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ORIGINAL PAPER

Dynamic Magnetic Properties of a Mixed Spin Ising Double-Walled Ferromagnetic Nanotubes: A Dynamic Monte Carlo Study

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Abstract Using the dynamic Monte Carlo simulation, the dynamic critical temperature of a ferromagnetic or ferrimagnetic double-walled nanotubes (DWNTs) is studied within the kinetic Ising model under the presence of a time-dependent oscillating external magnetic and crystal fields with mixed spins $S_A = 1$ and $S_B = 3/2$. The effects of the time-dependent oscillating external magnetic field, the period of the oscillating magnetic field, and the crystal field on the thermal behavior of the dynamic sub-lattice order parameters and the total dynamic order parameter, total dynamical magnetic susceptibility, dynamical specific heat, and dynamic hysteresis of a DWNTs are studied. Our theoretical predictions may be a reference for future experiment studies of the nanostructures.

Keywords Phase transition · Nanotubes · Hysteresis loop · Mixed spin system · Ising model · Monte Carlo method

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1 Introduction

Recently, magnetic nanostructures have received much attention [1–4] because of their great interest in various disciplines such as sensors, optics, spin electronics, thermoelectronic devices, molecular imaging devices, high density magnetic recorders [5–9], and biomedical applications (magnetic resonance imaging, drug delivery, and cell and tissue targeting or hyperthermia [10–16]).

On the other hand, from the theoretical point of view, many studies have been devoted to investigate the magnetic properties of various types of the magnetic nanostructure by using different methods by means of equilibrium and nonequilibrium Ising models. For example, mean-field theory [17], effective-field theory (EFT) [18–22], variational cumulant expansion [23], Green Functions formalism [24], and Monte Carlo (MC) simulations [25–28]. However, dynamic magnetic responses such as the dynamic hysteresis and the dynamic phase transition for a cooperative of these nanosystems in an oscillating external field have been widely studied [29–40]. These responses play an important role in modern research of nonequilibrium phenomena [41]. In the same dynamic aspect, many researchers have obtained interesting results on the dynamic phase transition and hysteresis loops of the Ising model in an oscillating field [33–40]. Using the EFT with correlation and the Glauber-type stochastic dynamics approach, Kantar et al. [42] have studied the dynamic phase diagrams of a cylindrical Ising nanowire. They have found a number of interesting properties, such as many dynamic critical points. Based on MC simulations, the magnetic properties of a ferrimagnetic nanostructure with mixed spin-(1/2, 1) were studied by Vatansever and Polat [43]. By the use of the same method, the temperature and the applied time-dependent magnetic field dependencies of the magnetic properties of the dynamic phase transition properties and hysteretic behavior of a ferrimagnetic core–shell nanoparticle system were investigated by Yüksel al. [44]. They have found the existence of triple hysteresis loops and the system exhibits the compensation-critical points. The authors have submitted the cubic nanoparticle to a time-dependent oscillating magnetic field and they have observed sharp transition regions with increasing applied field period. An early attempt to study the dynamic aspects of the kinetic Ising model was done by Kantar and Kocakaplan [45] who used the effective-field theory with correlations based on the Glauber-type stochastic dynamics (DEFT). They have investigated the time dependence of the order parameters and found that the dynamic behavior of the system strongly depends on the values of the interaction parameters.

Recently, Yuksel [46] has investigated the dynamic phase transition properties of ferromagnetic uniaxial nanowires with tunable radius r in the presence of both oscillating and biased magnetic fields. The author has found a number of interesting phenomena such as the existence of the compensation temperature. He has also investigated the magnetization dynamics in terms of magnetic hysteresis loops as functions of the bias field.

Despite these studies, as far as we know, the dynamic behaviors of a mixed spin Ising double-walled ferrimagnetic nanotubes (DWFNTs) Ising system have not been investigated. In this work, within the framework of the DMC, we study the dynamic behaviors of DWFNT. Indeed, the effects of the time-dependent oscillating external magnetic field, the period of the oscillating magnetic field, and the interaction parameters on the thermodynamic properties are discussed. The outline of this paper is as follows: in Section 2, we briefly present the used DMC method. The results and discussion are presented in Section 3 and Section 4 summarizes our conclusions.

2 Model and Dynamic Monte Carlo Simulation

We consider a ferrimagnetic mixed spin-(1, 3/2) Ising double-walled nanotube model consisting of a spin-1 ferromagnetic core which is surrounded by a spin-3/2 ferromagnetic surface shell (Fig. 1), in the presence of the time-dependent oscillating external magnetic and crystal fields. The Hamiltonian of the system is given by

$$H = -J_c \sum_{\langle ij \rangle} S_{i,z} S_{j,z} - J_s \sum_{\langle nm \rangle} S_{n,z} S_{m,z} - J_{sc} \sum_{\langle in \rangle} S_{i,z} S_{n,z} \\ -D\left(\sum_i (S_{i,z})^2 + \sum_n (S_{n,z})^2\right) - h(t)\left(\sum_i S_{i,z} + \sum_n S_{n,z}\right)$$

J_c and J_s are the exchange interaction parameters between two nearest-neighbor spins at the core and the surface shell,

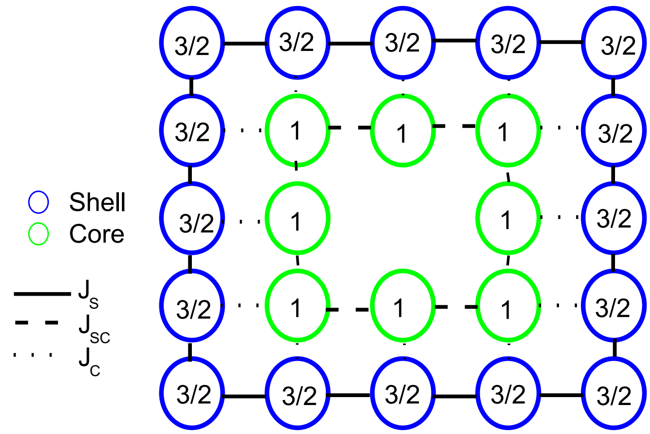


Fig. 1 Schematic representation of a transverse coup of a ferrimagnetic cubic nanotube double walled of surface shell (*blue circles*) and core (*green circles*) atoms

respectively. J_{sc} is the exchange interaction between two nearest-neighbor spins at surface shell and core. $S_i \equiv S_c$ spins take the values $\pm$ 1 and 0 at each site i and $S_n \equiv S_s$ spins take the values $\pm$ 3/2 and $\pm$ 1/2 at each site n of a ferrimagnetic mixed spin-(1, 3/2) Ising nanotube. The summations with indices $\langle ij \rangle$, $\langle nm \rangle$, and $\langle in \rangle$denote summations over all pairs of neighboring spins at the core, surface shell, and between shell and core, respectively. $\boldsymbol{D}$ represents the crystal field. The last term in the Hamiltonian of the system is taken over all lattice sites and represents the interactions due to time-dependent external field $\boldsymbol{h(t)}$, which has the form $\boldsymbol{h(t) = h_b + h_0 \cos(wt)}$, where h_b is the bias of the external field and h_0 denotes the oscillation amplitude. ω is the angular frequency of the oscillating field and the period of the oscillating magnetic field is given by $\tau = 2\pi/\omega$.

In the Monte Carlo simulations based on Heat-Bath algorithm, we apply periodic boundary conditions in the x and y directions. Free boundary conditions are applied in the z direction which is of finite thickness $\boldsymbol{L}$. The simulations are carried out for $\boldsymbol{N_s}$ spins-3/2 contained in the surface shell and for N_c spins-1 contained in the core. The total number of spins in the system is $N_T = N_s + N_c$, with $\boldsymbol{N_c} = 8 \times \boldsymbol{L}$ and $\boldsymbol{N_s} = 16 \times \boldsymbol{L}$. The results are reported for the size system $\boldsymbol{L} = 200$. When studying the double-walled nanotubes properties, the quantities of interest are:

– The instantaneous magnetization per spin in the core and shell defined by

$$m_c(t) = \frac{1}{N_c}\sum_{i=1}^{N_c} S_i, \text{ and } m_s(t) = \frac{1}{N_s}\sum_{i=1}^{N_s} S_n.$$

Using these equations, dynamic order parameters Q_c and Q_s can be written as

$$Q_c = \frac{2\pi}{\omega}\int m_c(t)dt \text{ and } Q_s = \frac{2\pi}{\omega}\int m_s(t)dt.$$

- The total dynamic order parameter per site is $Q_T = \frac{1}{N_T}(N_c \times Q_c + N_s \times Q_s)$.
- The total dynamical magnetic susceptibility is defined by $X_T = \beta N_T(\langle Q_T^2\rangle + \langle Q_T\rangle^2)$, with $\beta = \frac{1}{k_B T}$ and k_B is the Boltzmann constant.
- The dynamical specific heat C_T of the system is given by $C_T = \frac{\partial\langle E(t)\rangle}{\partial_T} = \frac{\beta}{T}[\langle E(t)^2\rangle + \langle E(t)\rangle^2]$, where the instantaneous internal energy of the system $\langle E(t)\rangle$ is defined by

$$\langle E(t)\rangle = \frac{1}{N_T}\sum_{i=1}^{N_T} E_{i,n}(S_{i,n})$$

At each temperature, the Monte Carlo steps per spin (MCS), which are supposed to vary between 2 $\times 10^5$ and 4 $\times 10^5$, were used for computing averages of thermodynamic quantities after 10^5 initial (MCS) has been discarded to achieve equilibrium.

3 Results and Discussion

In this section, we examine some interesting and typical results of time variations of the order parameters to find phases in the mixed Ising DWFNTs spin-1 core and spin-(3/2) shell structure with a crystal field under the influence of both bias and time-dependent magnetic fields. In this model, we take J_c as the unit of the energy, and for simplicity, we take $k_B = 1$.

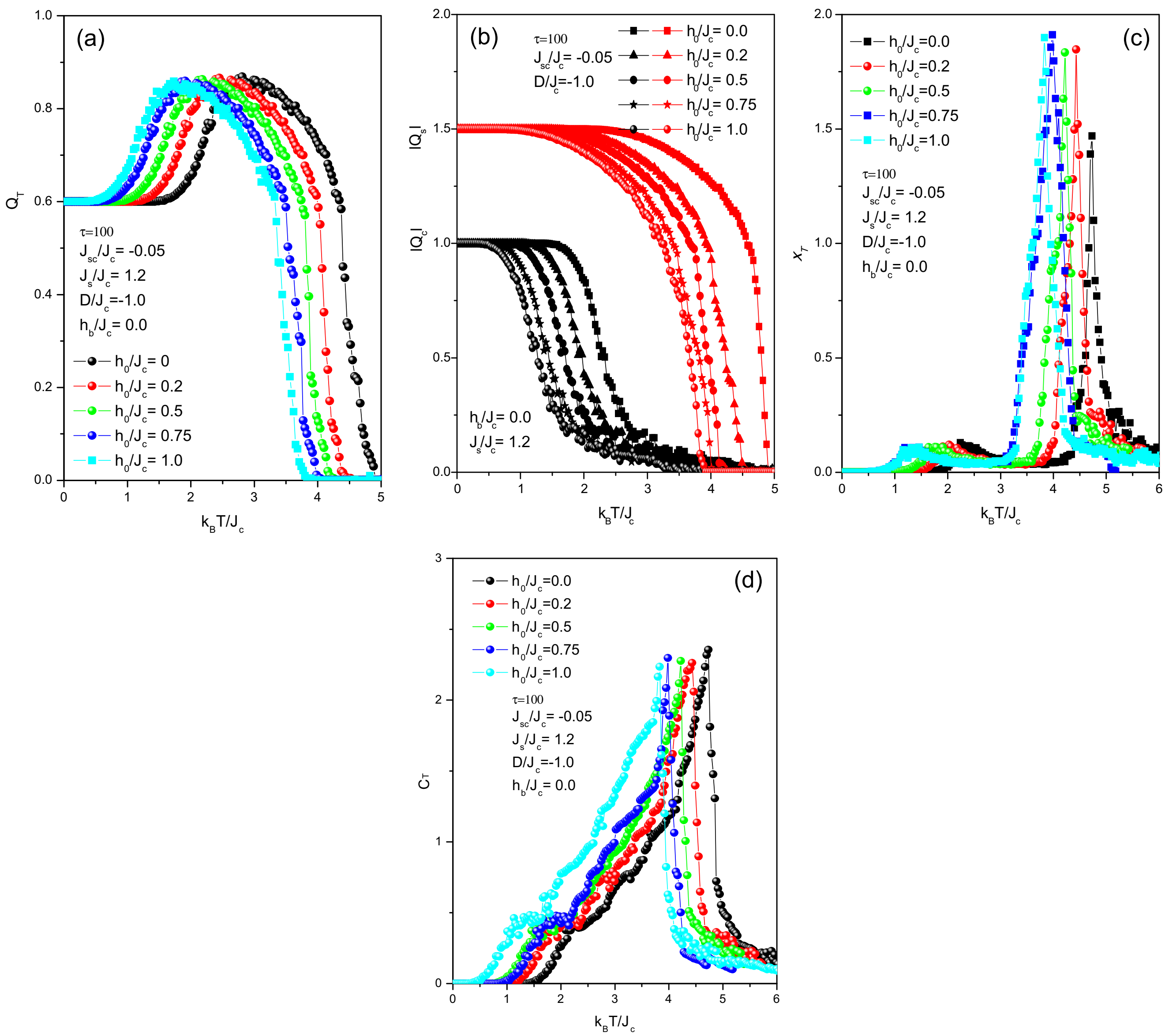


Fig. 2 Temperature dependence of the total (**a**), the core and the shell (**b**) dynamic order parameters, and the susceptibility (**c**) and the specific heat (**d**) for different values of h_0/J_c

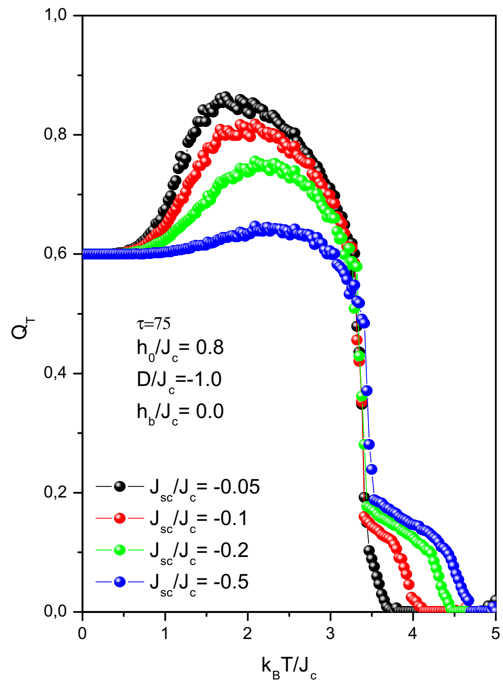


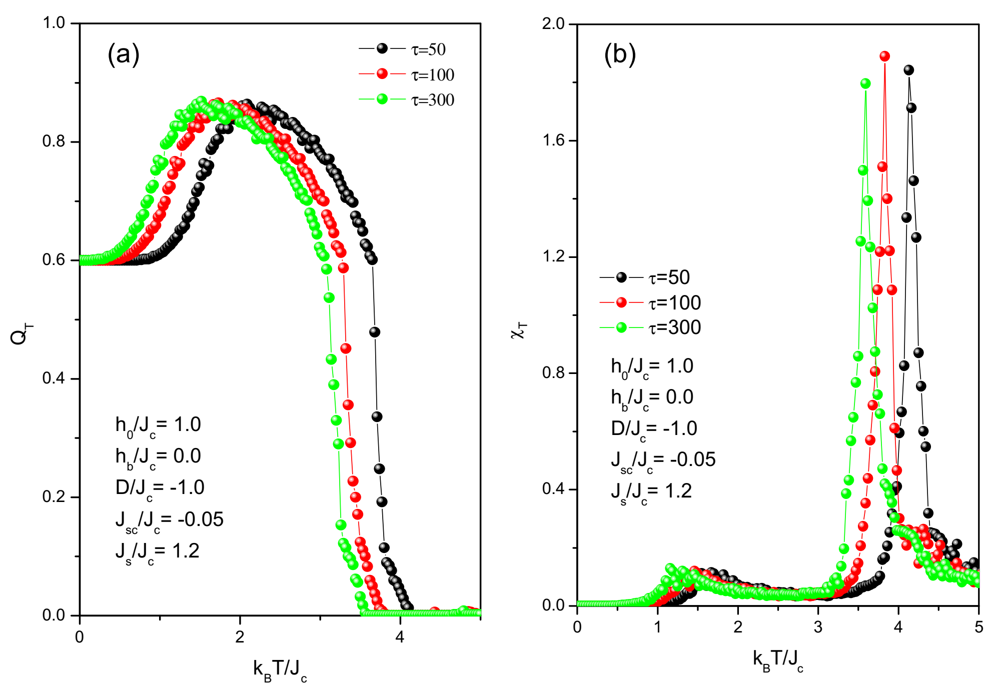
Fig. 3 Temperature dependence of the total dynamic order parameter of a DWFNTs system for different values of J_{sc}/J_c

At first, the effect of the oscillating magnetic field h_0/J_c on the total and the core–shell dynamic order parameters of a mixed spin-(1, 3/2) Ising double-walled nanotubes are investigated and discussed for selected values of J_{sc}/J_c, J_s/J_c, τ and D/J_c. The dynamic order parameters are defined as the time averaged magnetization over a full period of the oscillating magnetic field.

In Fig. 2a–b, we plot the total, the core, and the shell dynamic order parameters of a ferrimagnetic system as function of the temperature for different values of h_0/J_c and for selected parameters (D/J_c = −1.0, J_{sc}/J_c = −0.05, h_b/J_c = 0.0, τ = 100 and J_s/J_c = 1,). From Fig. 2a, we see that the total dynamic order parameter Q_T increases at first with the temperature reaching a maximum value and then decreases to vanish beyond the dynamic phase temperature, namely, second-order phase transition of the system.

However, the dynamic phase transition temperature of the system decreases with h_0/J_c. The similar behavior has also been observed in the previous work related to the core/shell nanowire in Ref. [46]. In Fig. 2b, we show the temperature dependence of the core and the shell dynamic order parameters. We remark that the shapes of Q_c and Q_s curves are similar regardless of h_0/J_c values and begin from the same value at zero temperature and decrease to become zero at the same critical temperatures obtained previously for the system. These temperatures are characterized by the divergence of the total dynamical susceptibility x_τ (Fig. 2c) also by the sharp drop of the total dynamical specific heat C_T (Fig. 2d). Note that this profile of C_T is observed for a ferrimagnetic nanoparticle with spin-(1/2, 1) Core–shell nanostructure [43]. x_T and C_T are interesting physical quantities that describe the characteristics of the change of the magnetization with the

Fig. 4 Temperature dependence of the total dynamic order parameter (**a**) and the susceptibility (**b**) of a ferrimagnetic DWNTs system for different values of τ



magnetic field and that of the internal energy and which can climb the phase transition properties, particularly its critical temperature.

In order to elucidate the influence of the ferrimagnetic interface core–shell coupling parameter on the dynamic evolution of the double-walled nanotube system, we present in Fig. 3 the total dynamic parameter versus reduced temperature for different values of $J_{sc}/J_c < 0$. It is obvious from this figure that the dynamic transition temperature increases when the strength of the ferrimagnetic interface coupling parameter increases. The behavior of these curves is similar to that obtained by Vatansever and Polat for a spherical ferrimagnetic core–shell nanoparticle under a time-dependent magnetic field [47].

In order to study the effect of the period of the oscillating magnetic field τ on the thermodynamic properties of the system for a ferrimagnetic case ($J_{sc}/J_c < 0$), we depict in Fig. 4 the temperature dependence of Q_T (Fig. 4a) and x_T (Fig. 4b) for the different values of τ, when the parameters are fixed as $J_{sc}/J_c = -0.05$, $D/J_c = -1.0$, $J_s/J_c = 1.2$, and $h_0/J_c = 1.0$.

In fact, for each value of the period of the oscillating magnetic field, we remark that the total dynamic order parameter begins from a saturation value and increases continuously with the temperature to reach the maximum, then decreases. The system loses its total dynamic order

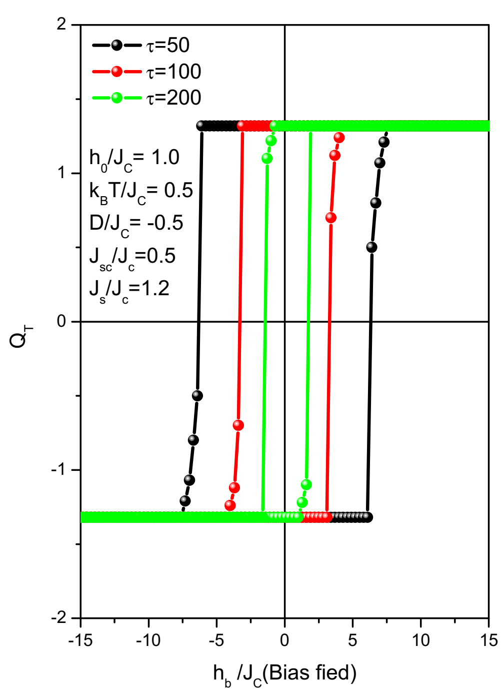


Fig. 5 Dependence of the hysteresis loops of a DWFNTs system for different values of τ

parameter after the critical temperature. The profile of Q_T depends on the difference in the number of "up" and "down" spins and on the competition between the core and surface shell parameters. The similar behavior has been also observed in the previous works related to the core/shell nanostructure in Refs. [46] and [47]. In addition to the above details, we remark that as the period of the oscillating magnetic field τ increases, the transition temperature for the dynamic phase transitions decreases because of the fact that decreasing field frequency leads to decrease of the phase delay between the total dynamic order parameter and the magnetic field and makes the occurrence of the dynamic phase transition easy. The temperature dependence of the total dynamical magnetic susceptibility is shown in Fig. 4b. Near the critical temperature, the total susceptibility increases abruptly and reaches its peak at T_c. From this figure, we can conclude that the dynamic transition temperature decreases with the period of the oscillating magnetic field which is a factor that promotes the magnetic phase of the system tends to shift dynamically to the paramagnetic phase [48].

Finally, we have discussed the influence of the period of the oscillating magnetic field τ on the hysteresis loop of the system, which is obtained by changing cyclically the values of the bias field h_b (Fig. 5). For $k_B T/J_c = 0.5$, the total dynamic order parameter curves are symmetric for both positive and negative values of the bias field h_b. The hysteresis loop of the system becomes narrower with an increases of τ. The similar results are obtained experimentally by Berger et al. [49] and theoretically by Vatansever and Polat [48].

4 Conclusion

In summary, we have studied the dynamic magnetic properties and the hysteresis loops of a mixed spin-(1, 3/2) Ising DWFNTs system with a ferromagnetic or ferrimagnetic interfacial coupling in the presence of the crystal field D/J_c and oscillating magnetic field $h(t)/J_c$. Within the dynamic Monte Carlo simulations, we have discussed the influence of the J_{sc}/J_c the period of the oscillating magnetic field τ, and the bias field h_b/J_c on the dynamic critical temperature and the hysteresis loop. We have also investigated their effect on the profiles of the dynamic magnetic susceptibility and the specific heat of the system.

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