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Hexagonal type Ising nanowire with mixed spins: Some dynamic behaviors

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ABSTRACT

The dynamic behaviors of a mixed spin (1/2–1) hexagonal Ising nanowire (HIN) with core–shell structure in the presence of a time dependent magnetic field are investigated by using the effective-field theory with correlations based on the Glauber-type stochastic dynamics (DEFT). According to the values of interaction parameters, temperature dependence of the dynamic magnetizations, the hysteresis loop areas and the dynamic correlations are investigated to characterize the nature (first- or second-order) of the dynamic phase transitions (DPTs). Dynamic phase diagrams, including compensation points, are also obtained. Moreover, from the thermal variations of the dynamic total magnetization, the five compensation types can be found under certain conditions, namely the Q-, R-, S-, P-, and N-types.

1. Introduction

Recently, magnetic nanomaterials (nanoparticles, nanofilms, nanorods, nanobelts, nanowires and nanotubes etc.) have attracted a great interest both theoretically and experimentally. The reason is that these materials can be used technological area, such as biomedical applications [1,2], sensors [3], nonlinear optics [4], permanent magnets [5], environmental remediation [6], and information storage devices [7–9]. In particular, magnetic nanowire systems have attracted considerable attention not only because of their academic interest, but also the technological applications. In the experimental area, the magnetic nanowires have been synthesized and their magnetic properties have been investigated, such as Fe–Co [10], Co–Pt [11], Ni [12], $Ga_{1-x}Cu_xN$ [13], Fe [14], Fe_3O_4 [15], Co [16], Fe–Pt [17], Ni–Fe [18], Co–Cu [19] etc. In theoretical area, the magnetic nanowires have been investigated within the various theoretical methods, such as effective-field theory (EFT) with correlations [20–24], Monte Carlo Simulations (MC_S) [25].

On the other hand, the mixed spin Ising systems have attracted a great deal of attention and intensively investigated within the concept of statistical physics. These systems have observed many new phenomena that cannot be exhibit in single-spin Ising systems. The most extensively mixed system is mixed spin $(1/2-1)$ Ising system. This model has been studied by the mean-field approximation (MFA) [26–29], MCs [30,31] and EFT with correlation [32–35]. Moreover, some further works about magnetic nanomaterials of mixed spin $(1/2-1)$ Ising system were given [36–40].

Finally, we should also mentioned that the dynamic phase transition (DPT) temperature has attracted much attention in recent years, both theoretically [41–49] and experimentally [50–54]. However, as far as we know, the DPT temperatures of the magnetic nanostructured materials have only been investigated a few works by usin EFT [55–58] and MCs [59–60]. Therefore, the aim of this paper is to investigate temperature dependence of the dynamic magnetizations and the dynamic phase diagrams, including compensation points, of the HIN in an oscillating magnetic field within the DEFT.

The paper is organized as follows. In Section 2, we define the model and give briefly the formulation of a mixed spin (1/2–1) HIN by using the DEFT. In Section 3, we present the numerical results and discussions. Finally, Section 4 contains the summary and conclusions.

2. Model and formulation

2.1. Model

The Hamiltonian of the hexagonal Ising nanowire (HIN) includes nearest neighbor interactions and the crystal field is given as follows:

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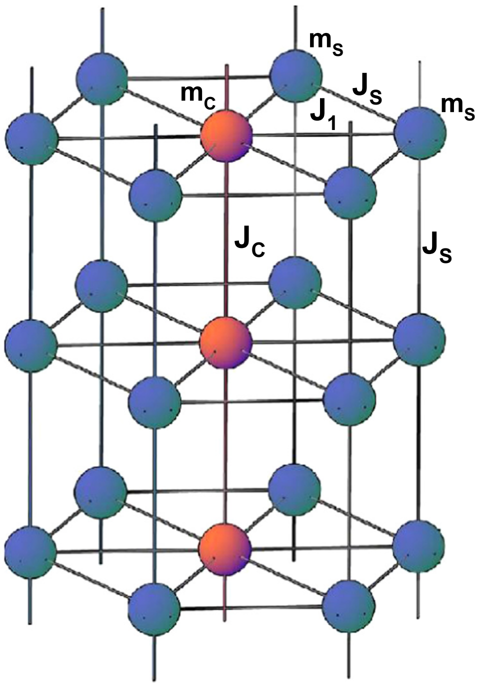

Fig. 1. Schematic presentation of hexagonal Ising nanowire. The blue and red spheres indicate magnetic atoms at the surface shell and core, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$H = -J_S\sum_{\langle ij\rangle} S_i S_j - J_C\sum_{\langle mn\rangle}\sigma_m\sigma_n - J_1\sum_{\langle im\rangle} S_i\sigma_m - D\sum_i S_i^2 - h(t)\left(\sum_i S_i + \sum_m \sigma_m\right) \tag{1}$$

where $\sigma = \pm 1/2$ and $S = \pm 1,\ 0$. The J_S, J_C and J_1 are the exchange interaction parameters between the two nearest-neighbor magnetic particles at the shell, core and between the shell and core, respectively (see Fig. 1). D is a Hamiltonian parameter and stands for the single-ion anisotropy (i.e. crystal field). The shell exchange interaction $J_S = J_C(1 + \Delta_S)$ and interfacial coupling $r = J_1/J_C$ are often defined to clarify the effects of the shell and interfacial exchange interactions on the physical properties in the nanosystem, respectively. $h(t)$ is a time-dependent external oscillating magnetic field and is given as

$$h(t) = h_0\ \sin(wt). \tag{2}$$

In here, h_0 and $\omega{=}2\pi\nu$ are the amplitude and the angular frequency of the oscillating field, respectively.

2.2. Formulations

We apply the Glauber-type stochastic dynamics [61], in particular we employ Glauber transition rates, to obtain the set of dynamic effective-field equations. Thus, the system evolves according to a Glauber-type stochastic process at a rate of $1/\tau$ transitions per unit time; hence the frequency of spin flipping, f, is $1/\tau$. Leaving the σ-spins fixed, we define $P^S(S_1,\ S_2,\ \ldots,\ S_N;\ t)$ as the probability that the system has the S-spin configuration, $S_1,\ S_2,\ \ldots,\ S_N$ at time t. Also, by leaving the S spins fixed, we define $P^C(\sigma_1,\ \sigma_2,\ \ldots,\ \sigma_N;\ t)$ as the probability that the system has the σ-spin configuration $\sigma_1,\ \sigma_2,\ \ldots,\ \sigma_N;\ t$, at time t. Then, we calculate $W_j^S\left(S_j \to S`_j\right)$ and $W_i^C\left(\sigma_i \to \sigma`_j\right)$, the probabilities per unit time that the ith σ spin changes from σ_i to $\sigma`_j$ (while the $S$ spins are momentarily fixed) and the $j$th S spin changes from $S_j$ to $S`_j$ (while the σ spins are momentarily fixed), respectively. Thus, if the σ spins on the core are momentarily fixed, the master equation for the S spins on shell can be written as

$$\frac{d}{dt}P^S(S_1,\ S_2,\ \ldots,\ S_N;\ t) = -\sum_i\left(\sum_{S_i\neq S_i^`} W_i^S\left(S_i \to S`_j\right)\right)P^S(S_1,\ S_2,\ \ldots,\ S_i,\ \ldots,\ S_N;\ t) + \sum_i\left(\sum_{S_i\neq S_i^`} W_i^S\left(S_i^` \to S_i\right)\right)P^S(S_1,\ S_2,\ \ldots,\ S`_j,\ \ldots,\ S_N;\ t), \tag{3}$$

where $W_i^S\left(S_i \to S`_j\right)$ is the probability per unit time that the $i$th spin changes from the value $S_i$ to $S`_j$. Since the system is in contact with a heat bath at absolute temperature T_A, each spin can change from the value S_i to $S`_j$ with the probability per unit time;

$$W_i^S\left(S_i \to S`_j\right) = \frac{1}{\tau}\frac{\exp\left[-\beta\ \Delta E^S\left(S_i \to S`_j\right)\right]}{\sum_{S`_j}\exp\left[-\beta\ \Delta E^S\left(S_i \to S`_j\right)\right]}, \tag{4}$$

where $\beta = 1/k_B T_A, k_B$ is the Boltzmann factor, $\sum_{S_i^`}$ is the sum over the three possible values of $S_i' = \pm 1$, 0, and

$$\Delta E^S\left(S_i \to S`_j\right) = -\left(S_i - S`_j\right)\left(J_S\sum_j S_j + J_1\sum_m \sigma_m + h(t)\right) - \left[\left(S`_j\right)^2 - \left(S_i\right)^2\right]D, \tag{5}$$

gives the change in the system's energy when the S_i-spin changes. The probabilities satisfy the detailed balance condition

$$\frac{W_i^S\left(S_i \to S`_j\right)}{W_i^S\left(S_j^` \to S_i\right)} = \frac{P^S(S_1,\ S_2,\ \ldots,\ S_i^`,\ \ldots,\ S_N)}{P^S(S_1,\ S_2,\ \ldots,\ S_i,\ \ldots,\ S_N)}, \tag{6}$$

and the probabilities $W_i^S\left(S_i \to S`_j\right)$ are presented in Ref. [65]. From the master equation associated with the stochastic process, it follows that the average $\left\langle S_i^A\right\rangle$ satisfies the following equation:

$$\tau\frac{d}{dt}\left\langle S_i^A\right\rangle = -\left\langle S_i^A\right\rangle + \left\langle\frac{2sinh\left(\beta\left(E_i + h(t)\right)\right)}{2\ \cos\ h\left(\beta\left(E_i + h(t)\right)\right) + \exp(-\beta D)}\right\rangle, \tag{7}$$

where $\langle\ldots\rangle$ denotes the canonical thermal average and $E_i = J_S\sum_j S_j + J_1\sum_m \sigma_m$. Now, assuming that the S spins on shell are momentarily fixed and that the σ spins on core change, we can obtain the second dynamic equation for the σ spins on core by using similar calculations as

$$\tau\frac{d}{dt}\left\langle\sigma_j^C\right\rangle = -\left\langle\sigma_j^C\right\rangle + \left\langle\frac{1}{2}\ \tanh\left(\frac{\beta}{2}\left(E_j + h(t)\right)\right)\right\rangle, \tag{8}$$

where $E_j = J_C\sum_n \sigma_n + J_1\sum_i S_i$.

Now, we use the EFT with correlations to obtain the set of dynamic effective-field equations. This method was first introduced by Honmura and Kaneyoshi [62] and Kaneyoshi et al. [63], where by a more advanced method is used in dealing with Ising systems than the MFT, because it considers more correlations. The main problem is to evaluate the thermal average of the last terms in Eqs. (7) and (8). The starting point to determine the statistics of the present spin system is the exact relation due to Callen [64]. The EFT with correlations is also convenient to introduce the differential operator technique into expressions of the last terms in Eqs. (7) and (8),