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Magnetic properties and thermodynamics in a metallic nanotube

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ABSTRACT

A metallic nanotube composed of the ferromagnetic spin-3/2 inner shell and spin-1 outer shell with a ferrimagnetic interlayer coupling has been studied by using the effective-field theory with correlations (EFT). With both existence of the magnetic anisotropy and transverse field, we have studied effects of them on the magnetic properties and the thermodynamics. Some interesting phenomena have been found in the phase diagrams. At low temperature, the magnetization curves present different behaviors. Two compensation points have been found for the certain values of the system parameters in the system. The research results of metallic nanotubes may have potential applications in the fields of biomedicine and molecular devices.

1. Introduction

Nanotube has attracted more attention since it found by Ijima in 1991 [1]. Because of the potential applications of nanotubes in different research fields, such as electronics, optics, mechanics, and even biology, many investigators have committed themselves to the nanotubes research [2–6]. In particular, metalliclic nanotubes have hollow structures with inner and outer active surface and magnetism, which gradually become an important kind of functional nanomaterials. For example, magnetic metallic nanotubes, which can be used to load drug, are expected to become an intelligent remote control of drugs and clinical diagnosis of new materials. They may have potential applications in molecular devices and because of hollow probe is more likely to reverse magnetization than solid probe. Magnetic metallic nanotubes can be composite by various experimental techniques [7,8]. Ni nanotube has been fabricated on silicon substrate using an anodic aluminum oxide/polypyrrole composite template. Magnetic measurements show that the magnetic anisotropic properties are strongly dependent on the wall thickness of nanotubes. Theoretical analysis and micromagnetic simulation have been performed to explain the wall thickness-dependent anisotropic behavior [9]. FeNi nanotubes have been successfully synthesized in pores of anodic aluminum oxide templates by the wetting template method [10]. And the macroscopic magnetic measurements show that FeNi nanotube arrays with obvious anisotropy, and the easy axis is parallel to the nanotube axis [11]. Steinhart et al. have prepared the Cr-doped Bi_2Te_3 nanotubes via wet chemical reaction. The nanotube appears ferromagnetic behavior, which exists even beyond room temperature, and large saturation magnetization. Also, these nanotubes exhibit infrared active modes in the Raman spectra due to its one-dimensional nature [12]. Experimental and theoretical results indicate that the magnetic anisotropy plays an important role in magnetic properties of the magnetic metallic nanotubes [13,14].

Seen from the perspective of the theory, these systems have been investigated by various numerical simulations [15–19]. Magnetic behaviors of ferromagnetic single-walled nanotubes are systematically investigated using the many-body Green's function method of the quantum statistical theory. The spontaneous magnetization, area of hysteresis loop and coercivity increase with diameter of the tubes and spin quantum number. Curie temperature increases with the diameter and the spin quantum number [20]. The properties of nanotubes have been studied by Monte Carlo simulations based on the plane with the square unit cell at low temperature [21,22]. We also studied the magnetic properties and critical behavior of a molecular-based magnetic film $AFe^{II}Fe^{III}(C_2O_4)_3(A{=}N(n-C_nH_{2n+1})_4,\ n{=}3\text{–}5)$ by using Monte Carlo simulations. The effects of surface exchange coupling, surface single-ion anisotropy and layer thickness on the compensation temperature and critical temperature of a ferrimagnetic mixed spin-2 and spin-5/2 Ising model on a honeycomb lattice have been discussed in detail [23]. Among these techniques, there is an efficient method called the effective field theory with correlations (EFT) [24,25]. Kaneyoshi has been using the EFT to discuss the phase diagrams and magnetizations of cylindrical transverse Ising nanotube. He has found that the phase diagrams of the system are strongly affected by the surface dilution.

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The possibility of two compensation points has also been found in his report [26,27]. Magnetizations and hysteresis loops of a cylindrical Ising nanotube in an oscillating magnetic field within the effective-field theory have been studied. And different types of compensation behaviors have been found [28]. However, the behavior of magnetic nanotubes with transverse fields and magnetic anisotropy existing simultaneously has not been studied. In our previous works [29–32], by using the EFT, we have succeeded in establishing the transverse Ising model with the magnetic anisotropy. The changing regularity of the phase diagrams and magnetizations depending on the physical parameters have been clearly found. Therefore, in the paper, we intend to continue to apply this theory (EFT) to study the magnetic properties and the thermodynamics of the magnetic metallic nanotubes.

The structure of this paper is as follows: In Section 2, we briefly introduce the basic framework of the effective field theory and the formulation for a double-wall hexagonal metallic nanotube. In Section 3, typical numerical results for the phase diagrams, the magnetizations and the internal energy of the system are studied in detail. Finally, Section 4 is devoted to the summary.

2. Formulation

Among many experimental results, we select a typical nanotube, double-wall hexagonal nanotube, as is depicted in Fig. 1 (a) and (b). The system consists of a ferromagnetic inner layer surrounded by a ferromagnetic outer layer. We suppose that the inner sites (big balls denote metallic Cr) are occupied by A sublattices with spin-3/2, while the outer sites (small balls denote metallic Ni) are occupied by B sublattices with spin-1. $J_a(>0)$ and $J_b(>0)$ are intralayer ferromagnetic exchange coupling, and $J_{ab}(<0)$ is the interlayer ferrimagnetic exchange coupling.

So the Hamiltonian of the system is expressed as follows:

$$H=-J_a\sum_{i,j}\sigma_i^z\sigma_j^z-J_{ab}\sum_{i,m}\sigma_i^zS_m^z-J_b\sum_{m,n}S_m^zS_n^z-\Omega_a\sum_i\sigma_i^x -\Omega_b\sum_m S_m^x-D_a\sum_i(\sigma_i^z)^2-D_b\sum_m(S_m^z)^2 \quad (1)$$

Where σ_i^z and S_j^z are spin-3/2 and spin-1 operator on sublattices A and B, respectively. $D_a(D_b)$ and $\Omega_a(\Omega_b)$ represent the magnetic anisotropy and the transverse field in the system, which comes from sublattice $A(B)$, respectively.

We can divide the model into three spins, as is shown in Fig. 1. Within the effective-field theory [26,31,33], their the longitudinal magnetizations (M_i, $i=1, 2, 3$) can be shown as

$$M_1=[n_1\times\exp(J_a\eta_1\nabla)+n_2\times\exp(-J_a\eta_1\nabla)]^4 \times[n_3\times\exp(J_{ab}\eta_2\nabla)+n_4\times\exp(-J_{ab}\eta_2\nabla)]^2 \times[n_5\times\exp(J_{ab}\eta_3\nabla)+n_6\times\exp(-J_{ab}\eta_3\nabla)]f_a(x)|_{x=0}, \quad (2)$$

$$M_2=[n_1\times\exp(J_{ab}\eta_1\nabla)+n_2\times\exp(-J_{ab}\eta_1\nabla)]^2 \times[n_3\times\exp(J_b\eta_2\nabla)+n_4\times\exp(-J_b\eta_2\nabla)]^2 \times[n_5\times\exp(J_b\eta_3\nabla)+n_6\times\exp(-J_b\eta_3\nabla)]^2f_b(x)|_{x=0}, \quad (3)$$

$$M_3=[n_1\times\exp(J_{ab}\eta_1\nabla)+n_2\times\exp(-J_{ab}\eta_1\nabla)] \times[n_3\times\exp(J_b\eta_2\nabla)+n_4\times\exp(-J_b\eta_2\nabla)]^2 \times[n_5\times\exp(J_b\eta_3\nabla)+n_6\times\exp(-J_b\eta_3\nabla)]^2f_b(x)|_{x=0}, \quad (4)$$

Here, M_1 is the longitudinal magnetization of the sublattices in the inner layer, and M_2 and M_3 are the longitudinal magnetizations of the two different sublattices in the outer layer. Then the corresponding transverse magnetizations of the system are defined by

$$M_{1x}=[n_1\times\exp(J_a\eta_1\nabla)+n_2\times\exp(-J_a\eta_1\nabla)]^4 \times[n_3\times\exp(J_{ab}\eta_2\nabla)+n_4\times\exp(-J_{ab}\eta_2\nabla)]^2 \times[n_5\times\exp(J_{ab}\eta_3\nabla)+n_6\times\exp(-J_{ab}\eta_3\nabla)]h_a(x)|_{x=0}, \quad (5)$$

$$M_{2x}=[n_1\times\exp(J_{ab}\eta_1\nabla)+n_2\times\exp(-J_{ab}\eta_1\nabla)]^2 \times[n_3\times\exp(J_b\eta_2\nabla)+n_4\times\exp(-J_b\eta_2\nabla)]^2 \times[n_5\times\exp(J_b\eta_3\nabla)+n_6\times\exp(-J_b\eta_3\nabla)]^2h_b(x)|_{x=0}, \quad (6)$$

$$M_{3x}=[n_1\times\exp(J_{ab}\eta_1\nabla)+n_2\times\exp(-J_{ab}\eta_1\nabla)] \times[n_3\times\exp(J_b\eta_2\nabla)+n_4\times\exp(-J_b\eta_2\nabla)]^2 \times[n_5\times\exp(J_b\eta_3\nabla)+n_6\times\exp(-J_b\eta_3\nabla)]^2h_b(x)|_{x=0}, \quad (7)$$

where $\nabla=\partial/\partial x$ is a differential operator in the differential operator technique, and η_1^2, η_2^2 and η_3^2 are

$$\eta_1^2=[n_1\times\exp(J_a\eta_1\nabla)+n_2\times\exp(-J_a\eta_1\nabla)]^4 \times[n_3\times\exp(J_{ab}\eta_2\nabla)+n_4\times\exp(-J_{ab}\eta_2\nabla)]^2 \times[n_5\times\exp(J_{ab}\eta_3\nabla)+n_6\times\exp(-J_{ab}\eta_3\nabla)]g_a(x)|_{x=0}, \quad (8)$$

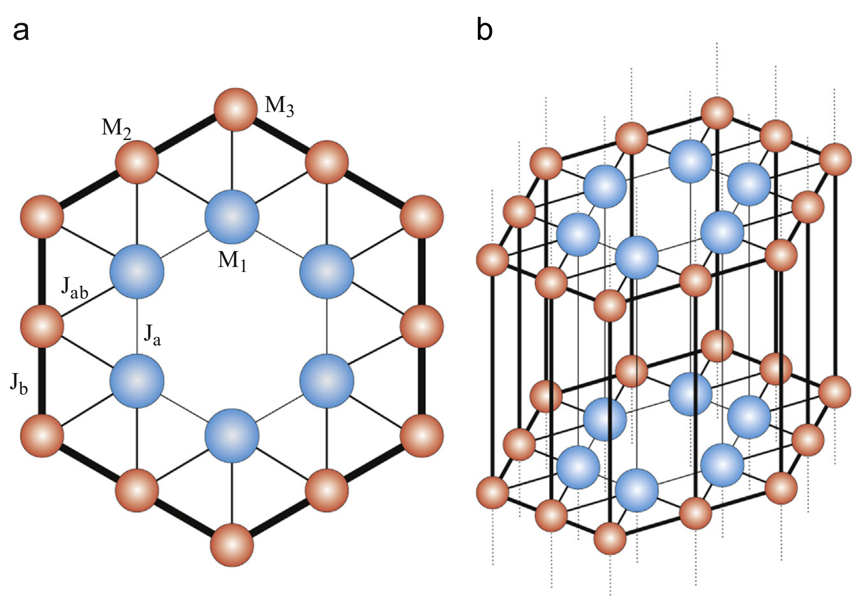

Fig. 1. Schematic diagram of a ferrimagnetic hexagonal nanotube with spin-3/2 inner layer (small balls denote metallic Ni) and spin-1 outer layer (big balls denote metallic Cr). (a) Cross-section and (b) three-dimensional.