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Magnetization of Nano-Size Subsystem in a Two-Dimensional Ising Square Lattice

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ABSTRACT

A two-dimensional Ising square lattice is modeled as a nano-size block array to study by Monte Carlo simulation the magnetic thermal stability of nano-structure magnetic media for data storage, thereon in the blocks $J_1 > 0$ is assigned for the interaction of a pair of nearest-neighbor spins, while $0 \le J_0 \le J_1$ for that in regions between the blocks and $(J_0 + J_1)/2$ for the nearest-neighbor pairs with one in the block and the other one out of but near-most the block. We show that the magnetic thermal stability of the block accrues with the increase of J_1 and with the decrease of $J_1 - J_0$ for a given J_1, but contrarily, the anchoring ability for the initial magnetic orientation in nano-size block trails off as $J_1 - J_0$ diminish. This phenomena and size dependence of such anchoring ability are discussed in detail.

Keywords: Magnetization; Ising Square Lattice; Nano-Size Subsystem

1. Introduction

Recently magnetic microstructure and nano-structure related to high-density magnetic recording, such as magnetic nanowires, chains, rings, planar arrays of magnetic nanoparticles and magnetic nano-structure thin film [1-3], is a topic of active research in material science. Practically, such microstructures are often imprinted on patterned substrate materials using lithography or beset in alloyed materials [4-6], which for practical applications are often imprinted using lithography on patterned substrate materials or doped with nanoparticles into alloyed ones [4-6]. That sophisticated techniques continue to be used to fabricate and characterize magnetic nano-structures assures the appearance of high density magnetic recording devices hereafter. Now, grains, as small as 7 - 8 nm, are used to store data at high signal-to-noise ratio (SNR) [7]. In the future, even smaller grains will be needed to store data at much higher areal densities. However, with the decreasing in size the particles will lose thermal stability, reaching the so called superparamagnetic limit, *i.e.*, the magnetic orientation of particle at some size point no longer acts as magnetic bit due to thermal fluctuations [8,9]. Therefore the thermal stability in magnetic media for high density magnetic recording is still an open question.

In general, magnetic materials for data storage are composed of tiny but isolated magnetic nanocrystalline grains, but for magnetic nano-structure materials and nanoparticle materials, dipolar interactions between particles are unavoidable becoming relevant when increasing the packing density of the particles. This means that bit relevant is not a piddling issue in magnetic media for high density magnetic recording and the thermal stability of nanoparticle/unite of nano-structure materials must be considered in all of the system rather than as an isolator. Recently, a model of a two dimensional monodispersed array of single domain magnetic nanoparticles arranged in a square lattice was thus investigated to simulate thermal stability of magnetic media [10]. In that model each nanoparticle is a unite of the nano-structure material and is modeled as a giant magnetic moment, possessing saturated magnetism, that is, the magnetic moment interactions between particles and thermal fluctuation work only on the magnetic orientation, not changing the magnetic quantity of nanoparticle. Indeed, a nanoparticle is a cluster consisting of decades or hundreds of atoms/ions whose magnetic orientation ensemble is responsible for magnetization of nanoparticle. With the increase of temperature its magnetization will die away, reaching the superparamagnetic limit. Furthermore, the particles must further close up when continuing to heighten the density of magnetic recording, consequently here the interaction between particles is not taken as that of giant magnetic moments. Alike in bulk crystal, the interaction between two particles comes from the nearest-neighbor spin-spin interaction of atoms/ions respectively in their outer layers. If consider the influence of the atoms of substrate materials the correlation of two particles, based on the view of nearest-neighbor interaction, results from the interaction of their outer atoms with the atoms of substrate materials insulating them.

The Ising model has an enormous impact on modern physics in general and statistical physics, as well as in condensed matter physics for understanding the magnetism of materials [11,12]. In this paper, we provide a two-dimensional Ising square lattice which is modeled as a nano-size block array to study the magnetic thermal stability of nano-structure unite in magnetic media for data storage. As schematically delineated in **Figure 1**, in the blocks $J_1 > 0$ is assigned for the interaction of a pair of nearest-neighbor spins, while $0 \le J_0 \le J_1$ for that in regions between the blocks and $(J_0 + J_1)/2$ for the nearest-neighbor pairs with one in the block and the other one out of but near-most the block. Here $J_1 > 0$ stipulates that the material in blocks/nanoparticles (acting as nano-bits) is ferromagnetic, and $0 \le J_0 \le J_1$ stands for the magnetic nature of media separating the particles from each other or for the interaction of nearest-neighbor spins in grain boundaries when they being close very much. For a binary Ag-Ni alloy, commonly the pairwise potential between different species of Ag and Ni atoms is assumed to be a mathematical or geometrical average function of the monoatomic potential [13,14]. Analogously we hence take the interaction of the nearest-neighbor pairs with one in the block and the other one out of but near-most the block as $(J_0 + J_1)/2$.

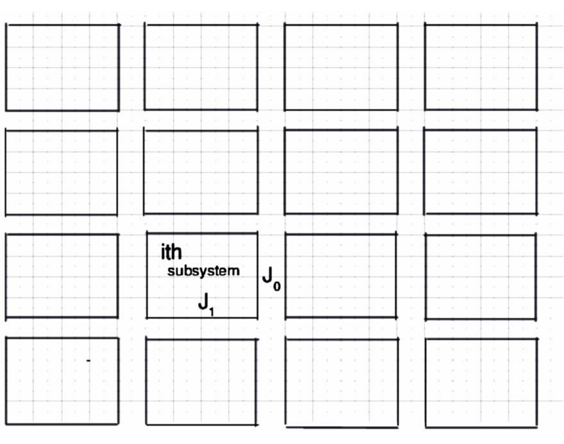

Figure 1. Schematic description of the Ising lattice model which is partitioned into blocks with each coated by patterned substrate material.

The Hamiltonian of our model is written as

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j , \tag{1}$$

where J_{ij} is the energy of spin-spin interaction which takes the values of J_1, J_0 and $(J_0 + J_1)/2$, respectively corresponding to the above three types of nearest-neighbor spin pairs. The spins can only be in one of two states, either spin-up, $S_i = +1$, or spin-down, $S_i = -1$. The notation $\langle i, j \rangle$ restricts the sum to run over all nearest-neighbor pairs. It is noted that periodic boundary condition is implemented in this model. This Hamiltonian does not contain any information about its temporal evolution. Nevertheless, one can obtain good estimates for the average value of an observable quantity such as magnetization, susceptibility, free energy and specific heat by applying Metropolis Monte Carlo (MMC) simulation.

2. Methods

MMC has been used extensively in the researches of Ising models [15], which are described by a simple recipe: 1) Choose an initial state; 2) choose a site i; 3) calculate the energy change ΔE which results if the spin at site i is overturned; 4) generate a random number r such that $0 < r < 1$; 5) if $r = \exp(-\Delta E / k_B T)$, flip the spin; 6) go to the next site and go to (III). For convenience in this paper, all energy scales are in units of the Boltzmann constant, which is set to $k_B = 1$. Focusing on the magnetization of subsystem, we first investigate a Ising model which is of the size of 56 × 56 and partitioned into 4 × 4 blocks. These blocks are segregated from each other by patterned substrate material with the thickness of 4 sites and possess the size of 10 × 10. The cases of the model with other size will be discussed at the end of this paper. As an example, the block locating on the second row and second column, named as particle A in the following for convenience, is considered in the cases of $J_1 = 4.0$ and $0 \le J_0 \le J_1$. It is well-known that for ferromagnetic bulk material, *i.e.*, $J_{ij} > 0$, there is a phase transition from a disordered (paramagnetic) high-temperature phase to an ordered (ferromagnetic) low-temperature phase, and a continuous but abrupt pick-up of the average magnetization per spin can be anticipated at a temperature T_C. In zero external field, the measured average magnetization would always be zero even for $T < T_C$, since a finite system which is necessarily performed to emulate the bulk material remains ergodic even for $T < T_C$. To surmount this puzzle, one of the simplest ways of emulating a system confined to a particular phase is to consider the average absolute magnetization per spin [11]. We found that when $J_1 \ge 4.0$ the time scaled by 10^5 MMC steps is long enough for system relaxing towards its equilibrium from an arbitrary initial state, during which the global spin inversion of the equilibrium state has not been observed. Therefore the average magnetization is still an observable quantity measured in the above time when $J_1 \geq 4.0$. Furthermore it is a necessarily quantity to character nanoparticle in the case of nanoparticle acting as nanobit. As mentioned above, we note that here the simulation results of the average magnetization, in terms of symmetry breaking, are suitable for bulk material consisting of the interacting nanoparticles. Under the same initial condition where S_i takes the value randomly from +1 and −1, for the system at an arbitrary temperature T we perform MMC 10^5 steps and sample the microscopic states after 5×10^4 steps with the interval of 100 steps to obtain the average magnetization and susceptibility of particle A.

3. Result and Discussion

We denote the absolute value of average magnetization per spin as $\left|\langle M_A \rangle\right| / N_A$ and susceptibility per spin of particle A as χ_A. In the cases of J_0 = 0.0, 1.5, 3.0, 4.0, the functions of the absolute value of average magnetization per spin and susceptibility per spin of particle A with respective to temperature T are plotted together in **Figure 2**. It is found from **Figure 2** that there exists a disordered (paramagnetic) high-temperature phase and an ordered (ferromagnetic) low-temperature phase. This can be interpreted by the free energy of particle A, $F_A = \langle E_A \rangle - TS_A$, where S_A is its entropy. At relatively high temperatures, the case of $J_{ij}/k_B T \ll 1$, the term TS_A dominates so that the free energy F_A is minimized by maximizing the entropy, corresponding to paramagnetic phase where the spins orientate randomly; while at relatively low temperatures, the case of $J_{ij}/k_B T \gg 1$, the interaction energy $\langle E_A \rangle$ dominates so that the free energy is minimized by minimizing the energy, corresponding to ferromagnetic phase where the spins orientate to the same direction; and when the thermal energy TS_A and the interaction energy $\langle E_A \rangle$ are comparable, *i.e.*, when $T \approx T_C$, phase transition between ferromagnetic phase and paramagnetic phase occurs. Theoretically, as T approaches the critical temperature T_C, the susceptibility per spin χ diverges. Therefore the temperature corresponding to the peak value of the function of χ versus T can be roughly taken as the value of T_C. It is well known that the susceptibility per spin χ can be obtained from the variance of the magnetization of system, formulated as follow [11],

$$\chi = \frac{1}{Nk_B T}\left(\langle M^2 \rangle - \langle M \rangle^2\right). \quad (2)$$

So as shown in **Figure 2(b)**, that T_C increases with the decreasing of $J_1 - J_0$ illuminates that the temperature variance range for the particle (nanobit) in ferromagnetic phase becomes larger and larger as $J_1 - J_0$ decreases, meaning that the magnetic thermal stability of the particle accrues when $J_1 - J_0$ trails off.

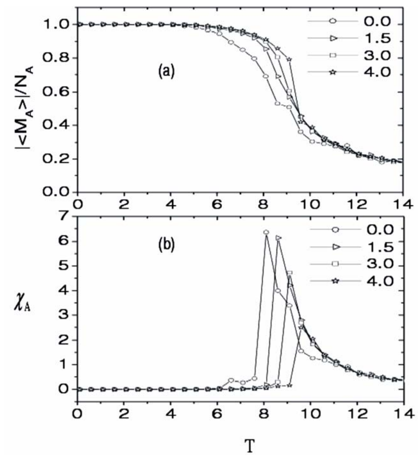

Figure 2. The functions of the absolute value of average magnetization per spin $\left|\langle M_A \rangle\right| / N_A$ and susceptibility per spin χ_A of particle A vs. temperature T, in the cases of J_1 = 4.0 and J_0 = 0.0, 1.5, 3.0, 4.0, respectively, where N_A is the number of sites in particle A, and the increment of T is 0.5.

What is related closely to the susceptibility is spin-spin correlation function defined as

$$g(i,j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle. \quad (3)$$

Based on Equation (3) the susceptibility χ can be written as

$$\chi = \left(\sum_{j=1}^{n} g(i,j)\right) / k_B T,$$

which is the analogue in percolation describing how site-site correlation function is related to the average cluster size or to the average correlation length [11]. It is known that for an infinite system, in the low temperature phase the correlation length increases with increasing of the temperature and diverges as the temperature approaches the critical temperature T_C; while for a finite system the correlation length reaches its peak value at the critical temperature T_C. To explore block-block correlation, we define the correlation of total spins of particle A with those of its four nearest-neighbor particles as

$$g = \frac{1}{4}\sum_{A_j}\left(\langle S_A S_{A_j} \rangle - \langle S_A \rangle \langle S_{A_j} \rangle\right),$$

where A_j = 1, 2, 3, 4 stand for the left, the right, the down, the up particles, respectively. **Figure 3** shows that the correlation of total spins of particle A with those of its four nearest-neighbor particles is a function of J_0. Comparing **Figure 3** with **Figure 2(b)**, one can see that at temperature $T = 9.0$, $g(J_0 = 3.0) > g(J_0 = 1.5) > g(J_0 = 0.0)$ accords with $\chi_A(J_0 = 3.0) > \chi_A(J_0 = 1.5) > \chi_A(J_0 = 0.0)$, as well as $g(J_0 = 4.0)$ versus $\chi_A(J_0 = 4.0)$. It accounts for that the magnetic thermal stability of the particle A having

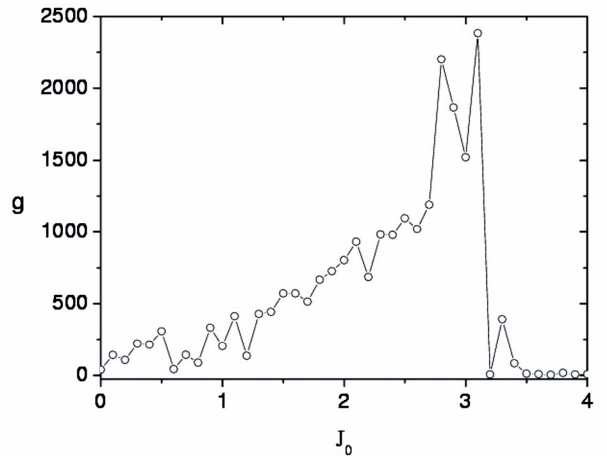

Figure 3. The plot for the mean value of the correlation function *g* in the fluctuation of total spins of particle *A* and those of its four nearest-neighbor particles (blocks) vs. J_0 at temperature *T* = 9.0, where J_1 = 4.0.

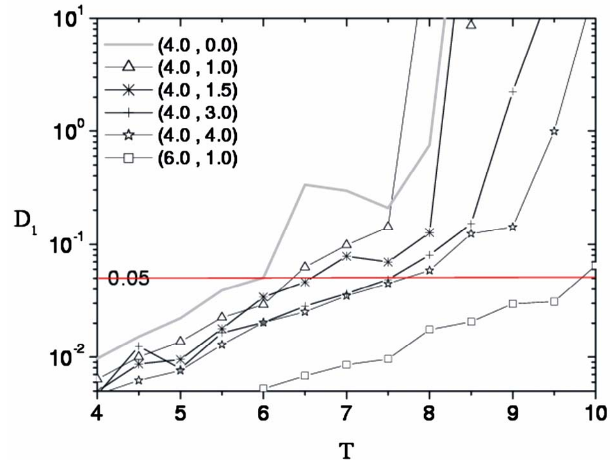

Figure 4. The functions of the fluctuation in magnetization of particle *A*, D_1, with respect to temperature *T* in the cases of (J_1, J_0): (4.0, 0.0) , (4.0, 1.0) , (4.0, 1.5) , (4.0, 3.0), (4.0, 4.0) and (6.0, 1.0).

relationship with J_0 indicates the relevance of the particle *A* with the other particles, bridged by substrate material.

Further to understand magnetic thermal stability of the block, the fluctuation in magnetization of particle *A*,

$$D_1 = \sqrt{\left\langle \left(M_A - \langle M_A \rangle \right)^2 \right\rangle} \Big/ \langle M_A \rangle,$$

with respect to temperature *T* are plotted on **Figure 4**. Here, D_1 describes the relative deviation of magnetization M_A to its average value. **Figure 4** shows that with increasing of temperature *T* the fluctuation of magnetization M_A becomes severe and particle *A* will lose its magnetization when it is in paramagnetic phase; further more, D_1 augments in the range of $0.05 \le D_1 \le 0.20$ as $J_1 - J_0$ reduces for a given J_1 or increases with the increasing of J_1. Thus one may conclude that in fluctuation criterion of $D_1 \le D_{1C}$, e.g., $D_1 \le 0.1$, particles acting as nanobits can be used to storage data at higher temperature when $J_1 - J_0$ is smaller than that when $J_1 - J_0$ is large in the case of J_1 being fixed.

However, in the magnetic media for data storage, what must be kept and be ensured not fluctuating intensity with the change of temperature *T* are particles' initial magnetic states. After the finish of the writing information on magnetic media, *i.e.*, with the applied field being switched off, the information bit has been recorded by the reversed spins S_i in particle and is represented by its total magnetization M_A with an orientation (say up or down). The fluctuation of magnetization D_1 does not contain any information about the initial magnetic state of particle. Therefore instead of D_1, we compute the fluctuation of magnetization D_2, which defined as

$$D_2 = \sqrt{\left\langle \left(M_A - M_A(0) \right)^2 \right\rangle} \Big/ M_A(0),$$

where $M_A(0)$ is the initial total magnetization of particle *A*. D_2 describes the relative deviation of magnetization M_A to its initial total magnetization. Note that here we initialize the system with $S_i(0) = 1$ if site in particle *A*, otherwise $S_i(0) = -1$. $D_2 = 0$ means that $M_A = M_A(0)$, while $D_2 = 2.0$ means that $M_A = -M_A(0)$. Thus **Figure 5** shows that in the cases of $J_1 - J_0$ being large, say (J_1, J_0): (4.0, 0), (4, 1), (4, 1.5) and (6, 1), the initial magnetic state of particle *A* can be kept down when it is in feromagnetic phase, but the initial magnetic state will be lost with the spin in particle *A* $S_i = -1 \ne S_i(0) = 1$ in the case of $J_1 - J_0$ being small, e.g., (J_1, J_0): (4, 3) and (4, 4). For clarity, sixteen microstates of the system being in equilibrium states evolving from the initial state mentioned above are shown in **Figure 6**, corresponding respectively to different J_1 and J_0 at temperature *T* = 2, 4, 6, 12. It is consistent with **Figure 5**. Up to now we thus conclude that the magnetic thermal stability of the block accrues with the increase of J_1 and with the decrease of $J_1 - J_0$ for a given J_1, but contrarily, the ability for the initial magnetic orientation kept in nano-size block, named as anchoring ability of initial magnetization, trails off as $J_1 - J_0$ diminishes.

The above discussions are based on the two dimensional Ising square lattice with size 56 × 56, in which the blocks with size 10 × 10 are segregated from each other by patterned substrate material with the thickness of 4 sites. With the decreasing of particle size the thermal fluctuations induce random flipping of the magnetic moment with time so that nanoparticles lose their stable magnetic order and become superparamagnetic. V. Skumryev and coworkers [16] had studied the systems where ferromagnetic cobalt nanoparticles of about 4 nm in diameter that are embedded in either a paramagnetic or an antiferromagnetic matrix. They found that the cobalt cores lose their magnetic moment at temperature being

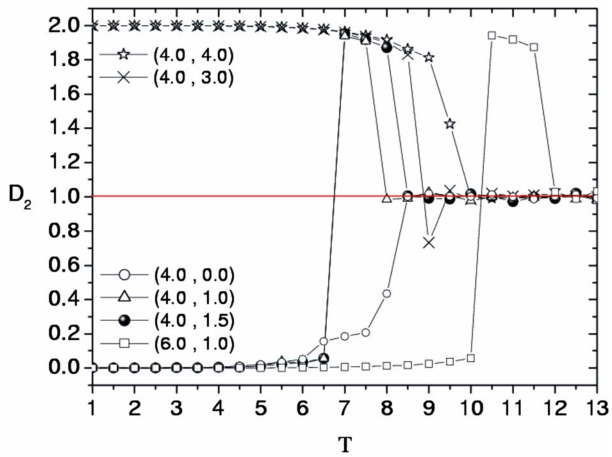

Figure 5. The functions of the fluctuation in magnetization of particle *A*, D_2, with respect to temperature *T* in the cases of (J_1, J_0): (4.0, 0.0), (4.0, 1.0), (4.0, 1.5), (4.0, 3.0), (4.0, 4.0) and (6.0, 1.0), respectively.

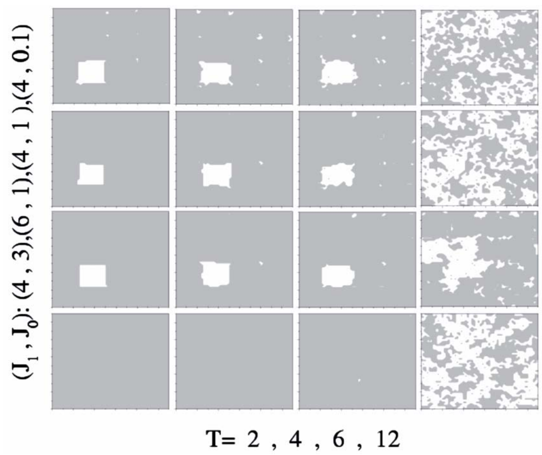

Figure 6. Sixteen microstates characterizing the system in equilibrium states for temperature $T = 2, 4, 6, 12$ from left to right and for (J_1, J_0): (4.0, 3.0), (6.0, 1.0), (4.0, 1.0), (4.0, 0.1) from bottom to top, respectively. Sites containing up-spins are white while sites containing down-spins are gray.

10 K in the first system but remain ferromagnetic up to about 290 K in the second. Similarly here for paramagnetic substrate material, we investigate theoretically the size dependence of temperature T_0 based on the criterion $D_1 \geq 0.1$, *i.e.*, $D_1 \geq 0.1$ if temperature $T \geq T_0$. For this purpose, the two-dimensional Ising square lattices are set to be 200 × 200, which are partitioned by the blocks with size of 6 × 6, 16 × 16, 21 × 21, 36 × 36 and 46 × 46, respectively, segregated from each other by patterned substrate material with the thickness of 4 sites. From **Figure 7** one can deduces 1) that for a given value of $J_1 - J_0$, T_0 increases with increasing the particle's size N_A and will reach its saturated value; 2) that for a given N_A, T_0 becomes large as $J_1 - J_0$ decreases if N_A is smaller and such change is not distinct anymore if N_A is larger. This

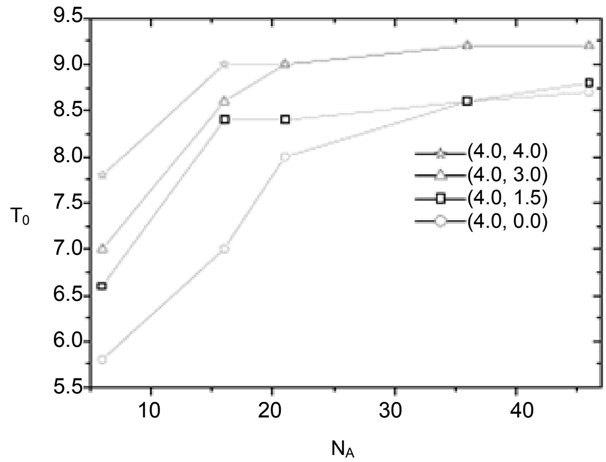

Figure 7. The size dependence of T_0 larger than which when temperature *T* is, $D_1 \geq 0.1$ corresponding respectively to different values of $J_1 - J_0$. The size of lattices are 200 × 200, thereon the size of blocks are $N_A \times N_A$ with N_A = 6, 16, 21, 36 and 46, respectively, segregated from each other by patterned substrate material with the thickness of 4 sites. Also, periodic boundary condition is implemented. The temperature increment for searching T_0 is 0.2.

may be explained as following. Reckon the sites in patterned substrate material coating the particle as its shell, with the increasing of the size of particle, the surface sites (shell's sites) to core sites (particle's sites) ratio decreases and the effects induced by surface become weak, that is, the properties of particle are dominated by itself, thereby it behaves like bulk material disregard of the patterned substrate material and can be considered as a isolated bulk system.

4. Conclusions

Based on the pair interaction of nearest neighbor spins in a two-dimensional Ising square lattice, we have investigated the thermal stability of magnetization of ferromagnetic nano-size subsystems separated by paramagnetic substrate material. The interaction for spins in subsystem is denoted as J_1 while that for spins in substrate material is J_0. It has been found that the magnetic thermal stability of the nano-subsystem accrues with the increase of J_1 and with the decrease of $J_1 - J_0$ for a given J_1, but contrarily, the anchoring ability for the initial magnetic orientation in nano-size subsystem trails off as $J_1 - J_0$ diminishes. In addition, with increasing the subsystem's size its magnetization behaves like that of bulk material, disregard of the patterned substrate material and being able to considered as a isolated bulk system. These results can be used to understand high-density magnetic nanoparticle material for data storage and superparamagnetic limit. Also, it may proposed some ways to enhance the storage density of recording magnetic media by reducing the size of particle: 1) Increasing the spin interaction in ferromagnetic nanoparticle, *i.e.*, increasing $J_1 - J_0$; 2) For a fixed spin interaction in ferromagnetic nanoparticle, selecting suitable J_0 to make nanoparticle meeting both thermal fluctuation criterions D_1 and D_2 is more available than that coating nanoparticle by non-magnetic substrate material (*i.e.*, the case of $J_0 = 0$), for in the former case the nanoparticle can keep its initial magnetization state at a higher temperature.

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