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The effects of random field at surface on the magnetic properties in the Ising nanotube and nanowire

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The phase diagrams and temperature dependences of total magnetization m_T in two nanosystems (nanotube and nanowire) with a random magnetic field at the surface shell are studied by the uses of the effective-field theory with correlations. Some characteristic phenomena (reentrant phenomena and unconventional thermal variation of total magnetization) are found in the two systems. They are rather different between the two systems, which mainly come from the structural differences of the cores

1. Introduction

Nowadays, a lot of theoretical works on the various types of magnetic nanowires and nanotubes have been investigated by using the core–shell concept, after the pioneer work [1]. In these works, the spin configurations in the core and shell are normally ferromagnetic or ferrimagnetic. In these systems, surface effects particularly give the distinct contributions to the magnetic properties, since a large fraction of the atoms in them exist at the surface. They become more important when reducing the size of the materials. In particular, one should notice that the magnetic nanosystems become single domain experimentally in contrast to multidomain structures of bulk magnetic materials, when the size reduces below a critical value. The magnetic properties of these systems have been studied by using a variety of theoretical techniques, mainly the mean-field theory (MFA), the effective-field theory with correlations (EFT) and the Monte Carlo simulation (MC) (For the references, see the recent works [2–5]). The recent works for nanosystems [6,7] prove that the results obtained from the EFT have the same topology as those obtained from the MC, while the results obtained from the MC are smaller than those of the EFT. The EFT corresponds to the Zernike approximation [8] and it is believed to give more exact results than those of the MFA, since it includes automatically some correlations between a central spin and the near neighbor spins.

In particular, the possibilities of various types of reentrant phenomena have been investigated theoretically for a variety of nanoscaled magnetic materials. In [9–12], the possibility of a new type of reentrant phenomena which is free from disorder induced frustration has been discussed by the use of the EFT. Traditionally, the reentrant phenomena have been found in a variety of disordered magnetic systems experimentally and theoretically [13,14], especially spin glass systems in which the effects of frustration due to the change of sign in exchange interactions play important ingredient. A ferromagnet in a random field also exhibits the reentrant phenomena, which is equivalent to the Ising antiferromagnet with randomly quenched exchange interactions in a uniform field [15]. In [16], the phase diagrams and thermal variations of magnetizations in the Ising nanowire with a spin glass like disorder at the surface have been examined within the EFT. We have found the two types of reentrant phenomena, induced by the surface effects, namely the spin glass like disorder at the surface shell and the core–shell coupling. In [17,18], within the theoretical framework of the EFT, the possibility of the reentrant phenomena, the phase diagram and the hysteresis have been investigated for the cylindrical Ising nanowire with the same structural aspect as that of [1], using the trimodal distribution [17] and the bimodal distribution [18] for the magnetic fields of the core and shell. In each case, there exist two transition temperatures (T_1 and T_2, $T_1 < T_2$), where the first-order transition occurs at $T=T_1$ and the second-order transition has been obtained at $T=T_2$. Using the trimodal distribution of magnetic fields acting on the

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core and the shell, the possibility of the reentrant phenomena and the magnetic properties in the spin-1 cylindrical Ising nanotube with the sane structural aspect as that of [1] have also been examined in [19], within the theoretical framework of the EFT. The reentrant phenomena obtained in the work are essentially similar to those of [17,18].

Recently, some experimental data [20,21] have been reported for magnetic nanoparticles, in which the reentrant spin glass state is predicted to exist at low temperatures. The experimental data [20] for the γ–Fe_2O_2 nanoparticles indicate that the phenomena can be well-described by the random-field model of exchange anisotropy. In particular, the experimental data of [21] for $TbCu_3$ nanoparticles imply that the phenomena come from the spin-glass like state at the surface shell. As far as we know, theoretically, the effects of random magnetic field at the surface shell on the magnetic properties in the cylindrical Ising nanotube and nanowire with the same structural aspects as those of [1] have not been discussed. Accordingly, the aim of this work is, within the theoretical framework of the EFT [22,23], to clarify whether the magnetic properties (phase diagram and thermal variation of total magnetization) of cylindrical Ising nanotube and nanowire with the same structural aspects as those of [1] show the same behaviors as those predicted in [17–19] or not. In Section 2, the models and formulations for the two Ising nanosystems are given. In Section 3, the phase diagram and the thermal variations of magnetizations in the nanotube are given. In Section 4, the phase diagram and the thermal variations of magnetizations in the nanowire are discussed. From these investigations, we have found that the results obtained in this work are rather different from those predicted in [17–19]. In Section 5, the summary of this work is given.

2. Models and formulations

The schematic representations of cylindrical Ising nanotube (A) and nanowire (B) are depicted in Fig. 1, which have the same structural aspects as those of [1]. It is consisted of the surface shell (white circles) and the core (black circles). The each site in the figure is occupied by a Ising spin. The each spin is connected to the two nearest neighbor spins on the above and below sections. The surface shell is coupled to the next shell in the core with an exchange interaction J_1.

The Hamiltonian of the two systems is given by

$$H = -J_S\sum_{(ij)}\mu_i\mu_j - J\sum_{(mn)}\mu_m\mu_n - J_1\sum_{(im)}\mu_t\mu_m - \sum_{(i)} H_i\mu_i, \tag{1}$$

where μ_i is the Ising spin operator with $\mu_i = \pm 1$. The J_S is the exchange interaction between two nearest-neighbor magnetic atoms at the surface shell and the J ($J > 0.0$) is the exchange interaction in the core. The surface exchange interaction J_S is here defined as

$$J_S = J(1 + \Delta_S) \quad . \tag{2}$$

The last term of (1) represents the random magnetic field acting only at the surface lattice sites. It is distributed according to the bimodal distribution, namely

$$P(H_i) = \left[\delta(H_i - H) + \delta(H_i + H)\right]/2.0 \tag{3}$$

Let us at first define the total magnetization m_T per site in the nanowire as follows;

$$m_T = \frac{1}{19}\left[12m_S + 7m_C\right] \quad , \tag{4}$$

with

$$m_S = \frac{1}{2}(m_{S1} + m_{S2}) \quad , \tag{5}$$

$$m_C = \frac{1}{7}(6m_{C1} + m_{C2}) \quad , \tag{6}$$

where m_S is the averaged magnetization per site at the surface shell and m_C is the averaged magnetization per site in the core. Also, the total longitudinal magnetization per site in the nanotube is given by

$$m_T = \frac{1}{2}[m_S + m_C] \quad , \tag{7}$$

where m_S is also defined by (5) and m_C represents the magnetization per site in the core (or black circle), which is given by the following Eq. (15).

As discussed in [1], within the framework of the EFT [22,23], the magnetizations in the nanowire can be given by

$$m_{S1} = \left[\cosh(A) + m_{S1}\sinh(A)\right]^2\left[\cosh(A) + m_{S2}\sinh(A)\right]^2 \left[\cosh(B) + m_{C1}\sinh(B)\right] F_S(x)\Big|_{x=0} \tag{8}$$

$$m_{S2} = \left[\cosh(A) + m_{S2}\sinh(A)\right]^2\left[\cosh(A) + m_{S1}\sinh(A)\right]^2 \left[\cosh(B) + m_{C1}\sinh(B)\right]^2 F_S(x)|_{x=0} \tag{9}$$

$$m_{C1} = \left[\cosh(C) + m_{C1}\sinh(C)\right]^4\left[\cosh(C) + m_{C2}\sinh(C)\right] \left[\cosh(B)+m_{S1}\sinh(B)\right]\left[\cosh(B)+m_{S2}\sinh(B)\right]^2 F(x)\Big|_{x=0,} \tag{10}$$

$$m_{C2} = \left[\cosh(C) + m_{C2}\sinh(C)\right]^2\left[\cosh(C) + m_{C1}\sinh(C)\right]^6 F(x)|_{x=0} \tag{11}$$

where A, B and C are defined by $A{=}J_SD$, $B{=}J_1D$ and $C{=}JD.D{=}\partial/\partial x$ is the differential operator. Here, the functions $F_S(x)$ and $F(x)$ are defined by

$$F_S(x) = \int F(x + H_i)\,P(H_i)\,dH_i \text{and} F(x) = \tanh(\beta x) \quad , \tag{12}$$

where $\beta = 1/k_BT$ and T is a temperature. The magnetizations in the nanotube are given by

$$m_{S1} = \left[\cosh(A) + m_{S1}\sinh(A)\right]^2\left[\cosh(A) + m_{S2}\sinh(A)\right]^2 \left[\cosh(B) + m_C\sinh(B)\right] F_S(x)\Big|_{x=0} \tag{13}$$

$$m_{S2} = \left[\cosh(A) + m_{S2}\sinh(A)\right]^2\left[\cosh(A) + m_{S1}\sinh(A)\right]^2 \left[\cosh(B) + m_C\sinh(B)\right]^2 F_S(x)|_{x=0} \tag{14}$$

$$m_C = \left[\cosh(C) + m_C\sinh(C)\right]^4\left[\cosh(B)+m_{S1}\sinh(B)\right] \left[\cosh(B)+m_{S2}\sinh(B)\right]^2 F(x)|_{x=0,} \tag{15}$$

At this place, the phase diagram (transition temperature T_C) can be obtained by expanding linearly the right-hand side of the coupled equations, namely from (8)–(11) for the nanowire and from (13)–(15) for the nanotube. The formulations of the two systems have been discussed in [1], so that it will not be given