Journal of Magnetism and Magnetic Materials 400 (2016) 266–270

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Cluster Monte Carlo methods for the FePt Hamiltonian

A. Lyberatos [a,*], G.J. Parker [b]

[a] Materials Science and Technology Department, P.O. Box 2208, 71003 Heraklion, Greece
[b] HGST, A Western Digital Company, 3403 Yerba Buena Road, San Jose, CA 95135, USA

ARTICLE INFO

Article history:
Received 20 June 2015
Received in revised form
3 July 2015
Accepted 11 July 2015
Available online 14 July 2015

PACS:
75.10.Hk
75.40.-s
75.40.Cx
75.50.Ss

Keywords:
Cluster Monte Carlo
FePt
Swensen-Wang
Wolff
Dynamic exponent
Spin autocorrelation time
Critical phenomena
Heat assisted magnetic recording

ABSTRACT

Cluster Monte Carlo methods for the classical spin Hamiltonian of FePt with long range exchange interactions are presented. We use a combination of the Swendsen–Wang (or Wolff) and Metropolis algorithms that satisfies the detailed balance condition and ergodicity. The algorithms are tested by calculating the temperature dependence of the magnetization, susceptibility and heat capacity of $L1_0$-FePt nanoparticles in a range including the critical region. The cluster models yield numerical results in good agreement within statistical error with the standard single-spin flipping Monte Carlo method. The variation of the spin autocorrelation time with grain size is used to deduce the dynamic exponent of the algorithms. Our cluster models do not provide a more accurate estimate of the magnetic properties at equilibrium.

1. Introduction

The temperature dependence of the magnetic and thermal properties of FePt nanoparticles in the critical region close to the Curie temperature T_c is of interest in the theory of critical phenomena and also of practical relevance in thermomagnetic writing on granular thin films. The high uniaxial perpendicular magnetic anisotropy $K \approx 10^8$ erg/cm^3 makes FePt a good candidate for next generation hard disk drives. Application of the finite size scaling theory [1–3] allows an estimate of the critical exponents describing the divergence of the magnetization $m \sim |t|^{\beta}$, susceptibility $\chi \sim |t|^{-\gamma}$, specific heat $c \sim |t|^{-\alpha}$ and spin correlation length $\xi \sim |t|^{-\nu}$ of the bulk material at the phase transition point, where $t = (T - T_c)/T_c$ is the reduced temperature. Monte Carlo simulations of FePt nanoparticles have suggested that the critical exponents appear to be in agreement with the universality class of the 3D Ising model [3], however, the accuracy of the calculations was insufficient to resolve this issue beyond doubt. The critical exponent ν is required to determine the grain size dependence of the Curie temperature [2] which is a major concern in thermomagnetic writing where the trend is toward smaller grains with wider T_c dispersions. To first approximation, Curie point writing occurs when the medium has cooled to T_c, so local variations of the Curie temperature result in wider transition width. In multiscale modeling, atomistic simulations based on a classical spin Hamiltonian of FePt were used to calculate the temperature dependence of the magnetic properties m, χ of nanoparticles and the data were fitted to functions that extrapolate to the critical behavior of an infinite system [4]. The fitted functions $m(T)$, $\chi(T)$ were then used as an input in micromagnetic models of the thermomagnetic writing process using the Landau–Lifshitz Bloch equation that allows efficient simulation of heat-assisted recording assuming homogeneous magnetization within each grain to reduce the CPU time.

Statistical errors using the standard Metropolis Monte Carlo methods are significant in simulations of magnetic systems in the critical region as a result of two reasons:

1. Critical fluctuations arise from the presence of large clusters of spins pointing in the same direction. The divergence of the spin correlation length at T_c results in divergence of the size

* Corresponding author.
E-mail address: lyb@materials.uoc.gr (A. Lyberatos).

http://dx.doi.org/10.1016/j.jmmm.2015.07.020
0304-8853/

of fluctuations in magnetization and energy. Critical fluctuations increase the size of the statistical errors in the simulations, for instance for a multispin system consisting of N atomic spins with moment μ_s the error in the magnetic susceptibility per spin is $\delta\chi = \beta\mu_s N \,\mathrm{Var}(\mathrm{Var}(m))$, where $\beta = 1/k_B T$ and $\mathrm{Var}(m) = \langle m^2\rangle - \langle m\rangle^2$ is the variance of the distribution which is known to be of gaussian form [5]. Critical fluctuations are an intrinsic feature of any Monte Carlo model which correctly samples the Boltzmann distribution and cannot be avoided.

2. Critical slowing down, i.e. the spin autocorrelation time τ that is defined from the time-displaced autocorrelation function

$$\phi(t) = \langle m(0)m(t)\rangle - \langle m\rangle^2 = \phi(0)e^{-t/\tau} \tag{1}$$

diverges at T_c for bulk material as $\tau \sim \xi^z$, where z is a dynamic exponent. For finite systems a cut-off is imposed by the linear size $\xi = L$, so $\tau \sim L^z$. The error on the magnetization $\sigma = \sqrt{(2\tau/t_{max})\mathrm{Var}(m)}$ is dependent on the number $n = t_{max}/2\tau$ of uncorrelated spin configurations in a run of duration t_{max} after equilibration. The time to generate a single uncorrelated state is $\tau_{CPU} \sim L^{d+z}$ where $d=3$ is the dimensionality of our system (FePt nanoparticles) and is therefore strongly dependent on the dynamic exponent.

The fundamental reason for the large value of the dynamic exponent z in the Metropolis algorithm is the divergence of the spin correlation length. For instance, in the Ising model, large domains of spins pointing in the same direction are flipped slowly starting with spins close to the domain boundary where the exchange coupling is lower, whereas the flip probability of spins in the interior of a domain is low.

Cluster flipping algorithms were proposed that reduce the exponent z and solve the problem of critical slowing down. The basic idea is to look for clusters of similarly oriented spins and flip them in their entirety. Cluster algorithms were applied to Ising and Heisenberg Hamiltonians with nearest neighbor interactions [6,7] and Ising models with long range interactions [8]. The classical spin Hamiltonian of FePt, which is of the Heisenberg type with long range exchange interactions and also includes magnetic anisotropy and antiferromagnetic coupling for some Fe–Fe pairs [9] has not been considered before. In this paper, we show that it is possible to construct cluster-flipping algorithms for the FePt Hamiltonian that satisfy detailed balance and ergodicity.

2. The model

A detailed description of the atomic spin model of the chemically ordered $L1_0$ phase of FePt using ab initio calculations of non-collinear magnetic configurations [9] and the application to small nanoparticles [3] is given elsewhere. It consists of a superlattice of alternating Fe and Pt atomic planes along the (001) direction with fct structure. The itinerant Pt atomic moments are incorporated into effective Fe atomic moments $\mu_s = 3.23\mu_B$ where μ_B is the Bohr magneton. The effective classical spin Hamiltonian is

$$\mathcal{H} = -\sum_{i<j,\alpha} \tilde{J}_{ij}^{\ \alpha}\sigma_i^{\alpha}\cdot\sigma_j^{\alpha} - \sum_i K_i\left(\sigma_i^z\right)^2, \quad \alpha = x, y, z \tag{2}$$

Here $\vec{\sigma}_i$ are the Fe sublattice spin moments treated as unit vectors in the classical limit, $K_i = k_{Fe}^{(0)} + m_i K'$ are effective single ion anisotropy parameters, m_i is the number of Pt nearest neighbors, $k_{Fe}^{(0)} = -0.097$ meV and

$$\tilde{J}_{ij}^{\ \alpha} = J_{ij} + 2n_{ij}\left[I + \delta_{\alpha z}K'\right] \tag{3}$$

where J_{ij} are effective Fe–Fe exchange integrals that decay slowly with distance as a result of the Pt itinerant electrons and $I=0.351$ meV. The term $2n_{ij}K'$ arises from two-ion magnetic anisotropy, where n_{ij} is the number of Pt atoms that mediate additional exchange coupling between Fe spins at sites i and j and $K' = 0.0223$ meV.

The FePt nanoparticles in the present model are cubic and their magnetic state is described by an array of $N_x \times N_y \times N_z$ Fe spins where the x and z axes are along the [110] and easy (c)-axis, respectively. The mean spin polarization of the grain is $\vec{m} = (1/N)\sum_1^N \vec{\sigma}_i$ where $N = N_x N_y N_z$ is the total number of Fe atoms. The lattice parameters $a=3.88$ Å and $c=3.7$ Å are considered in the calculation of the exchange integrals J_{ij}. The range of the Fe–Fe exchange coupling, up to 10 unit cells, is more extended than previous models [2,3] and is the same as in Ref. [1]. Beyond this cut-off region, the coupling is negligible.

The temperature dependence of the magnetic properties of FePt nanoparticles and finite size effects were studied using the Monte Carlo method [3]. The Monte Carlo method calculates the thermodynamic average of an observable $A(\mu)$ where the state μ is here defined by the set of Fe spins in the grain $\{\vec{\sigma}_i,\ i = 1, \ldots N\}$, by generating a Markov process to construct a random sequence of states leading to equilibrium. A transition probability $W(\mu \to \nu)$ is specified between successive states μ, ν that satisfies the condition of detailed balance

$$p_\mu W(\mu \to \nu) = p_\nu W(\nu \to \mu) \tag{4}$$

where p_μ and p_ν are the probabilities of the states μ and ν at equilibrium respectively. The transition probability is determined by the selection probability of the Monte Carlo move $g(\mu \to \nu)$ providing freedom to choose a Markov process and the acceptance ratio $A(\mu \to \nu)$ [10]

$$W(\mu \to \nu) = g(\mu \to \nu)A(\mu \to \nu) \tag{5}$$

The ratio of the transition probabilities for Boltzmann distribution at equilibrium is therefore

$$\frac{g(\mu \to \nu)A(\mu \to \nu)}{g(\nu \to \mu)A(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)} \tag{6}$$

The moves $g(\mu \to \nu)$ should be selected so that the acceptance ratio is maximized. A successful cluster algorithm was formulated by Wolff for the Heisenberg model with nearest neighbor interactions [7] and is extended here to the case of the FePt spin Hamiltonian.

We consider two spin configurations μ and ν that differ by the flipping of a single cluster, by reflection of all spins in the cluster in the plane perpendicular to a random direction specified by a unit vector $\vec{n}$. The group of spins constituting the cluster may not be simply connected. We denote by $\{\vec{\sigma}_i,\ i \in A\}$ spins belonging to the cluster and the rest of the spins in the grain by $\{\vec{\sigma}_j,\ j \in B\}$. The change in the energy following the flip of the cluster is

$$\Delta E = \Delta E_{ex} + \Delta E_{cl} \tag{7}$$

The first term is the change in the energy of the exchange interaction between the spins in the cluster and the exterior region. By symmetry $\tilde{J}_{ij}^{x} = \tilde{J}_{ij}^{y} = \tilde{J}_{ij}$ and it can be shown that

$$\Delta E_{ex} = \sum_{\langle ij\rangle} 2\tilde{J}_{ij}\left(\vec{\sigma}_i\cdot\vec{n}\right)\left(\vec{\sigma}_j\cdot\vec{n}\right) + 2\left(\tilde{J}_{ij}^{z} - \tilde{J}_{ij}\right)\left(\vec{\sigma}_i\cdot\vec{n}\right)\sigma_j^z n_z \tag{8}$$

The second term is the change in the internal energy of the cluster