



Effects of the biaxial transverse crystal-field on the phase diagrams of a spin-1 nanowire

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ABSTRACT

By using the effective field theory based on a probability distribution method, the phase diagrams and the magnetic properties of an Ising nanowire in the presence of the biaxial transverse crystal-field are investigated. The effects of the biaxial transverse crystal field, the interfacial coupling and the exchange interaction in the surface on the phase diagram, the magnetization and the internal energy are examined. Some characteristic phenomena are found such as the tricritical behavior, the critical end point and the re-entrant phenomenon.

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1. Introduction

In recent years, there has been growing interest both theoretically and experimentally in the magnetic nanomaterials [1–3]. The reason is that these materials have many peculiar and unexpected physical properties compared with those of bulk materials [4].

Nowadays, the growing interest is continuously directed to the nanowires and nanotubes. This is motivated by numerous possibilities of their applications in nanotechnology [5,6]. Nanowires can be used as an ultrahigh density magnetic recording media [7–9] and they have potential applications in biotechnology [10,11], such as Ni nanowires can be used for bio-separation [12,13].

Theoretically, Akinci has used the effective field theory (EFT) with correlation to study the effects of the randomly distributed magnetic field on the phase diagrams of a spin-1/2 Ising nanowire [14]. Some interesting results have been found, such as re-entrant behavior and first-order phase transitions. The hysteresis behavior of the Blume–Capel nanowire have been examined using Monte Carlo simulations (MCS) based on heat-bath algorithm, [15]. A number of characteristic behaviors have been obtained such as the existence of double and triple hysteresis loops for appropriate values of the system parameters. By using the EFT based on the probability distribution method, the influence of the trimodal random longitudinal field, on the magnetic properties and the phase diagrams of a spin-1 Ising nanotube have been examined [16], the results show that the system can exhibit first-order phase transitions, tricritical point, re-entrant and even double re-entrant phenomena. MCS based on Metropolis algorithm, has been used [17] to investigate the critical behavior of a magnetic

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nanowire on a hexagonal lattice structure. It have been found that the system can exhibit first-order phase transitions, tri-critical and critical end points and compensation temperatures. Using the two theoretical frameworks of the effective field theory, based on a probability distribution method and the MCS based on Metropolis algorithm, we have investigated the magnetic properties of a nanoscaled ferrimagnetic thin film [18]. It was found that the results of the EFT are in qualitative agreement with those of the MCS. With the framework of the EFT and the mean field theory, Kaneyoshi [19] has studied a cylindrical nanowire. It was shown that, the phase diagram of the system is strongly affected by the physical parameters in the surface shell. The dynamic phase transitions in a cylindrical Ising nanowire under a time-dependent oscillating external magnetic field for both ferromagnetic and antiferromagnetic exchange interactions have been investigated within the EFT with correlations and the Glauber-type stochastic dynamics approach [20]. Depending on the values of the Hamiltonian parameters, five different types of compensation behaviors in the Néel classification nomenclature exist in the system.

Furthermore, Ising models with transverse crystal field have been widely studied in the literature [21,22]. It is known that the effects of the transverse crystal field are very different from those of the longitudinal counterpart, because the transverse crystal field can produce the quantum effects [23]. Since both the longitudinal and the transverse crystal fields have been found in particular materials, there must exist a kind of material in which both the absolute value of the longitudinal crystal-field interaction and that of the transverse counterpart may not be very small. Using the EFT with self-spin correlations and the differential operator technique, physical properties of the spin-2 Ising model with biaxial crystal field on the simple cubic, body-centered cubic, as well as faced-centered lattice have been studied in Ref. [24]. It was found that, the magnetization in the ground state shows quantum effects produced by the biaxial transverse crystal field. Within the framework of the effective-field theory with correlations, the ferromagnetic spin-1 Ising model with biaxial crystal-field is studied in Refs. [25–27]. The results show that the tricritical points and re-entrant phenomena may appear in certain ranges of biaxial crystal-field interactions. The hysteresis loops and the longitudinal magnetic susceptibility of the ferromagnetic spin-1 Ising model on a honeycomb lattice with a biaxial crystal field have been studied in Ref. [28] by the use of the EFT based on the probability distribution technique. It was found that the sign and the value of the biaxial crystal field have effects on the critical temperature, on the hysteresis behavior and on the area of the hysteresis loops. The appearance of the crystal field was also experimentally confirmed by changing the thickness of the nonmagnetic TaN inter-layer in FeTaN/TaN/FeTaN sandwiches [29]. There are also some materials which display evidences for the existence of the biaxial crystal fields, for example, on the magnetic properties of some polymeric molecular-based magnetic materials, such as $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ [30], $\text{Mn}(\text{CH}_3\text{COO})_2 \cdot 3\text{H}_2\text{O}$ [31], and $\text{Ni}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ [32].

However, as far as we know, Ising nanoparticle with biaxial transverse crystal-field have not been studied yet. The aim of this paper is, within the theoretical framework of the EFT based on the probability distribution technique, to investigate the influence of the biaxial transverse crystal-field on the magnetic properties of a spin-1 Ising nanowire. In section 2, the model and formulation based on the EFT for the Ising nanowire with a ferromagnetic spin configuration have been discussed. In section 3, the phase diagrams, the magnetization and the internal energy are reported. The system may exhibit some characteristic phenomena which hasn't been observed in Refs. [20–22], for example the appearance of the re-entrant phenomenon, of a second first-order phase transition line and of critical end point. Finally we give the conclusion.

2. Model and formalism

We consider a spin-1 ferromagnetic nanowire with core-shell structure (Fig. 1). The Hamiltonian of the system is given by

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z - D_x \sum_i (S_i^x)^2 - D_y \sum_i (S_i^y)^2 \quad (1)$$

Where the first sum runs over all pairs of nearest neighbors. J_{ij} is the exchange interaction constant between neighboring spins; we assume $J_{ij} = J_s$ if both spins belong to the surface shell, $J_{ij} = J_{int}$ between the core and the surface shell and $J_{ij} = J_c$ in the core. S_i^x , S_i^y and S_i^z are the components of a quantum spin $\vec{S}$ of magnitude $S = 1$ at each site i of the Ising nanoparticle. D_x and D_y are the two transverse uniaxial anisotropy parameters that denote the biaxial transverse crystal field.

Using the EFT with probability distribution method which is based on a simple site cluster comprising just a simple selected spin labeled i and the neighboring spins with which it directly interacts. The total Hamiltonian can be split into two parts $H = H_i + H'$, the part H_i includes all those terms in the hamiltonian containing the spin i ; it can be written in the form of a 3×3 matrix as:

$$H_i = \begin{pmatrix} X + \frac{1}{2}(D_x + D_y) & 0 & -\frac{1}{2}(D_x - D_y) \\ 0 & -(D_x + D_y) & 0 \\ -\frac{1}{2}(D_x - D_y) & 0 & -X - \frac{1}{2}(D_x + D_y) \end{pmatrix} \quad (2)$$

where $X = J_{ij} \sum_j S_j^z$

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