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Thermal and magnetic properties of a nanotube with spin-1/2 core and spin-3/2 shell structure

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HIGHLIGHTS

- Surface shell and core magnetization of mixed spin-1/2 and spin-3/2 Ising nanotube is studied by EFT with correlations.
- This is the first investigation on mixed spin-1/2 and spin-3/2 Ising nanotube.
- The effects of crystal field on the system are investigated as well.
- Both first-order and second-order phase transitions and critical end point are observed.
- Magnetic susceptibilities, specific heat, internal energy and free energy of the system have also been studied in detail.

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ABSTRACT

The magnetic properties of a cylindrical Ising nanotube with a spin-1/2 core surrounded by a spin-3/2 shell system have been studied by means of the effective field theory (EFT). We have investigated the effects of crystal-field coupling at the surface shell and bilinear interactions among the core and surface shells to the order parameters, susceptibility, internal energy, specific heat, and free energy. Some characteristic phenomena are examined in terms of thermal or crystal-field variations when the other system parameters are fixed. Moreover, we have observed first-order and second-order transitions and critical end points in the (D/J, kT/J) plane, where D/J and kT/J are crystal-field and temperature, respectively.

1. Introduction

The Ising model and its variations have played an important role in the deeper understanding of phase transitions and critical phenomena. Ferrimagnetic systems resulting from the combination of different magnitudes of spins can be mimicked by the mixed-spin Ising model. The mixed-spin Ising model has attracted significant attention in the past decades because of its fascinating and novel properties. Moreover, ferrimagnetic or magnetic layered systems, especially those produced from rare earth or transition metals with different magnitudes of spins or sequential orders, have been investigated extensively as they can possess significantly different properties from their constituting components [1–5].

Enormous and splendid developments in the experimental techniques and technologies have recently enabled us to produce nanostructures. It is well known that the properties of a material are strictly related to its size and dimensions, and they exhibit some different characteristics from their bulk counterparts when they are reduced to a few atomic lengths.

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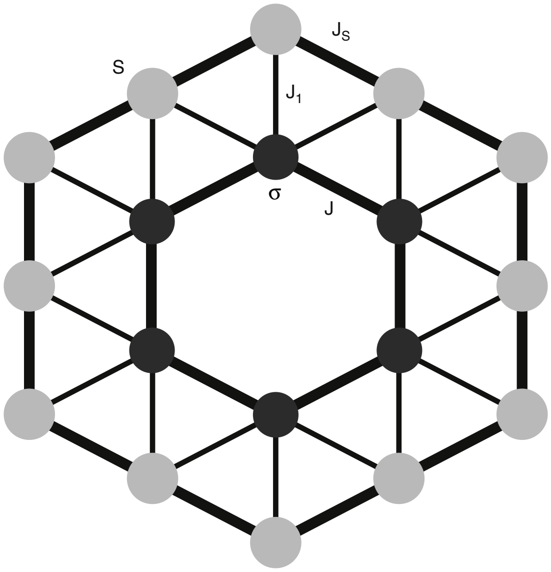

Fig. 1. Schematic representation of cylindrical nanotube. The gray and black circles indicate magnetic atoms at the surface and core shell, respectively.

Therefore, there is no doubt that nanoparticles would be an active research field for both theoreticians and experimentalists due to their interesting physical properties and possible technological application areas. Sensors [6], medical applications [7], permanent magnets [8], and ultra-high-density magnetic storage devices [9] etc. are among the interesting research areas and technological applications of nanoparticles. In addition, magnetic nanotubes can be fabricated by various methods and has attracted great interest because of their beneficial applications in nanotechnology and biotechnology [10,11].

Recently, a theoretical core–shell model has been introduced to explain some characteristic phenomena in the magnetism of the nanoparticle [12–16]. The magnetic properties of a ferrimagnetic core–shell Ising nano-cube model have been studied by using Monte Carlo simulations [17]. Ising nano-wires and nanotubes have been studied using the effective field theory (EFT) with correlations [18–20]. The initial susceptibility and magnetization of a cylindrical Ising nanotube are investigated, and the Neel hyperbola has been found [21]. Furthermore, the magnetic behaviors of complex spin systems have been studied by using EFT [22,23].

The mixed-spin Ising systems are also one of the most actively studied subjects in statistical physics. One of the reasons is their less translation symmetry compared with their single counterparts. Another reason is that many new phenomena are observed in these systems, which cannot be seen in the single-spin Ising model [24]. To the best of our knowledge, the role of bilinear interaction between nano-cylindrical layers and the effect of crystal-field interaction on the magnetic properties of a cylindrical Ising nanotube have not yet been discussed. Therefore, the aims of this paper are to investigate both cylindrical nanostructure and ferrimagnetism. We should also mention that the order parameters and susceptibilities are mainly investigated in the vicinity of the second-order phase transition point in recent studies [18–21]. Hence, this study will focus on the investigation of the magnetic behaviors of the system near the first-order phase transition and critical end point as well. Recently, a first-order phase transition has also been found in the core–shell models [25–27].

The rest of the paper is organized as follows. In Section 2, we define the model and give briefly the formulations of the magnetic properties of the cylindrical Ising nanotube within the theoretical framework of the EFT. In Section 3, the numerical solutions, that is, temperature and crystal-field dependencies of these properties are given. These studies enabled us to obtain the phase diagrams of the system. Finally, the last section is devoted to a brief summary and conclusion.

2. Model and formulation

A nanotube, from Fig. 1, consists of a core and surface shell in which the core is surrounded by a surface shell. Each site on the figure is occupied by an Ising spin. Each spin is connected to the two nearest-neighbor spins in the upper and lower sections, that is, constituting an infinite cylindrical geometry. The sites on the surface shell are not identical positions since the numbers of their nearest neighbors are different.

The Hamiltonian of the system is given by

$$H = -J_s \sum_{\langle ij \rangle} S_i S_j - J_1 \sum_{\langle kl \rangle} \sigma_k S_l - J \sum_{\langle mn \rangle} \sigma_m \sigma_n - h \left(\sum_i S_i + \sum_k \sigma_k \right) - D \sum_i S_i^2, \tag{1}$$

where S and σ are the Ising operator with $S = \{\pm 3/2, \pm 1/2\}$ and $\sigma = \pm 1/2$, respectively. The first three $\sum_{\langle\rangle}$ refer to the summation over the nearest neighbor pairs; the other summations, however, are taken over the lattice points. J_s is the