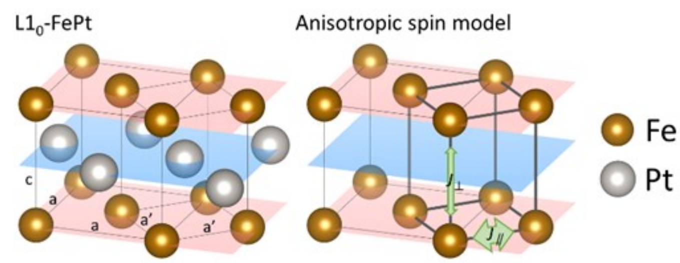

Fig. 1. Schematic diagram of the anisotropic spin model.

The Hamiltonian governing the magnetic dynamics is defined as follows:

$$H = -\frac{1}{2}\left[\sum_{\langle i,j\rangle ||} J_{||}(s_i \cdot s_j) + \sum_{\langle i,j\rangle \perp} J_{\perp}(s_i \cdot s_j)\right] - k_u \sum_i (s_i \cdot \hat{e})^2 - \sum_i \mu_i (s_i \cdot \mathbf{B}) \quad (1)$$

Here $\Sigma\langle i,j\rangle_{//}$ and $\Sigma\langle i,j\rangle_\perp$ d denote summations over nearest-neighbor sites within the same atomic layer and between adjacent layers, respectively. The term si represents the unit spin vector at site i, ku is the uniaxial anisotropy constant, μ_i is the magnetic moment corresponding to spin i, and B is the external magnetic field. By increasing the $J_{//}/J_{\perp}$ ratio, the model explicitly captures the differences between intralayer and interlayer couplings. Furthermore, the Metropolis Monte Carlo method [7] was employed to determine the thermal equilibrium magnetization distribution at temperature. T_c was estimated by fitting magnetization data [8].

Simulations were performed for various sizes and heights of rectangular L10-FePt nanoparticles to analyze the dependence of T_c on particle size.

III. Results and Discussions

To assess the exchange interaction anisotropy in L10-FePt, Density Functional Theory (DFT) calculations were performed using the Quantum ESPRESSO package [9]. These simulations revealed a pronounced anisotropy ratio, where the in-plane exchange $J_{//}$ is approximately 7.06 times larger than the out-of-plane exchange $J_{\perp}$. Based on these considerations, the exchange interaction parameters for the anisotropic spin model were set to $J_{//}$=10.033 J/link and $J_{\perp}$=1.422. Using these parameters, T_c of the bulk crystal was reproduced as approximately 685 K, which aligns well with experimental observations.

Using the established anisotropic spin model, we explored the size-dependent variation in T_c for three sample sets: Prototype (Legacy In-house), Current In-house, and Current External. These samples were distinguished by their differences in particle size and height distributions. The model demonstrated that the size-dependent dispersion of the Curie temperature, $\sigma T_{c,size}$, accounted for approximately 70–80% of the experimentally observed total T_c dispersion, σT_c. This finding suggests that variations in particle size and height are the primary drivers of the observed T_c distribution.

TABLE I

Measured grain sizes and Curie temperatures for several samples, and predictions of the Curie temperatures from the anisotropic spin model.

A) Measured data

Sample	Width (nm)	σ_Width (%)	Hight (nm)	σ_Hight (%)	T_c (K)	σT_c (%)
Prototype In-house	7.8	20	10.0	12	650	2.5
Current In-house	6.6	23	10.4	4.8	650	2.5
Current External	5.7	23	11.6	14	650	3.5

B) Predicted by anisotropic spin model

Sample	T_c (K)	σ$T_{c,size}$ (%)	σ$T_{c,size}$/σT_c
Prototype In-house	638.9	1.7	0.68
Current In-house	632.3	2.0	0.80
Current External	630.1	2.5	0.71

The remaining ~30% of σT_c is likely attributed to secondary factors such as chemical ordering and lattice strain. Nonetheless, the numerical simulations effectively isolated the dominant contribution of size effects to T_c variations, providing valuable insights into controlling these dispersions for HAMR media design. By minimizing T_c dispersion through approaches such as regulating particle dimensions or refining material composition, significant advancements in recording stability and ADC could be achieved. These results underscore the practical importance of the developed atomistic spin model in optimizing next-generation magnetic storage systems.

IV. Conclusion

This study investigated the dispersion of Curie temperature (T_c) in L10-FePt nanoparticles by developing an anisotropic spin model and examining the influence of particle size distribution on Tc variability. The findings revealed that finite-size effects are responsible for approximately 70%–80% of the experimentally observed T_c c dispersion (σT_c), with particle size and height distributions identified as the main contributors.

Non-equilibrium dynamics during HAMR processes, such as rapid thermal fluctuations, significantly impact recording performance. Future research will focus on incorporating temperature- and time-dependent simulations to gain deeper insights into the transient behaviors tied to these processes.

The proposed model and its results provide actionable guidelines for minimizing Tc dispersion through optimized particle size management and material modifications, paving the way for enhanced performance in next-generation high-density storage systems.

At the conference, we will present a comprehensive simulation analysis of the nonlinear impact of particle size on Tc dispersion and look forward to discussing practical strategies for reducing σT_c by optimizing grain-size distributions.

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