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Reentrant phenomena in a transverse Ising nanowire (or nanotube) with a diluted surface: Effects of interlayer coupling at the surface

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ABSTRACT

The phase diagrams and magnetizations of two transverse Ising nanosystems (nanowire and nanotube) with a dilution at the surface are investigated by the use of the effective field theory with correlations. In particular, the effects of interlayer coupling between the surface and the core on them are discussed for the two systems. We find that the reentrant phenomena are obtained for the two systems with pure surface, while they immediately disappear when the surface dilution has been introduced.

1. Introduction

The reentrant phenomena have been found in a variety of disordered magnetic systems experimentally and theoretically [1,2], especially spin glass systems in which the effects of frustration due to the change of sign in exchange interactions play as an important ingredient. A ferromagnet in a random field also exhibits the reentrant phenomena, which are equivalent to the Ising antiferromagnet with randomly quenched exchange interactions in a uniform field [3,4]. Free from these disorder induced frustrations, the reentrant phenomena of another type have been found in decorated Ising spin systems [5–7].

Nowadays, the growing interest is continuously directed to the magnetic properties of a material with a nanostructure, such as nanoscaled thin films, nanoparticles, nanotubes and nanowires. This is motivated by numerous possibilities of their applications in nanotechnology. When the size of a magnetic material decreases to a nanometer scale, magnetic properties of a simple magnetic material (for example, ferromagnetic material such as Fe or Co) will be a complex function of finite-size, defects, and surface effects. The physics of these effects governs the nanomagnetism of a material and point to the new way of finding important possible applications. In a series of recent works [8–16], we have examined the magnetic properties of these nanoscaled magnetic systems by the use of the effective-field theory with correlations (EFT) [17,18]. The EFT corresponds to the Zernike approximation [19] and it is believed to give more exact results than those of the mean field theory. In these works, we have found that the magnetic properties in nanoscaled Ising materials are strongly influenced by finite-size, dilution and surface effects. A variety of characteristic phenomena has been obtained for these systems, such as the possibility of two compensation points, which originate from the negative interlayer coupling J_1 between the surface and the next inner layer. Furthermore, the phase diagrams (or transition temperature versus $|r|$ plot) in nanoscaled systems have exhibited a broad maximum in the region with $|r| > 1.0$, where $r = J_1/J$ and J is the exchange interaction in the inner layer. As far as we know, however, the possibility of reentrant phenomena has not been discussed for these nanoscaled systems except for few works [20,21].

The aim of this work is, within the theoretical framework of the EFT, to investigate the effects of r on the phase diagram in the two transverse Ising nanosystems (nanowire and nanotube) with a dilution at the surface, when the value of p ($p = \Omega_S/\Omega$) is changed. Ω_S and Ω are the transverse fields at the surface and in the inner layers. In Section 2, we define the model and give briefly the formulations of the two systems, since they have been given in Refs. [8–16]. The numerical results of the phase diagrams and the magnetizations in the two systems are discussed in Section 3, especially in order to clarify whether the reentrant phenomena are possible in the present systems or not.

2. Model and formulation

We consider a Ising nanowire (or nanotube) with a dilution at the surface, as depicted in Fig. 1, in which the wire (or tube) is consisted of the surface shell and the core. The each site on the figure is occupied by a Ising spin, while the surface shell is diluted

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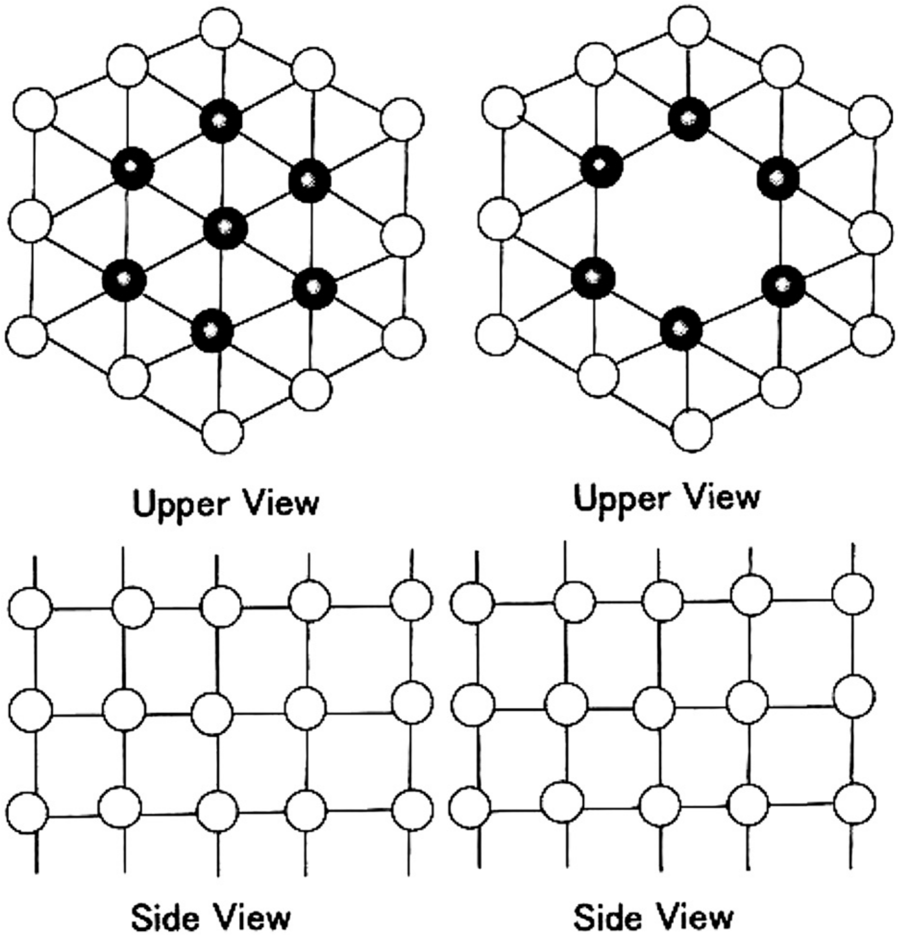

Fig. 1. Schematic representations of a cylindrical nanowire (left hand side) and a cylindrical nanotube (right hand side). The white circles represent magnetic (or non-magnetic) atoms at the surface shell. The black circles are magnetic atoms constituting the core. The lines connecting the white and black circles represent the nearest-neighbor exchange interactions (J_S, J_1 and J).

by non-magnetic atoms. 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 system is given by

$$\mathrm{H} = -J_S \sum_{(ij)} \sigma_i^z \sigma_i^z \xi_i \xi_j - J \sum_{(mn)} \sigma_m^z \sigma_n^z - J_1 \sum_{(im)} \sigma_i^z \xi_i \sigma_m^z - \Omega_S \sum_{(i)} \sigma_i^x \xi_i - \Omega \sum_{(m)} \sigma_m^x, \tag{1}$$

where σ (α=z, x) is the Pauli spin operator with $\sigma_i{}^z = \pm 1$. J_S is the exchange interaction between two nearest-neighbor magnetic atoms at the surface shell and J is the exchange interaction in the core. Ω_S and Ω represent the transverse fields at the surface shell and in the core, respectively. The parameter ξ_i is a site occupancy number that is 1 or zero, depending on whether the site is occupied or not. Since only the surface is diluted in the present system, ξ_i takes unity with a probability q when the site i is occupied by a magnetic atom and takes 0 with a probability $(1-q)$ when the site i on the surface is occupied by a non-magnetic atom. The surface exchange interaction J_S is often defined as

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

in order to clarify the effects of surface on the physical properties in the system.

Let us first define the total magnetization m_T^α (α=z and x) per site in the two systems. They are given by

$$m_T^\alpha = \frac{1}{(12q+7)}\left[6q(m_{S1}^\alpha + m_{S2}^\alpha) + 6m_{C2}^\alpha + m_{C1}^\alpha\right] \tag{3}$$

for the nanowire and,

$$m_T^\alpha = \frac{1}{(2q+1)}\left[q(m_{S1}^\alpha + m_{S2}^\alpha) + m_C^\alpha\right] \tag{4}$$

for the nanotube, where m_{S1}^α, m_{S2}^α and m_C^α, m_{C1}^α, m_{C2}^α are, respectively, the longitudinal (z) and transverse (x) magnetizations at the surface and the core.

As has been discussed in Refs. [8–16], within the theoretical framework of the EFT [17,18], we can easily obtain these magnetizations at the surface shell and the core, such as for the longitudinal magnetizations (m_{S1}=m_{S1}^z, m_{S2}=m_{S2}^z and m_C=m_C^z) in the nanotube

$$m_{S1} = [q\{\cosh(A) + m_{S1}\sinh(A)\} + 1 - q]^2 [q\{\cosh(A) + m_{S2}\sinh(A)\} + 1 - q]^2 [\cosh(B) + m_C \sinh(B)] f_S(x)|_{x=0} \tag{5}$$

$$m_{S2} = [q\{\cosh(A) + m_{S2}\sinh(A)\} + 1 - q]^2 [q\{\cosh(A) + m_{S1}\sinh(A)\} + 1 - q]^2 [\cosh(B) + m_C \sinh(B)]^2 f_S(x)|_{x=0} \tag{6}$$

$$m_C = [\cosh(C) + m_C \sinh(C)]^4 [\cosh(B) + m_{S1}\sinh(B)][\cosh(B) + m_{S2}\sinh(B)]^2 f(x)|_{x=0} \tag{7}$$

with

$$f_S(x) = (x/y_S)\tanh(\beta y_S) \text{ and } f(x) = (x/y)\tanh(\beta y) \tag{8}$$

with

$$y_S = (x^2 + \Omega_S{}^2)^{1/2} \text{ and } y = (x^2 + \Omega^2)^{1/2}, \tag{9}$$