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The phase diagrams and the magnetic properties of a ferrimagnetic mixed spin 1/2 and spin 1 Ising nanowire

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ABSTRACT

In this work, we have used Monte Carlo Simulation technique (MCS) and effective field theory (EFT) to study the critical and the compensation behaviors of a ferrimagnetic cylindrical nanowire. The system consists of a ferromagnetic spin $S_A=1/2$ core and a ferromagnetic spin $S_B=1$ surface shell coupled with an antiferromagnetic interlayer coupling J_1 to the core. The effects of the uniaxial anisotropy, the shell coupling and the interface negative coupling on both the critical and compensation temperatures are investigated.

1. Introduction

During the last few years, one could observe a growing interest in the experimental and theoretical investigations of various new structures at nano-scale [1–4]. This is motivated by numerous possibilities of their applications in nanotechnology [5–8]. These structures include different geometric configurations such as fullerenes, nanotubes and nanowires. The exploration of different properties of these objects opens wide perspectives for applications. Due to their potential application in high density magnetic recording media, high attention is paid to the magnetic nanowire and nanotube based on the transition metals, such as Co–Pt, Co–Pd, Fe–Pt and Fe–Pd alloys [9–13]. Besides technological applications, the magnetic properties of nanoparticles are scientifically interesting research areas since their magnetic properties are quite different from those of the bulk and greatly affected by the particle size [14].

Theoretically, the core–shell model has been accepted to explain many characteristic phenomena in nanoparticle magnetism [15–19]. The same concept has been applied to the investigation of magnetic nanowires and nanotubes [20–22]. In particular, the magnetic properties of a nanocube [23], which consists of a ferromagnetic spin 1/2 core and a ferromagnetic spin 1 shell coupled with an antiferromagnetic interlayer coupling J_{int} to the core, have been investigated by the use of Monte Carlo simulation (MCS). Some characteristic feature have been obtained in it. The system consists of L_c layers in the core and two layers in the spin 1 shell, so that the total number of layers L is given by $L=L_c+4$. The authors have examined the effects of shell coupling and interface coupling on both the compensation and magnetization profiles. They have observed that as the shell thickness increases, both critical and compensation temperatures of the system increase and reach a saturation values for high values of the thickness. The magnetic properties of the ferromagnetic (FM)-antiferromgnetic (AFM) core–shell morphology were studied by using MC Metropolis method [24]. Kaneyoshi has investigated phase diagrams [25] and magnetizations [26] of the transverse Ising nanowire by using the effective field theory with correlation (EFT). He has found that the magnetic properties are strongly influenced by surface effects and finite size. Keskin et al. [27] have studied the hysteresis behaviors of the cylindrical Ising nanowire by EFT. They have obtained phase transition temperatures and found that the results of hysteresis behaviors of the nanowires are in good agreement with both theoretical and experimental results. In another work, Zaim and Kerouad [28] have simulated a spherical particle consisting of a ferromagnetic spin 1/2 core and a ferromagnetic spin 1 or 3/2 shell with antiferromagnetic interface coupling. They have focused on the effect of the shell and the interface coupling and found that two compensation temperatures can occur when the sites of the shell sublattice are occupied by $S=3/2$ spins. In a series of recent works [29–33], the hysteresis behavior and the susceptibility of the nanowire have been investigated by using EFT [29,30], the effect of the diluted surface on the phase diagrams and the magnetic properties of the nanowire and

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nanotube have been also studied [31–33]. Beside these, higher spin nanowire or nanotube have been investigated, e.g. spin-1 nanowire [34,35] and nanotube [36], mixed spin 1/2, 1 nanotube [37].

The aim of this work is to study the effects of the crystal field, the shell and the interface coupling on the phase diagrams and the magnetic properties of a cylindrical ferrimagnetic nanowire with a spin $-1/2$ core surrounded by a spin -1 shell layer. In our analysis we use Monte Carlo (MC) technique according to the heat bath algorithm [38] and compare the simulation results with those of the effective field theory.

The outline of this paper is as follow: In Section 2, we define the model and give briefly the formulation of magnetic properties within the Monte Carlo simulation and the effective field theory. The results and discussions are presented in Section 3, and finally Section 4 is devoted to the conclusion.

2. Model and formalism

We consider a ferrimagnetic cylindrical nanowire consisting of a spin 1/2 ferromagnetic core which is surrounded by a spin -1 ferromagnetic shell layer. At the interface, we have an antiferromagnetic interaction between core and shell spins. A cross-section of the wire is depicted in Fig. 1. The Hamiltonian of the system is given by

$$H=-J_s\sum_{i,j}S_i^zS_j^z-J\sum_{m,n}\sigma_m^z\sigma_n^z-J_1\sum_{i,m}\sigma_m^zS_i^z-D\sum_i(S_i^z)^2 \quad (1)$$

where 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 S_i^z in the surface shell and the spins σ_m^z in the next shell in the core. D represents the single ion anisotropy terms of the surface shell sublattice.

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 -1, and the core contains $N_c\times L$ spins $-1/2$. The total number of spins in the wire is $N_T=(N_s+N_c)L$. $N_s=12$, $N_c=7$ and $L=500$. N_s and N_c are the spin numbers of the nanowire cross-section, of the surface and of the core, respectively. L denotes the wire length's. We use the Monte Carlo Simulation and we flip the spins once a time, according to the heat bath algorithm [38]. 4×10^4 Monte Carlo steps were 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 [40] by taking all the measurements and grouping them in 20 blocks. This error bar is negligible, so it does not appear in our plots.

The sublattice magnetizations per site in the core and in the shell surface are defined by

$$M_{1/2}=\frac{1}{N_cL}\sum_{m=1}^{N_cL}\sigma_m^z \quad (2)$$

and

$$M_1=\frac{1}{N_sL}\sum_{i=1}^{N_sL}S_i^z \quad (3)$$

The total magnetization per site is defined by

$$M_T=\frac{1}{19}(12M_1+7M_{1/2}) \quad (4)$$

The total susceptibility χ_T is defined by

$$\chi_T=\beta N_T(\langle M_T^2\rangle-\langle M_T\rangle^2) \quad (5)$$

with $\beta=1/K_BT$.

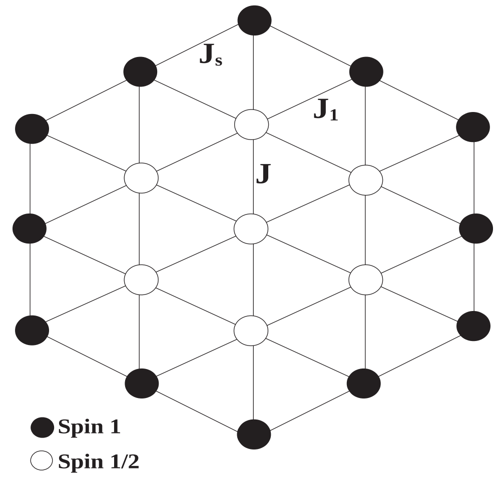

Fig. 1. Schematic representation of a cross section of a cylindrical nanowire. Solid circles indicate spin -1 atoms at the surface shell and open circle are spin $-1/2$ atoms constituting the core.

On the other hand, in the framework of the well known effective field theory, based on the use of a probability distribution technique [39], the longitudinal site order parameters are given by

For the central site:

$$m_{\sigma1}=\sum_{i1=0}^{N2}\sum_{i2=0}^{N4}C_{i1}^{N2}C_{i2}^{N4}(1/2-m_{\sigma1})^{i1}(1/2+m_{\sigma1})^{N2-i1}(1/2-m_{\sigma2})^{i2}$$
$$\times(1/2+m_{\sigma2})^{N4-i2}F(0.5((N2+N4)-2(i1+i2)),T) \quad (6)$$

For the first shell of the core:

$$m_{\sigma2}=\sum_{i1=0}^{N3}\sum_{i2=0}^{N1}\sum_{i3=0}^{N1}\sum_{j3=0}^{N1-i3}\sum_{i4=0}^{N2}\sum_{j4=0}^{N2-i4}C_{i1}^{N3}C_{i2}^{N1}C_{i3}^{N1}C_{j3}^{N1-i3}C_{i4}^{N2}C_{j4}^{N2-i4}(1/2-m_{\sigma2})^{i1}$$
$$\times(1/2+m_{\sigma2})^{N3-i1}(1/2-m_{\sigma1})^{i2}(1/2+m_{\sigma1})^{N1-i2}(1-q_1)^{i3}(q_1-m_1)^{j3}$$
$$\times(q_1+m_1)^{N1-i3-j3}(1-q_2)^{i4}(q_2-m_2)^{j4}(q_2+m_2)^{N2-i4-j4}$$
$$\times F(0.5(N3+N1-2(i1+i2))+R_1(N1+N2-i3-i4-2(j3+j4)),T) \quad (7)$$

For the surface shell:

$$m_1=\sum_{i1=0}^{N2}\sum_{j1=0}^{N2-1}\sum_{i2=0}^{N2}\sum_{j2=0}^{N2-i2}\sum_{i3=0}^{N1}C_{i1}^{N2}C_{j1}^{N2-i1}C_{i2}^{N2}C_{j2}^{N2-i2}C_{i3}^{N1}(1-q_2)^{i1}(q_2-m_2)^{j1}$$
$$\times(q_2+m_2)^{N2-i1-j1}(1-q_1)^{i2}(q_1-m_1)^{j2}(q_1+m_1)^{N2-i2-j2}(1/2-m_{\sigma2})^{i3}$$
$$\times(1/2+m_{\sigma2})^{N1-i3}G1(R_S(2N2-i1-2j1-i2-2j2)+(R_1/2)(N1-2i3),D,T) \quad (8)$$

$$q_1=\sum_{i1=0}^{N2}\sum_{j1=0}^{N2-1}\sum_{i2=0}^{N2}\sum_{j2=0}^{N2-i2}\sum_{i3=0}^{N1}C_{i1}^{N2}C_{j1}^{N2-i1}C_{i2}^{N2}C_{j2}^{N2-i2}C_{i3}^{N1}(1-q_2)^{i1}(q_2-m_2)^{j1}$$
$$\times(q_2+m_2)^{N2-i1-j1}(1-q_1)^{i2}(q_1-m_1)^{j2}(q_1+m_1)^{N2-i2-j2}(1/2-m_{\sigma2})^{i3}$$
$$\times(1/2+m_{\sigma2})^{N1-i3}G2(R_S(2N2-i1-2j1-i2-2j2)+(R_1/2)(N1-2i3),D,T) \quad (9)$$

$$m_2=\sum_{i1=0}^{N2}\sum_{j1=0}^{N2-1}\sum_{i2=0}^{N2}\sum_{j2=0}^{N2-i2}\sum_{i3=0}^{N2}C_{i1}^{N2}C_{j1}^{N2-i1}C_{i2}^{N2}C_{j2}^{N2-i2}C_{i3}^{N2}(1-q_1)^{i1}(q_1-m_1)^{j1}$$
$$\times(q_1+m_1)^{N2-i1-j1}(1-q_2)^{i2}(q_2-m_2)^{j2}(q_2+m_2)^{N2-i2-j2}(1/2-m_{\sigma2})^{i3}$$
$$\times(1/2+m_{\sigma2})^{N2-i3}G1(R_S(2N2-i1-2j1-i2-2j2)+(R_1/2)(N2-2i3),D,T) \quad (10)$$

$$q_2=\sum_{i1=0}^{N2}\sum_{j1=0}^{N2-1}\sum_{i2=0}^{N2}\sum_{j2=0}^{N2-i2}\sum_{i3=0}^{N2}C_{i1}^{N2}C_{j1}^{N2-i1}C_{i2}^{N2}C_{j2}^{N2-i2}C_{i3}^{N2}(1-q_1)^{i1}(q_1-m_1)^{j1}$$
$$\times(q_1+m_1)^{N2-i1-j1}(1-q_2)^{i2}(q_2-m_2)^{j2}(q_2+m_2)^{N2-i2-j2}(1/2-m_{\sigma2})^{i3}$$
$$\times(1/2+m_{\sigma2})^{N2-i3}G2(R_S(2N2-i1-2j1-i2-2j2)+(R_1/2)(N2-2i3),D,T) \quad (11)$$

where q_1 and q_2 are the quadrupolar moments, $R_1=J_1/J$ and $R_s=J_s/J$. $N1=1$, $N2=2$, $N3=4$ and $N4=6$ denote respectively the