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Phase diagrams and magnetic properties of a cylindrical Ising nanowire: Monte Carlo and effective field treatments

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ABSTRACT

The Monte Carlo simulation (MCS) technique has been used to study the phase diagrams and the magnetic properties of a cylindrical core/shell spin 1/2 Ising nanowire. The system mainly consists of two parts: the core and the surface shells, and the core is surrounded by the surface shell. The effects of the surface parameters and the random longitudinal field, on the critical and compensation behaviors, are examined. The results present rich critical behavior, which includes the first- and second-order phase transitions. It is also found that the compensation point can appear for appropriate values of the system parameters. The hysteresis curves are obtained for different temperatures (T). The triple hysteresis loops can be seen in the system for antiferromagnetic interactions. The effective filed theory (EFT) results are compared to those obtained by using the Monte Carlo Simulations. However, EFT predicts the same topology of the phase diagrams as the Monte Carlo Simulations.

1. Introduction

One focus of the physics today is the investigation of the properties of a small assembly of atoms. Notably, nanoparticle magnetism is one of these topics under study, especially due to the large variety of new structures that can be produced with interesting physical properties. The investigation and improvement of these properties can lead to the discovery of advanced magnetic materials with great impact on the new technologies [1,2]. From the technological point of view, their potential application in magnetic recording media [3,4] is responsible for a great interest. Indeed, sufficiently small ferromagnetic nanoparticles are single domain [5,6] and are good candidates for high density storage.

The magnetic nanowires have been successfully fabricated by various methods. They have received considerable attention experimentally due to their distinctive properties and potential applications [7,8]. There is now experimental evidence concerning deviations from bulk behavior. The magnetic properties are strongly influenced by finite size and surface effects, a fact that has given a strong motivation for the investigations of magnetic nanowires.

The Ising model has been applied successfully to the investigation of a nanostructure materials, such as nanowire and nanotube. These systems can be modeled by core–shell models which can also be solved by EFT, MFA and MC. Recently, Kaneyoshi has studied the phase diagrams and the magnetic properties of magnetic nanostructure, such as nanowire, nanotube and nanoparticle by using the effective field theory [9–15] and by using MFA and EFT [16,17]. In Ref. [16], Kaneyoshi has studied the phase diagrams of a cylindrical nanowire composed of two layers in the core and a single layer on the surface. Some characteristic phenomena are found in the phase diagram, depending on the ratio of the physical parameters in the surface shell and the core. The initial susceptibility of the nanowire and nanotube has been investigated by using EFT [12,13], the hysteresis behavior of the nanowire within EFT [18,19], the effect of the diluted surface on the phase diagrams and the magnetic properties of the nanowire and nanotube have been also studied [20–23]. Beside these, higher spin nanowire or nanotube has been investigated, e.g. spin-1 nanowire [24,25] and nanotube [26], and mixed spin 1/2, 1 nanotube or nanowire [27,28].

In this work, the phase diagrams and the magnetic properties of a cylindrical Ising nanowire with three ($S=3$) shells are examined. In our analysis, we have used Monte Carlo technique according to the heat bath algorithm [29] and we have compared the simulation results with those of effective field theory [30]. The outline of this paper is as follows: In Section 2, we define the model and review the basic points of the Monte Carlo approach and the effective field theory. In Section 3, the numerical results are discussed and we present our concluding remarks in Section 4.

2. Model and formalism

We consider a cylindrical Ising nanowire, as depicted in Fig. 1, in which the wire consists of the surface shell and the core.

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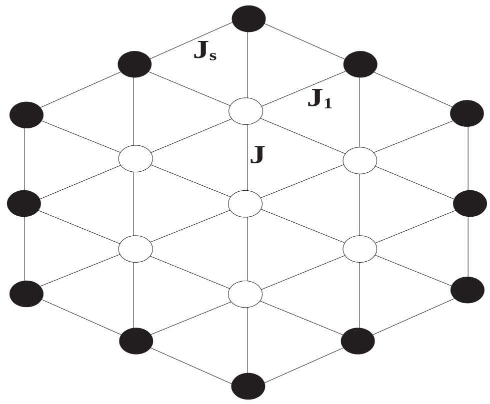

Fig. 1. A schematic cross-section of a cylindrical nanowire. The black and the white circles represent the surface shell and the core spin 1/2 atoms.

Each site on the figure is occupied by a spin 1/2 Ising particle. The hamiltonian of the system is given by

$$H=-J_s\sum_{i,j}\sigma_i^z\sigma_j^z-J\sum_{m,n}\sigma_m^z\sigma_n^z-J_1\sum_{i,m}\sigma_i^z\sigma_m^z-\sum_i H_i\sigma_i^z-H\left(\sum_i\sigma_i^z+\sum_m\sigma_m^z\right) \quad (1)$$

where σ_i is the z component of the spin at a lattice site i and it takes the values $\sigma_i=\pm1$ for the spin 1/2 system; J_s is the exchange interaction between two nearest neighbor magnetic atoms at the surface shell; J is the exchange interaction in the core and J_1 is the exchange interaction between the spins in the surface shell and the next shell in the core. H is an external magnetic field; H_i is the random magnetic fields acting on σ_i, distributed according to a bimodal distribution:

$$p(H_i)=\tfrac{1}{2}(\delta(H_i-H_0)+\delta(H_i+H_0)) \quad (2)$$

Our system consists of three shells, namely one shell of the surface and two shells in the core, the surface shell contains $N_s\times L$ spins, and the core contains $N_c\times L$ spins. The total number of spins in the wire is $N_T=(N_s+N_c)L$. $N_s=12$, $N_c=7$ and $L=300$. N_s and N_c are the spin numbers, of the nanowire cross section, of the surface and of the core, respectively, and L denotes the wire lengths. We use Monte Carlo Simulation and we flip the spins once a time, according to the heat bath algorithm [29]. 4×10^4 Monte Carlo steps are used to obtain each data point in the system, after discarding the first 10^4 steps. The magnetization M of a configuration is defined by the sum over all the spin values of the lattice sites, the critical temperature is determined from the peak of the susceptibility. The error bars are calculated with a jackknife method [31] by taking all the measurements and grouping them in 20 blocks. The magnetizations of the surface shell, the core and the total system per site are defined by

$$M_{\mathrm{Shell}}=\frac{1}{N_S}\sum_{k=1}^{N_S}\sigma_k \quad (3)$$

$$M_{\mathrm{Core}}=\frac{1}{N_C}\sum_{m=1}^{N_C}\sigma_m \quad (4)$$

$$M_T=\frac{12M_{\mathrm{Shell}}+7M_{\mathrm{Core}}}{19} \quad (5)$$

The total susceptibility χ_T is defined by

$$\chi_T=\beta N_T(\langle M^2\rangle-\langle M\rangle^2) \quad (6)$$

with $\beta=1/K_BT$, K_B is the Boltzman constant.

On the other hand, in the framework of the well known effective field theory based on the use of a probability distribution technique [30]. The longitudinal site order parameters are given by

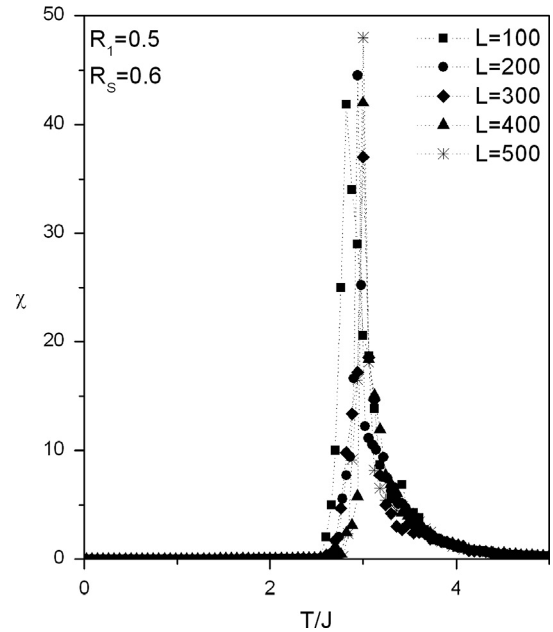

Fig. 2. The total susceptibility versus T/J for $R_1=0.5$, $R_S=0.6$, $H_0/J=0.0$ and for different lengths of wire.

For the central site:

$$m_{c1}=2^{-(N2+N4)}\sum_{i1=0}^{N2}\sum_{i2=0}^{N4}C_{i1}^{N2}C_{i2}^{N4}(1-2m_{c1})^{i1}(1+2m_{c1})^{N2-i1}\times(1-2m_{c2})^{i2}(1+2m_{c2})^{N4-i2}\times\left(\frac{F(X_{c1},H,H_0)+F(X_{c1},H,-H_0)}{2}\right) \quad (7)$$

For the first shell of the core:

$$m_{c2}=2^{-(N2+2N1+N3)}\sum_{i1=0}^{N3}\sum_{i2=0}^{N1}\sum_{i3=0}^{N1}\sum_{i4=0}^{N2}C_{i1}^{N3}C_{i2}^{N1}C_{i3}^{N1}C_{i4}^{N2}(1-2m_{c2})^{i1}\times(1+2m_{c2})^{N3-i1}\times(1-2m_{c1})^{i2}(1+2m_{c1})^{N1-i2}(1-2m_{S1})^{i3}(1+2m_{S1})^{N1-i3}\times(1-2m_{S2})^{i4}(1+2m_{S2})^{N2-i4}\times\left(\frac{F(X_{c2},H,H_0)+F(X_{c2},H,-H_0)}{2}\right) \quad (8)$$

For the spins of type-1 surface shell:

$$m_{s1}=2^{-(2N2+N1)}\sum_{i1=0}^{N2}\sum_{i2=0}^{N2}\sum_{i3=0}^{N1}C_{i1}^{N2}C_{i2}^{N2}C_{i3}^{N1}(1-2m_{s1})^{i1}(1+2m_{s1})^{N2-i1}\times(1-2m_{s2})^{i2}(1+2m_{s2})^{N2-i2}(1-2m_{c2})^{i3}(1+2m_{c2})^{N1-i3}\times\left(\frac{F(X_{s1},H,H_0)+F(X_{s1},H,-H_0)}{2}\right) \quad (9)$$

For the spins of type-2 surface shell:

$$m_{s2}=2^{-3N2}\sum_{i1=0}^{N2}\sum_{i2=0}^{N2}\sum_{i3=0}^{N2}C_{i1}^{N2}C_{i2}^{N2}C_{i3}^{N2}(1-2m_{s2})^{i1}(1+2m_{s2})^{N2-i1}\times(1-2m_{s1})^{i2}(1+2m_{s1})^{N2-i2}(1-2m_{c2})^{i3}(1+2m_{c2})^{N2-i3}\times\left(\frac{F(X_{s2},H,H_0)+F(X_{s2},H,-H_0)}{2}\right) \quad (10)$$

where

$X_{c1}=(N2+N4)-2(i1+i2)$

$X_{c2}=(N3+N1-2(i1+i2))+R_1(N1+N2-2(i3+i4))$

$X_{s1}=R_s(2N2-2(i_1+i_2))+R_1(N1-2i3)$

$X_{s2}=R_s(2N2-2(i_1+i_2))+R_1(N2-2i3)$