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Random crystal field effect on the magnetic and hysteresis behaviors of a spin-1 cylindrical nanowire

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ABSTRACT

In this work, the magnetic behavior of the cylindrical nanowire, consisting of a ferromagnetic core of spin-1 atoms surrounded by a ferromagnetic shell of spin-1 atoms is studied in the presence of a random crystal field interaction. Based on Metropolis algorithm, the Monte Carlo simulation has been used to investigate the effects of the concentration of the random crystal field p, the crystal field D and the shell exchange interaction J_s on the phase diagrams and the hysteresis behavior of the system. Some characteristic behaviors have been found, such as the first and second-order phase transitions joined by tricritical point for appropriate values of the system parameters, triple and isolated critical points can be also found. Depending on the Hamiltonian parameters, single, double and para hysteresis regions are explicitly determined.

1. Introduction

In the past few decades the attractiveness of magnetic behaviors of nanomaterials i.e. nanowires, nanoparticles, nanotubes, thin film and nanorods …etc, has been increased and their experimental and theoretical studies have been intensified [1–8]. The motivation in these papers is mainly due to the fact that nanomaterials have many peculiar physical properties compared with those of the bulk materials; and there are many potential applications where nanomaterials may become very important [9–12]. On the experimental side, a lot of inquiries have been undertaken to fabricate such nanomaterials by electron beam lithography, vapor liquid solid and wet chemical method [13–15]. On the theoretical side, a large variety of techniques and methods have been applied to determine the magnetic properties of these systems [16–22]. The phase diagrams and the magnetic properties of nanowire systems have been studied by means of the effective field theory EFT in many works [23–26]. It has been shown that, many interesting phenomena such as, the existence of the tricritical point, the critical end point and the reentrant behavior can be found. Albayrak [27] has studied the triangular Ising nanowire on the Bethe lattice by using the core-shell structure. The phase diagrams of the model are constructed only by second-order phase transition lines because of the frustration at low temperatures. In Ref. [28], the phase diagrams of a nanowire with mixed spin (1, 3/2) have been studied by EFT. Two compensation points can exist for certain values of the system parameters.

The randomness of the crystal field may change the critical behavior of the system considerably, therefore, the random crystal field RCF on the Blume-Capel model was studied by several authors [29–34]. Besides the approach adopted, in some of these papers and the choice of the RCF distribution is also different. However, in all cases the phase diagrams display a rich behavior with the presence of tricritical point, critical end point, as well as reentrant and double reentrant phenomena. Likewise, Boughrara et al. [35] have studied the magnetic properties of a spin-1 Blume-Capel thin film in the presence of a random crystal field within the framework of Monte Carlo simulation. They have shown that the phase diagram exhibits a rich variety of behaviors such as the double reentrant phenomena and the existence of tricritical points. The mixed spin-1 and spin-3/2 ferrimagnetic Ising system under the effects of different random crystal fields is studied in Ref. [36] within the mean field approach. It was found that the system presents phase transitions of second- and first-order types separated by tricritical points.

On the other hand, considerable progress has been recently made in the understanding of the magnetic hysteresis behaviors of nanomaterials. In particular, the hysteresis behaviors of these systems have been studied from both experimental [37–39] and theoretical point of view [40–42]. Magnetic hysteresis behaviors have been studied by various methods [43–47]. Jiang et al. [48] have studied the various shapes of the hysteresis loop of a cubic nanowire in the presence of the crystal field by using the effective field theory. For certain values of the system parameters at low temperature, a number of characteristic behaviors

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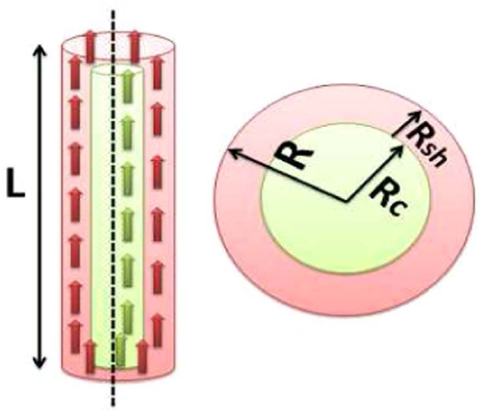

Fig. 1. Schematic representation of a ferromagnetic nanowire with cylindrical shape of length L and radius R.

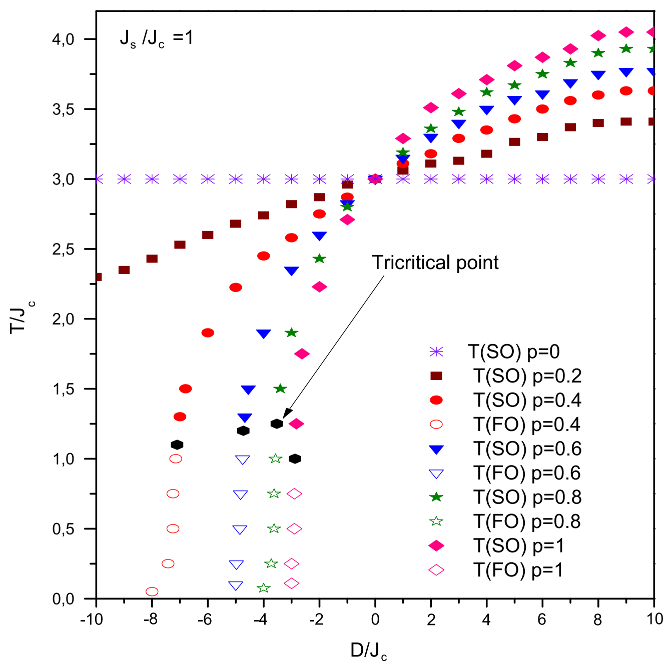

Fig. 2. The phase diagrams on the $(T/J_c, p)$ plane for $J_s/J_c = 1$ and for several values of random crystal field D (D=−5, −4, −3, −2, −1, 0, 1, 3 and 5).

are obtained especially for the triple and multiple hysteresis loop patterns. Recently, Akıncı [49] has investigated the hysteresis behaviors of the Blume-Capel model within the effective field approximation. The effect of the crystal field on the hysteresis behaviors was examined. The regions of the single, double, triple and paramagnetic hysteresis behaviors in $(d - t)$ plane are explicitly obtained in the space of the Hamiltonian parameters. Furthermore, in several studies based on the effective field theory [50,51], the authors paid attention to the effects of crystal field on the magnetic hysteresis behavior of the systems and they observed that the systems may exhibit multi-hysteresis loops, as well as singly hysteresis loop. Using Quantum Monte Carlo simulation, the hysteresis properties of a ferroelectric nanowire have been investigated [16]. It was found that for appropriate parameters, the system can exhibit triple hysteresis loops.

To our knowledge, no works have been directed to the study of phase diagrams and hysteresis behavior of a spin-1 nanowire with core/shell structure in the presence of random crystal field by using Monte Carlo simulation based on Metropolis algorithm. Therefore, the goal of this work is to study the effects of the random crystal field on the phase diagrams and the magnetic hysteresis behavior of a cylindrical nanowire with core/shell structure.

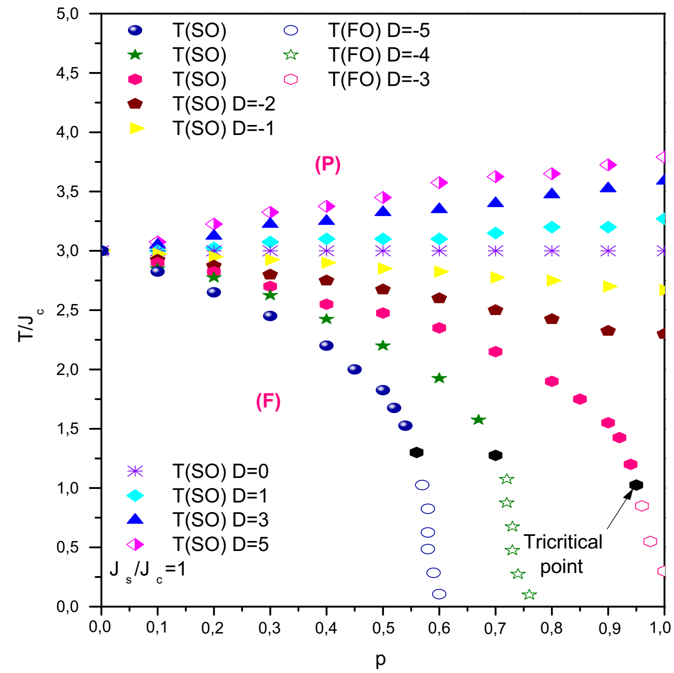

Fig. 3. The phase diagram on the $(T/J_c, D/J_c)$ plane for J_s/J_c1 and for different values of the concentration of crystal field p (p=0, 0.2, 0.4, 0.6, 0.8 and 1).

The organization of this work is as follows: In Section 2, we give the formalism and Monte Carlo simulation. In Section 3, we present the results and discussions, while Section 4 is devoted to a brief conclusion.

2. Model and Monte Carlo simulation

We have considered a ferromagnetic core/shell Ising nanowire model with cylindrical shape of length L and radius R, located on a simple cubic lattice. Two regions are distinguished inside the nanowire: a ferromagnetic core with radius R_c and a ferromagnetic shell of thickness $R_{sh} = R - R_c$. The sites of the nanowire are occupied by atoms of spin-1. The Hamiltonian of the system is given by:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - \sum_i D_i S_i^2 - H \sum_i S_i \tag{1}$$

where $S = \pm 1$, 0 are spin variables in the core and the shell. J_{ij} is the exchange interaction between two nearest neighbor magnetic atoms, it takes the value J_s in the shell and the value J_c otherwise (core and interface). We assume that H is the external magnetic field, D represents the crystal field interaction and D_i satisfy the random distribution defined by:

$$P(D_i) = p\delta(D_i - D) + (1 - p)\delta(D_i) \tag{2}$$

where p indicates the concentration of the random crystal field.

We use Monte Carlo simulation (MCS) based on Metropolis Algorithm [52,53]. We flip the spins once a time, according to the Metropolis algorithm. 3×10^4 Monte Carlo steps were used to obtain each data point in the system, after discarding the first 10^4 steps. We apply free boundary conditions in the x, y directions and periodic boundary conditions in the z direction. The results are reported for a cylindrical nanowire of length L=120. A number of additional simulations were performed for L=150 and L=200, but no significant differences have been found from the results presented here.

The magnetizations per site M_c of the core, M_{sh} of the shell for the nanowire within the framework of the MCS are given by:

$$M_c = \langle m_c \rangle = \frac{1}{N_c} \left\langle \sum_{i=1}^{N_c} S_i \right\rangle, \tag{3}$$