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Compensation behaviors and magnetic properties in a cylindrical ferrimagnetic nanotube with core-shell structure: A Monte Carlo study

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ABSTRACT

Compensation temperature T_{comp} and transition temperature T_C have significant applications for the experimental realization of magnetic nanotube structure in the field of thermal magnetic recording. In this work, we use the Monte Carlo simulation to investigate the phase diagrams, magnetizations, susceptibilities, internal energies, specific heats and hysteresis behaviors of a cylindrical ferrimagnetic nanotube with core-shell structure. The effects of the single-ion anisotropies (D_C, D_S) and the exchange couplings (J_{int}, J_S) on the magnetic and thermodynamic properties of the system are examined. A number of characteristic behaviors are discovered in the thermal variations, depending on different physical parameters. In particular, the triple hysteresis loops behavior has been found for appropriate physical parameters. These findings are qualitatively in good agreement with related experimental and the other theoretical results.

1. Introduction

Magnetic nanotubes are of great interest for researchers owing to their unique characters, such as the electrical energy storage [1,2], the superpara magnetism at room temperature [3,4] and permanent magnets [5,6]. Furthermore, they also have extensive applications in medical fields [7–9]. So far, great progress has been made in the studies of physical performance of magnetic nanotubes whether in experiment or in theory [10–14]. In experiment, there are many achievements on the investigations of core-shell structure magnetic nanotubes such as Co-Ni nanotubes [15–19]. D. Zhou et al. prepared a series of FeNi magnetic nanotubes by using the pore wetting template method [20]. Ye used one-dimensional mesoporous SiO_2 as an effective template to obtain the SnO_2 nanotube in controllable form by hydrothermal method. The results show that the SnO_2 nanotubes, as the anode material in the lithium ion battery, show better performance than the ordinary SnO_2 nanoparticles [21].

On the other side, without theoretical explanations, the experimental evidences obtained could not be clarified in depth. Theoretically, the magnetic properties of nanomaterials such as nanowires and nanotubes have been widely investigated by the use of various techniques, including the mean-field theory (MFT), effective-field theory (EET), Monte Carlo (MC) simulations and so on. It is remarkable to mention that there may be possible of existence of compensation temperature in the ferrimagnetic materials, which is of great importance in applications of thermal magnetic recording. T. Kaneyoshi has investigated the phase diagrams and the variations of magnetizations in the transverse Ising nanowire with simple core-shell structure, within the theoretical framework of EFT [22]. Furthermore, T. Kaneyoshi has investigated magnetic properties compensation temperature and phase diagrams of a ferrimagnetic cylindrical transverse Ising nanotube with a negative core-shell interaction, by EET [23–25]. Using EFT, interesting investigations have been directed to the initial susceptibility and reduced total magnetization of a cylindrical Ising nanotube in order to clarify their distinctions between the ferromagnetic and ferrimagnetic behaviors [26]. Y. Kocakaplan et al. have studied the compensation behaviors and hysteresis loops of the cylindrical transverse core-shell spin-1 Ising nanowire in detail with EFT. And comparing the results with some experimental and theoretical results and a qualitatively good agreement has been obtained [27]. Numan Şarlı has investigated the temperature and the applied field dependence of the magnetic properties including magnetization, susceptibility, specific heat and internal energy of the ferromagnetic and the antiferromagnetic cylindrical mixed spin-1/2 core and spin-1 shell Ising nanotube system by EET [28]. H. Magoussi et al. has investigated the hysteresis behavior of a nanotube, consisting of a ferromagnetic core of spin-1 atoms surrounded by a ferromagnetic shell of spin-1 atoms with ferro- or anti-ferromagnetic interfacial coupling by using EET. Some characteristic behaviors have been observed, such as the existence of double or

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triple hysteresis loops for appropriate values of the system parameters [29].

As we all know, the Monte Carlo simulation is a successful and effective random simulation method for understanding the physical properties of the mixed-spin Ising systems [30–33]. E. Konstantinova have found that some magnetic and thermodynamic properties of magnetic nanotubes based on the plane structures with the square unit cells, manifesting strong dependence on the form of rolling up (armchair or zigzag) by using MC method [34]. Zaim et al. studied magnetic properties and hysteresis loops of a single nanocube Ising model, consisting of a ferromagnetic core of spin- 1/2 surrounded by a ferromagnetic shell of spin-1 with antiferromagnetic interface coupling by MC simulation [35].Y. Benhouria et al. have used Monte Carlo simulation technique to indicate the dielectric properties and hysteresis behaviors of the negative core/shell coupling on the spin-1 Ising nanowire system with a square surface area, and studied the effects of temperature and exchange coupling on the critical and compensation behaviors of ferroelectric and ferrielectric nanowire [36]. Despite tremendous successes have been achieved in the studies of magnetic nanotubes, fewer explorations have been carried out to examine the magnetic and thermodynamic properties of the ferrimagnetic single spin-1 Ising nanotube with core-shell structure by the MC simulation. In particular, the effects of various physical parameters such as the single-ion anisotropies and the exchange couplings on the magnetization, the susceptibility, the internal energy, the specific heat and the hysteresis loop of the system also request further discussion. It is remarkable that the experimental observations of core-shell nanotube have exhibited a series of excellent magnetic behaviors [15–19], which simulates us to carry out related theoretical explorations to better understand these magnetic properties in the core-shell nanotube. We have successfully studied magnetic and thermodynamic properties of various mixed-spin Ising nanoscaled systems by MC simulation in recent researches [37–40]. The results demonstrate the physical parameters including single-ion anisotropy and exchange coupling have critical implications for the phase diagrams, the magnetizations and the thermodynamics properties. Therefore, our purpose of this paper is to present a theoretical MC simulation of the effects of the anisotropies, the exchange couplings and temperature on the compensation and magnetic properties of the ferrimagnetic core-shell nanotube. The paper is organized as follows: in Section 2, we defined model and give briefly MC simulations for the system. In Section 3, we present the numerical results and discussion. Finally, Section 4 is devoted to a brief summary and conclusions.

2. Model and formalism

We here study a cylindrical a ferrimagnetic Ising nanotube of the spin-1 core and shell structure, as depicted in Fig. 1. The total number of spins is $N = (N_C + N_S) \times L$ with the number of N_C is 6 and N_S is 12 at each cross section. $L = 2000$ is regarded as the length of the nanotube in the z-direction. We should take notice of the similar structure of the nanotube which described in Refs. [22–26], but we also observed the differences with ETT in the values of spins for core and shell sublattices in Ref. [28]. The Hamiltonian of the Ising nanotube can be defined as

$$H = -J_C \sum_{i,j} \sigma_{iC}^z \sigma_{jC}^z - J_{\text{int}} \sum_{i,m} \sigma_{iC}^z \sigma_{mS}^z - J_S \sum_{m,n} \sigma_{mS}^z \sigma_{nS}^z - D_C \sum_i \left(\sigma_{iC}^z\right)^2 - D_S \sum_m \left(\sigma_{mS}^z\right)^2 - h\left(\sum_i \sigma_{iC}^z + \sum_m \sigma_{mS}^z\right) \tag{1}$$

where $\sigma_{iC(mS)}^Z = \pm 1, 0$ mean the spin variables of the core and shell sublattices. $< \ldots >$ represent the summation over all pairs of nearest-neighbor spins. J_C (>0), J_S (>0) and J_int (<0) is a representative of the exchange coupling parameters between the two nearest contiguous magnetic atoms at the core-core, shell-shell and core-shell, respectively (see Fig. 1). D_C and D_S are the single-ion anisotropies for core and shell sublattices. h denotes the external longitudinal magnetic field.

With free boundary conditions in *xy*-plane and periodic boundary condition in the *z*-direction, we applied the standard Monte Carlo simulation with the Metropolis algorithm [41] to simulate the model. It is worth mentioning that some additional simulations are influential in determining the effect of L on the results, but we haven't obtained the exact differences when L increasing from 2000 to 5000. Our data were generated with 25000 Monte Carlo steps per spin, discarding the first 5000 Monte Carlo steps for balancing the system.

The magnetizations per site of core and shell are calculated by

$$\begin{aligned} M_C &= \frac{1}{N_C} \sum_{i=1}^{N_C} \sigma_{iCi} \\ M_S &= \frac{1}{N_S} \sum_{m=1}^{N_S} \sigma_{mS} \end{aligned} \tag{2}$$

Thus the total magnetization per site M is

$$M = \frac{6M_C + 12M_S}{18} \tag{3}$$

The internal energy and the specific heat per site are:

$$U = \frac{1}{N} \langle H \rangle \tag{4}$$

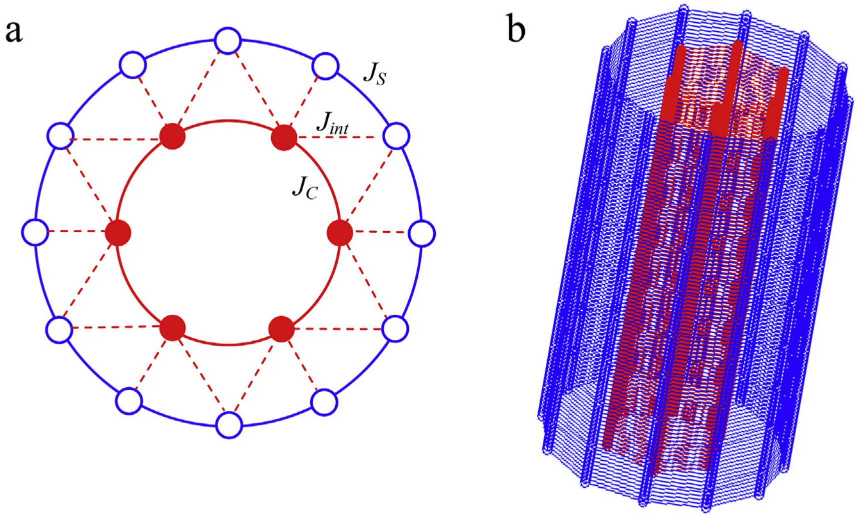

Fig. 1. Schematic representations of a cylindrical ferrimagnetic nanotube with core-shell structure. (a) cross-section and (b) three-dimensional. The red filled and the open green circles represent magnetic atoms (spin$\sigma_{iC}^z = 1$) in the core and magnetic atoms (spin $\sigma_{mS}^z = 1$) in the shell. The lines connecting the red and green circles denote the nearest-neighbor exchange couplings J_C, J_{int} and J_S, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)