Monte Carlo study of a mixed spin (1, 3/2) ferrimagnetic nanowire with core/shell morphology

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In this work, Monte Carlo simulation based on Metropolis algorithm was used to study the magnetic behavior of a ferrimagnetic nanowire on a hexagonal lattice with a spin-3/2 core surrounded by a spin-1 shell layer with antiferromagnetic interface coupling in the presence of the crystal field interactions. The influences of the crystal field interactions, the interfacial and core couplings on the critical and compensation behaviors of the nanowire, are investigated. The results present rich critical behavior, which includes the first-and second-order phase transitions, the tricritical and critical end points. In addition, the compensation points can appear for appropriate values of the system parameters.

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1. Introduction

Nowadays, growing interest is continuously directed towards the magnetic properties of nanomaterials. Among these nanomaterials, core/shell nanowires and nanotubes such as ZnO [1], FePt, and Fe3O4 [2] are of considerable interest for both theoretical and experimental studies because of their potential technological application such as ultrahigh-density recording, biology and medicine [3,4]. From the theoretical point of view, these systems have been studied by a wide variety of techniques such as mean field theory (MFT) [5,6], effective field theory (EFT) [7,8], Green functions formalism (GF) [9], variational cumulant expansion (VCE) [10,11], and Monte Carlo simulations (MCS) [12–17]. Some studies show that we can find in these systems a very rich critical behavior and many interesting phenomena. Recently, Magoussi et al. [18] have investigated the effect of the trimodal longitudinal field on the critical behavior of a spin-1 nanotube. It has been found that the system exhibits tricritical point and reentrant phenomena. Zaim et al. [19] have investigated the magnetic properties of a cubic Ising nanocube which consists of a ferromagnetic spin-1/2 core and a ferromagnetic spin-1 shell coupled with an antiferromagnetic interlayer coupling J⊥ to the core by the use of Monte Carlo method. A number of characteristic phenomena are found, in particular, compensation temperature may occurs in this system.

The occurrence of a compensation point is of great technological importance, since at this point only a small driving field is required to change the sign of the resultant magnetization. This property is very useful in thermomagnetic recording. Canko et al. [20] have investigated the crystal field dependence of the magnetic properties of the mixed spin-(1/2,1) Ising nanotube using the EFT. Some characteristic phenomena are found such as the tricritical points. Akunci et al. [21,22] have studied the effects of a randomly distributed magnetic field on the phase diagrams of Ising nanowires and the dynamic behavior of a site diluted Ising ferrimagnet in the presence of a periodically oscillating magnetic field using EFT. It has been shown that the system exhibits reentrant phenomena, as well as a dynamic tricritical point which disappears for sufficiently weak dilution.

In recent years, much attention has been paid to the study of the mixed spin nanoparticles. The phase diagrams of a ferrimagnetic cubic nanoparticle with spin-3/2 core and spin-1 shell structure have been investigated in Refs. [23,24]. It was observed that the occupation of the sites of the particle core by the spin-3/2 plays an important role on the shape of the phase diagrams. Other work studied by using Monte Carlo simulation [25], the dynamic phase transition properties of a single spherical ferrimagnetic core–shell nanoparticle. It has been found that the dynamic phase boundaries depend strongly on the Hamiltonian parameters such as the high amplitude and the period of the external field. In Refs. [26,28], the magnetic properties of an hexagonal nanowire, cubic nanowire and multisublattice cubic nanowire with mixed spin (1, 3/2) have been examined by the EFT. Two compensation points can exist for certain values of the system parameters. Zaim et al. [29] have studied the magnetic behavior of a mixed spin (1, 3/2)
ferrimagnetic spherical nanoparticle using Monte Carlo simulations. The results present rich critical behavior, which includes the first- and second-order phase transitions, thus also the tricritical and critical end points. In Ref. [30] the authors have used the effective field theory to study the hysteresis loops of a mixed spin (1, 3/2) cubic nanowire in the presence of the crystal field and the transverse field. The triple, pentamerous and heptamerous hysteresis loops have been observed at low temperature. In other recent work, Jiang et al. [31] have investigated the compensation behavior, and magnetic properties of a ferrimagnetic nanotube, which includes ferromagnetic spin-3/2 inner shell and spin-1 outer layer with the ferrimagnetic interlayer coupling. Two compensation points have been found for certain values of the system parameters.

Despite these studies, as far as we know, the phase diagrams and the compensation behavior of a mixed spin (1, 3/2) hexagonal Ising nanowire have not been investigated. Therefore, in this

Fig. 1. Schematic representation of core/shell nanowire (two and three dimensional) with a spin-3/2 core and a spin-1 shell.

Fig. 2. The temperature dependencies of (a) total magnetizations, (b) core and shell magnetizations $M_c, M_s$, and (c) total susceptibility for $J_c/J_{sh} = 0.2$ and $D/J_{sh} = 0.5$ and for different values of $J_{int}/J_{sh}$. (d) Phase diagram of the system in $(T, J_{int}/J_{sh})$ plane for $J_c/J_{sh} = 0.2$, $D/J_{sh} = 0.5$, and $D/J_{sh} = -0.5$. 
