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Phase diagrams and magnetic properties of ferrimagnetic mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising nanowire

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HIGHLIGHTS

- The mixed cylindrical Ising nanowire is investigated using the MCS.
- The effects of the crystal field on the phase diagrams have been examined.
- The compensation phenomena are found.
- The tricritical and the isolated critical points are also observed.

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ABSTRACT

A hexagonal nanowire consisting of a ferromagnetic spin–$\frac{1}{2}$ core and spin–$\frac{3}{2}$ outer shell coupled with ferrimagnetic interlayer coupling has been studied by the use of the Monte Carlo simulation based on the heat bath algorithm. Particular emphasis is given to the effects of the size, the crystal field, the shell and the interface coupling constants on the critical and the compensation phenomenon. Some interesting behaviors have been observed which include the first and second order phase transitions. The isolated critical points are also observed. We have also found that the system exhibits the compensation phenomenon for appropriate values of the system parameters. The critical exponent has also been calculated.

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1. Introduction

In the last two decades, mixed spin Ising systems have attracted a great deal of attention, these systems have been of interest because they have less translational symmetry than their single-spin counter parts, since they consist of two inter-penetrating inequivalent sublattice. They have been proposed as possible models to describe a certain type of ferrimagnetic systems such as molecular systems based magnetic materials [1]. Moreover, the importance of these systems is mainly related to the potential technological applications in the area of thermomagnetic recording [2]. One of the well-known mixed spin Ising systems is the mixed spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ Ising model. Amorphous $V(\mathrm{TCNE})_x$. y (solvent), where TCNE is tetracyanoethylene, are organometallic compounds that seem to have a $\frac{1}{2}$–$\frac{3}{2}$ ferrimagnetic structure and order ferrimagnetically as high as 400 K [3,4]. Several techniques have been used to study the equilibrium and non-equilibrium magnetic properties of the mixed spin $(\frac{1}{2}, \frac{3}{2})$ Ising systems, such as mean field theory [5], effective field theory [6–8], Monte Carlo simulation [9] and Oguchi approximation [10].

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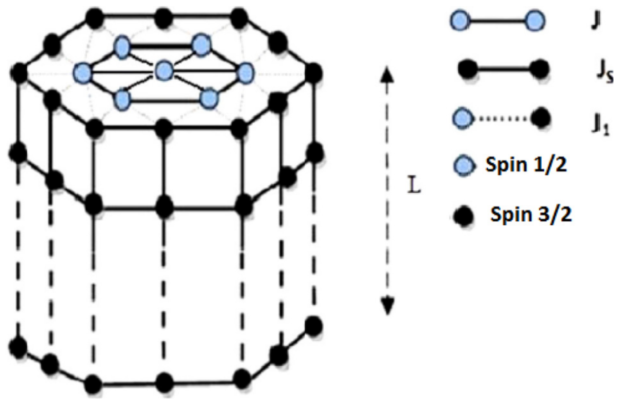

Fig. 1. Schematic representation of a cylindrical nanowire. The black circles denote the spin-$\frac{3}{2}$ surface shell atoms. The blue circles are the spin-$\frac{1}{2}$ atoms constituting the core. L denotes the length of the wire.

Recently, magnetic nanoparticle systems have been the subject of a large number of experimental and theoretical studies, because of their great potential for technological [11,12] and biomedical [13–15] applications. In particular, magnetic nanowires have many applications in nanotechnology [16,17]. Nanowires can be used as ultrahigh density magnetic recording media [18–20] and they have potential applications in biotechnology [21,22]. Some methods were explored to prepare large area nanowire, such as the print process [23,24], vapor–liquid–solid (VLS) [25], dielectrophoresis [26] and electron beam lithography [27]. Among those, the dielectrophoresis was a controllable and effective method to fabricate large quantity of nanodevices.

The magnetic nanowires can be modeled by core–shell models which can also be solved by various methods such as Monte Carlo simulation [28,29], mean field theory [30], effective field theory [31–33]. The phase diagrams of a cylindrical nanowire have been studied by the use of the mean field method and the effective field theory [34]. Some characteristic phenomena are found in the phase diagrams, depending on the ratio of the physical parameters in the surface shell and the core. Using the effective-field theory and the Monte Carlo Simulation, Boughazi et al. have studied the magnetic properties of a small particle on a hexagonal substrate [35]. The study of the magnetization shows that the system exhibits a compensation phenomenon and the compensation temperature increases with increasing the absolute value of the interface exchange interaction. Using Monte Carlo Simulation and effective field theory, Boughrara et al. have discussed the magnetic properties of a mixed spin (1/2,1) Ising nanowire [36]. They have shown that the phase diagrams obtained by the two methods have the same topology. It was found that the system presents very rich critical behaviors, which includes the first and second order phase transitions. They have also shown that, depending on the values of R_S, R_1 and $\frac{D}{J}$, the system can exhibit a compensation point.

The aim of this paper is to study the effect of the uniaxial anisotropy, the surface and the interfacial coupling constants on the magnetic properties and the phase diagrams (the critical and the compensation behaviors) of a cylindrical ferrimagnetic nanowire with a spin 1/2 core surrounded by a spin 3/2 shell layer. In our analysis, we use Monte Carlo (MC) technique according to the heat bath algorithm [37]. The outline of this paper is as follows: In Section 2, we give the model and review the basic points of the Monte Carlo approach. In Section 3, we present the results and discussions, while Section 4 is devoted to a brief conclusion.

2. Model and formalism

We consider hexagonal nanowire which consists of a spin 1/2 ferromagnetic core surrounded by a spin 3/2 ferromagnetic outer shell, as depicted in Fig. 1. The sites of the core are occupied by the spins $\sigma_i = \frac{1}{2}$, while those of the shell are occupied by the spins $S_i = \frac{3}{2}$.

The Hamiltonian of the system is expressed as follows:

$$H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - J_S\sum_{\langle ij\rangle}S_iS_j - J_1\sum_{\langle ij\rangle}S_i\sigma_j - D\sum_{\langle i\rangle}S_i^2 \quad (1)$$

where the first sum runs over all pairs in the core of the nanowire, the second sum runs over pairs neighboring in the outer shell, and the third runs over pairs which interact across the interface between the core and the outer shell. J_1 is the exchange coupling between nearest-neighbors magnetic atoms across the core and the outer shell, J_S is the exchange coupling between two nearest-neighbor magnetic atoms at the outer shell and J is the exchange coupling in the core. D is the single-ion anisotropy that comes from the outer shell sublattice.

Our system consists of one centric wire and two shells, namely one shell in the core and one shell of the surface (Fig. 1), the surface shell contains N_{Shell} spins-$\frac{3}{2}$, and the core contains N_{Core} spins-$\frac{1}{2}$. The total number of spins in the wire is $N_{\text{Total}} = N_{\text{Core}} + N_{\text{Shell}}$. $N_{\text{Core}} = 7 \times L$, $N_{\text{Shell}} = 12 \times L$. L denotes the wire length. We use Monte Carlo Simulations and

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