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Hysteresis and compensation behaviors of mixed spin-2 and spin-1 hexagonal Ising nanowire core–shell structure

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ABSTRACT

The magnetic behaviors of a mixed spins (2-1) hexagonal Ising nanowire with core–shell structure are investigated by using the Monte Carlo simulations. The thermal magnetizations, the magnetic susceptibilities and the transition temperatures of core–shell are studied for different values of crystal field and exchange interactions. The thermal and magnetic hysteresis cycles are given for different values of the crystal field.

1. Introduction

Recently, the research on the bimagnetic core/shell nanoparticles is steadily increasing, since it has brought about interesting physical and chemical properties of the nanostructured materials that have shown important technological applications [1]. The bimagnetic core/shell nanoparticles are widely used to improve the hard magnetic properties [3] and to enhance the coercivity and squareness in permanent magnet powders [2], as well as to pin the ferromagnetic reference magnetization into a well-defined direction by means of exchange bias [4–6]. Another reason is that they have important potential technological applications in various areas, e.g. they can be used for medical applications [7,8], environmental remediation [9], and permanent magnets [10]. Deviren and Keskin [11] investigated thermal behavior of dynamic magnetizations, hysteresis loop areas and correlations of a cylindrical Ising nanotube. Deviren et al. [12,13] investigated dynamic phase transitions temperature of cylindrical Ising nanowire [12], transverse cylindrical Ising nanowire [13] and the dynamic phase diagrams of the kinetic cylindrical Ising nanotube [14] using dynamic effective-field theory. The hysteresis behaviors have been studied for nanomaterials from both the experimental and theoretical points of view. Experimentally, the hysteresis behaviors have been studied for the ferromagnetism in nanowires [15,16], in $La_{2/3}Sr_{1/3}MnO_3$ nanoparticle, assembled nanotubes [17] and for carbon nanotubes [18–21]. Theoretically, hysteresis behaviors have been investigated in the ferromagnetic single-walled nanotubes [22], nanomagnets [23] and noninteracting nanoparticles [24]. The Monte Carlo simulations have been used to study the magnetic properties of Ni/Au core/shell by Ref. [25]. Multicritical dynamic phase diagrams and dynamic hysteresis loops in a Mixed Spin-2 and Spin-5/2 Ising ferrimagnetic system with repulsive biquadratic coupling: Glauber dynamic approach have been reported in Ref. [26]. In the present work, the thermal magnetizations and magnetic susceptibilities of core–shell are given with different values of exchange interactions. The total magnetizations and total magnetic susceptibilities were also established. The transition temperatures are obtained for different values of crystal field and exchange interactions. The thermal magnetizations and magnetic susceptibilities in core and shell are given for different values of exchange interactions for different values of crystal field. The thermal and magnetic hysteresis cycle are also given. The magnetizations versus the external field are also obtained.

2. Model and formulation

The Hamiltonian of the hexagonal Ising nanowire with core–shell structure including nearest neighbors interactions, external

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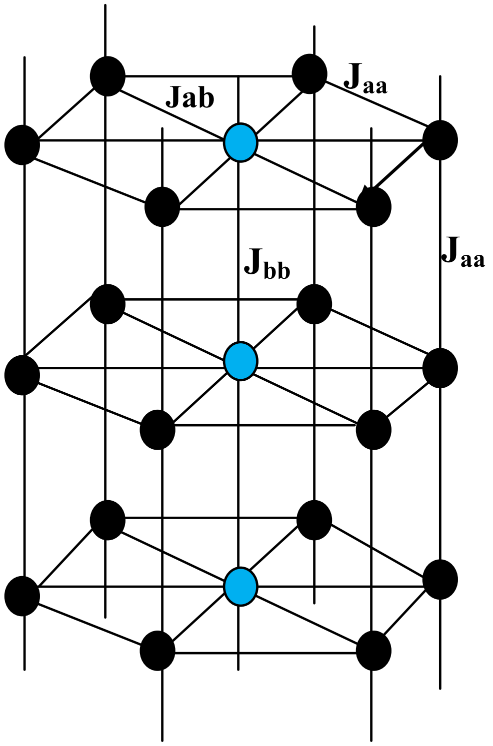

Fig. 1. Schematic presentation of hexagonal Ising nanowire with core–shell structure. The black and blue spheres indicate magnetic atoms at the surface shell and core, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

magnetic field and the crystal field is given by:

$$H = -J_{aa}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - J_{ab}\sum_{\langle i,j\rangle}\sigma_i S_j - J_{bb}\sum_{\langle i,j\rangle}S_i S_j - H\sum_i (S_i+\sigma_i) - \Delta\sum_i (S_i^2+\sigma_i^2) \quad (1)$$

where $\langle i,j\rangle$ stand for the first nearest neighbor sites i and j, Δ represents the crystal field and H is the external magnetic field. The J_{aa}, J_{ab} and J_{bb} are the exchange interactions parameters between the two nearest neighbor magnetic particles at the shell surface, core and between shell surface and core, respectively (see Fig. 1). The spin moments of core and shell ions are: $\sigma_C = \pm 1$, 0 and $S_S = \pm 2$, ± 1, 0, respectively.

3. Monte Carlo simulations

The hexagonal Ising nanowire with core–shell structure are assumed to reside in the unit cells and the system consists of the total number of spins $N=(N_S(\text{shell})+N_C(\text{core}))\text{x}L$, with $N_S=1$, $N_C=6$ where $L=16$ is the system size in the z-direction. We apply a standard sampling method to simulate the Hamiltonian given by Eq. (1). Cyclic boundary conditions on the lattice were imposed and the configurations were generated by sequentially traversing the lattice and making single-spin flip attempts. The flips are accepted or rejected according to a heat-bath algorithm under the Metropolis approximation. Our data were generated with 10^5 Monte Carlo steps per spin, discarding the first 10^4 Monte Carlo simulations. Starting from different initial conditions, we

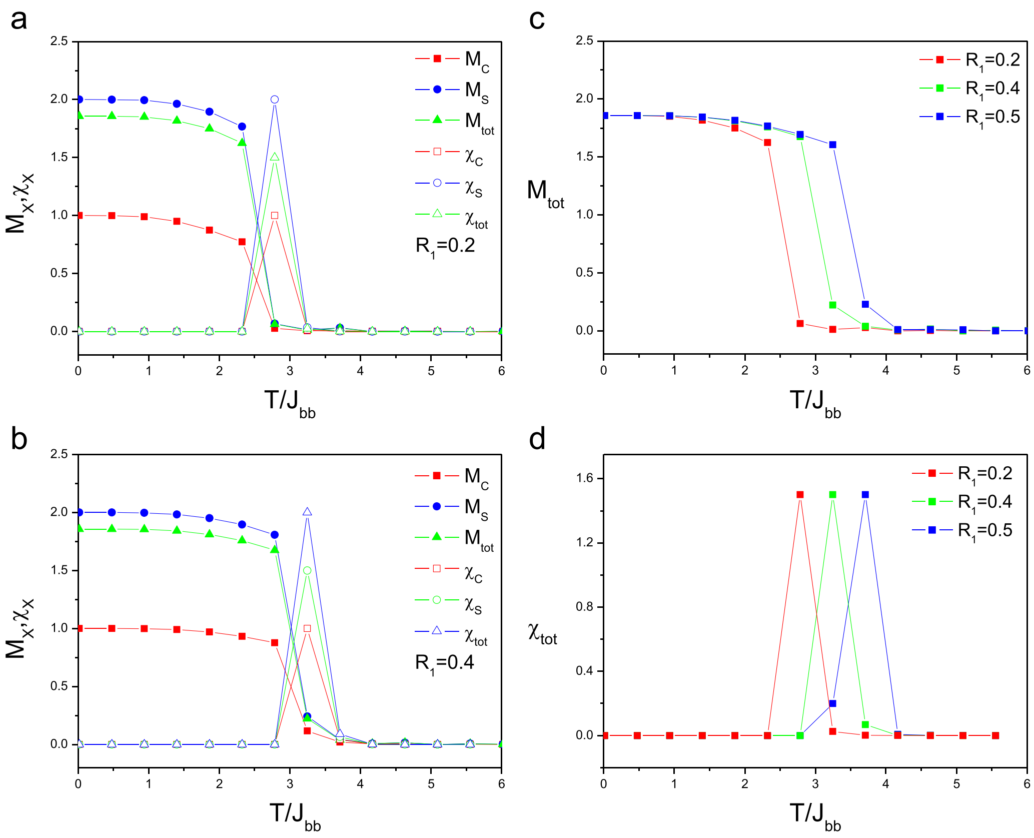

Fig. 2. The thermal magnetizations and magnetic susceptibilities of core and shell with different values of exchange interactions $R_1=0.2$ (a), $R_2=1.0$ (b) and $\Delta/J_{bb}=0.0$. The variation of total magnetization (c) and total magnetic susceptibilities (d) of core–shell for $R_1=0.2$, 0.4, 0.5 with $R_2=1.0$ (b) and $\Delta/J_{bb}=0.0$.