DYNAMICS OF $S = \frac{1}{2}$ AND $S = 1$ ISING SPIN SYSTEM IN RESTANGULAR NANOWIRE

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The dynamic behaviors are studied, within a mean-field approach, in the kinetic mixed spin (1/2, 1) Ising nanowire system with core-shell structure under the presence of a time varying (cosinusoidal) magnetic field by using the Glauber-type stochastic dynamics. The time variations of the average shell and core magnetizations are investigated to obtain the phases in the system. In order to determine the behaviors of time variotions of the average magnetization, the stationary solutions of the dynamic effective filed coupled equations have been studied for various values of interaction parameters, temperature and external magnetic field. It has been determined that the system contain paramagnetic (*p*), ferrimagnetic (*i*), nonmagnetic (*nm*) phases, and also coexistence regions, which strongly depend on interaction parameters.

Keywords: Nanowire; Ising model; Mixed spin system; Mean-field approach; Glauber-type stochasticdynamic.
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1. INTRODUCTION

Researchers have made great efforts analytically [1], experimentally [2] and computer simulations [3] to provide a better understanding of the magnetic behavior of nanowires. Theoretically, the Ising model with a core /shell structure has been accepted in the literature to explain many characteristic phenomena in magnetic nanomaterials, such as magnetic nanoparticles, nanotubes and nanowires, and has begun to be applied in many fields [4-9]. Moreover, the magnetic behaviors of various magnetic nanowires have been investigated in detail using mean field approach [10], correlated effective field theory [11], Green function formalism [12], Bethe Peierls approach [13], Monte Carlo simulation (MCS) [14] and others statistical physics methods. More recently, Boughrara et al. [15] investigated the phase diagrams and magnetic behaviors of the mixed spin (1/2, 1) Ising nanowire and obtained phase diagrams that displayed very rich critical behaviors, such as first-, second-order phase transitions, compensation temperatures, depending on the interaction parameters. Albayrak [16] studied the Ising nanowire system with core-shell structure mixed spin (1/2, 1) in the Bethe weave, and the resulting phase diagrams showed first-, second-order phase transitions and triple critical point behavior.

Although enough studies have been done to understand the balance properties of nanostructured systems using the Ising model, there have not been enough studies for its dynamic properties and especially in recent years, the dynamic properties of these nanostructured systems have been started to be studied. Dynamic phase transitions of cylindrical Ising nanowires under the oscillating outer magnetic field for the ferromagnetic and antiferromagnetic interaction parameters were investigated using Glauber-type stochastic dynamic based effective field theory [17-19].

In this paper, the dynamic behavior of the mixed spin (1/2, 1) Ising nanowire system will be examined using the mean-area dynamic and Glauber-type stochastic dynamic. In order to find the phases, present in the system, time dependent behaviors of the average order parameters will be examined. Thus, it will be possible to interpret dynamic phase transitions and dynamic phase diagrams of the mixed spin (1/2, 1) Ising nanowire system, which is one of the main objectives of this paper.

2. DESCRIPTION OF THE METHOD AND MODEL

Glauber-type stochastic dynamic based mean field approach method is used to investigate the dynamic magnetic behavior of complex spin systems such as ferrimagnetic mixed spin (1/2, 1) Ising nanowire. The schematic representation with rectangular structure that will be used in this paper is given in figure 1.

The model of interest is alternatively composed of three repetitive substrates, A, B and C. The first substrate A, belonging to the spin-1/2 magnetic atoms in the core, takes the values of ± 1/2. The other two substrates B and C, take the values of ± 1, 0, and the S spins in the shell take the values of spin-1. The core of the core is occupied by the σ spins, while the shell is surrounded by the S spins. Hamiltonian expression of the cylindrical mixed spin (1/2, 1) Ising nanowire system, which includes the closest neighbor interactions, the term crystalline or single ion anisotropy, and the term dependent outer magnetic field is defined as

$$H = -J \sum_{<ij>} \sigma_i \sigma_j - J \sum_{<im>} \sigma_i S_m - J_s \sum_{<mn>} S_m S_n - D \sum_{<m>} S_m^2 + h(t)\Big(\sum_{<i>} \sigma_i + \sum_{<m>} S_m \Big) \quad (1)$$

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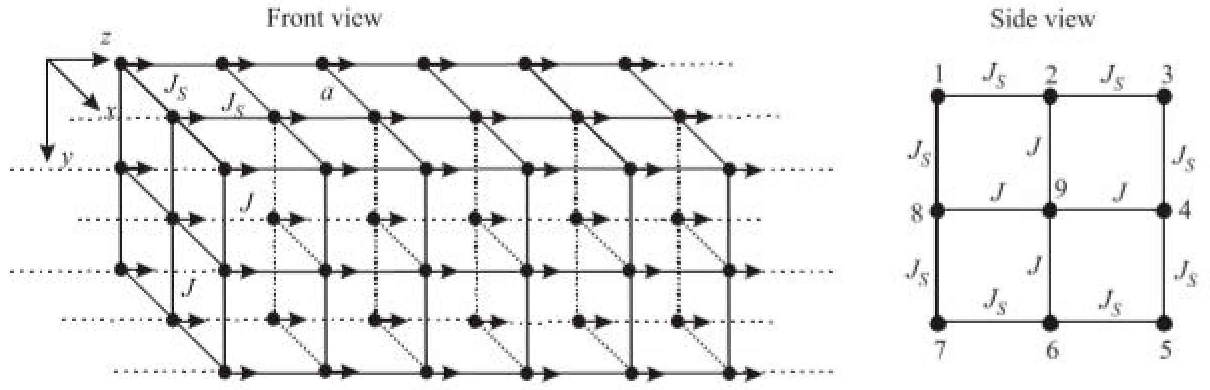

Fig. 1. Model of simple cubic rectangular nanowires. The nanowires are infinite in the direction to the axes z

where $\sigma = \pm 1/2$, $S = \pm 1, 0$. The sum of $< ij >$, $< im >$ and $< mn >$ means that the adjacent spins between the core, core-shell, and at the shell surface. J is the exchange coupling between spins labeled 9 and its nearest neighbors, and J_s is that between surface spins. D denotes the crystal-field or single-ion anisotropy interaction term, and $h(t) = h_0 cos\omega t$ is the time-dependent oscillating external magnetic field. Since the atoms on the surface of the shell have a great influence on the physical properties of nanostructured materials, the term of the bi-linear interaction between magnetic atoms on the surface of the nanostructured materials is defined as follows $J_s = J(1 + \Delta_s)$.

In the presence of time-dependent oscillating external magnetic, we will use the Glauber dynamics and use the Master equation to obtain the mean-field dynamic equations describing the dynamic behavior of the system for the mixed spin (1/2, 1) Ising nanowire system. The mixed spin (1/2, 1) Ising nanowire system changes at a rate of 1 / τ per unit time according to the Glauber-type stochastic dynamic. When the spins in the substrates *B* and *C* remain constant, at time t, the probability function when the system has the spin configuration $\sigma_1, \sigma_2, \dots, \sigma_j, \dots, \sigma_N$ is defined by $P^A(\sigma_1, \sigma_2, \dots, \sigma_j, \dots, \sigma_N, t)$. When the spins on the *A* and *C* substrates remain constant, the probability function at time t of the system when it has the spin configuration $S_1, S_2, \dots, S_j, \dots, S_N$ is defined by $P^B(S_1, S_2, \dots, S_j, \dots, S_N, t)$. Finally, when the spins on the substrates *A* and *B* remain constant, the probability function at time t of the system is defined by $P^C(S_1, S_2, \dots, S_j, \dots, S_N, t)$.

Considering that the spins in the *B* and *C* substrates are fixed for a moment, the master equation for the substrates *A* is writen as

$$\frac{d}{dt} P^A(\sigma_1, \sigma_2, \dots, \sigma_j, \dots, \sigma_N, t) = -\sum_j \left(w_j(\sigma_j \to -\sigma_j)\right) P^A(\sigma_1, \sigma_2, \dots, \sigma_j, \dots, \sigma_N, t) + \\ + \sum_j \left(w_j(-\sigma_j \to \sigma_j) P^A(\sigma_1, \sigma_2, \dots, -\sigma_j, \dots, \sigma_N, t)\right) \quad (2)$$

Here $w_j(\sigma_j \to -\sigma_j)$ is the probability that the spin of ith will change from σ_j state to $-\sigma_j$ state per unit time. Using the canonical set probability distribution expression probability $w_j(\sigma_j \to -\sigma_j)$ can be written as

$$w_j(\sigma_j \to -\sigma_j) = \frac{1}{\tau} \frac{\exp[-\beta \Delta E(\sigma_j \to -\sigma_j)]}{\exp[-\beta \Delta E(\sigma_j \to -\sigma_j)] + 1} \quad (3)$$

Here, $\beta = 1/k_B T$, T is the absolute temperature and k_B is the Boltzmann constant. The change in energy corresponding to following situation

$$\Delta E(\sigma_j \to -\sigma_j) = E(-\sigma_j) - E(\sigma_j) = 2\sigma_j x$$

$$\Delta E(-\sigma_j \to \sigma_j) = E(\sigma_j) - E(-\sigma_j) = -2\sigma_j x$$

where

$$x = 2J < \sigma_j > + 4J \sum_{<i,j>} S_i + h(t)$$

If these energy change expressions found are substituted in the equation (3), $w_j(\sigma_j \to -\sigma_j)$ probability densities

$$w_j\left(\frac{1}{2} \to -\frac{1}{2}\right) = \frac{1}{2\tau} \frac{\exp[-\beta x/2)]}{\cosh[\beta x/2)]} \quad (4a)$$

$$w_j\left(-\frac{1}{2} \to \frac{1}{2}\right) = \frac{1}{2\tau} \frac{\exp[\beta x/2)]}{\cosh[\beta x/2)]} \quad (4b)$$

Using the master equation, the general average-area dynamic equation for sub-*A* is obtained as follows:

$$\tau \frac{d}{dt} < \sigma_j > = -< \sigma_j > + \frac{1}{2} \tanh[\beta\, x/2)] \quad (5)$$

If we make substitutions $m_c = < \sigma_j >_A$, $m_{s1} = < S_j >_B$, $\Omega = \tau\omega$ and $\xi = \omega t$, then we can write equation (5) as follows

$$\Omega \frac{d}{d\xi} m_c = -m_c + \frac{1}{2}\tanh\left[\beta\left(2Jm_c + 4Jm_{s1} + h(\xi)\right)/2\right] \qquad (6)$$

In the mixed spin (1/2, 1) Ising nanowire system, considering the spin in the *A* and *C* substrates remains constant for one, we can also obtain the average area dynamic equations for the *B* substrate using similar calculations as below. In this case, the master equation for *B* substrate

$$\frac{d}{dt} P^B\left(S_1, S_2, \dots, S_j, .., S_N, t\right) = -\sum_j \sum_{S_j \neq S_j'} w_j^B\left(S_j \to S_j'\right) P^B(S_1, S_2, \dots, S_j, .., S_N, t) +$$
$$+\sum_j \sum_{S_j \neq S_j'} w_j^B\left(S_j' \to S_j\right) P^B(S_1, S_2, \dots, S_j', .., S_N, t) \qquad (7)$$

While the system is in balance, with the help of the master equation and general definition of the canonical distribution, the probability of each spin to pass from S_j to S_j' per unit time

$$w_j^B\left(S_j \to S_j'\right) = \frac{\exp[-\beta \Delta E^B(S_j \to S_j')]}{\tau \sum_{S_j'} \exp[-\beta \Delta E^B(S_j \to S_j')]} \qquad (8)$$

Then the expression of $\Delta E^B(S_j \to S_j')$ is found by using the Hamiltonian expression:

$$\Delta E^B\left(S_j \to S_j'\right) = -\left(S_j' - S_j\right)\left(J \sum_{<i,j>} \sigma_i + J_s \sum_{<i,j>} S_i + h(t)\right) - D\left({S_j'}^2 - {S_j}^2\right) \qquad (9)$$

If these energy change expressions found are substituted in the equation (8), probability densities for each *Sj* state are obtained as follows.

$$w_j^B(1 \to 0) = w_j^B(-1 \to 0) = \frac{\exp[-\beta D]}{\tau(\exp[-\beta D] + 2\cosh[\beta y])}$$

$$w_j^B(-1 \to 1) = w_j^B(0 \to 1) = \frac{\exp[\beta y]}{\tau(\exp[-\beta D] + 2\cosh[\beta y])}$$

$$w_j^B(0 \to -1) = w_j^B(1 \to -1) = \frac{\exp[-\beta y]}{\tau(\exp[-\beta D] + 2\cosh[\beta y])}$$

where $y = J \sum_{<i,j>} \sigma_i + J_s \sum_{<i,j>} S_i + h(t)$

If the mean-area approach is used, the mean-area dynamic equation for the *B* substrate,

$$\Omega \frac{d}{d\xi} m_{s1} = -m_{s1} + \frac{2\sinh\left[\beta\left(Jm_c + 2J_s m_{s1} + 2J_s m_{s2} + h(\xi)\right)\right]}{\exp[-\beta D] + 2\cosh\left[\beta\left(Jm_c + 2J_s m_{s1} + 2J_s m_{s2} + h(\xi)\right)\right]} \qquad (10)$$

Similar to the equation (10), the following equation can be obtained for the *t C* substrate

$$\Omega \frac{d}{d\xi} m_{s2} = -m_{s2} + \frac{2\sinh\left[\beta\left(2J_s m_{s1} + 2J_s m_{s2} + h(\xi)\right)\right]}{\exp[-\beta D] + 2\cosh\left[\beta\left(2J_s m_{s1} + 2J_s m_{s2} + h(\xi)\right)\right]} \qquad (11)$$

3. NUMERICAL RESULTS AND DISCUSSION

In order to find the phases, present in the system, the stable solutions of the mean-field dynamical equations given by equation (6), (10) and (11) will be examined for different crystal field *(d)*, magnetic field amplitude *(h)* and temperature *(T)* values. The stationary solutions of equations (6), (10) and (11) are a periodic function of ξ for the period 2π of a periodic function, so it will be, so $m_c(\xi) = m_c(\xi + 2\pi)$, $m_{s1}(\xi) = m_{s1}(\xi + 2\pi)$ and $m_{s2}(\xi) = m_{s2}(\xi + 2\pi)$. Moreover, they can be one of the three types according to whether they have or not have the properties

$$m_c(\xi + \pi) = -m_c(\xi) \qquad (11a)$$

$$m_{s1}(\xi + \pi) = -m_{s1}(\xi) \qquad (11b)$$

and

$$m_{s2}(\xi+\pi) = -m_{s2}(\xi) \qquad (11c)$$

The first type solution of equation (11a) here is called the symmetric solution, and this solution corresponds to the irregular or paramagnetic *(p)* solution. In this solution, the average order parameters, namely the average sublattice magnetizations m_c, m_{s1} and m_{s2} are equal to each other and oscillate around the zero value, conforming to the external magnetic field. The second type of solution does not fit the equation given by (11a), but obeys the equations given by (11b) and (11c). This solution corresponds to the non-magnetic (nm) solution and oscillates around $m_c = \pm 1/2$ values in this solution, while m_{s1} and m_{s2} oscillates around zero. In the third type of solution, the solution we obtained does not obey equations (11) and this is the unsymmetrical solution, which corresponds to the ferrimagnetic *(i)* solution. In this solution, m_c, m_{s1} and m_{s2} are not equal and they oscillate around non-zero values, i.e. $m_c = \pm 1/2$ and $m_{s1(2)} = \pm 1$ and do not conform to the external magnetic field. These solutions are clearly seen by numerically solving the mean-area dynamic equations given by (6), (10) and (11). These equations are solved for the given parameters and initial values, besides paramagnetic (p), non-magnetic *(nm)* and ferrimagnetic (i) base phases in the system *i+ nm*, *nm + p*, *i+nm +p* and *i+p* mixed phases were found. Some solutions corresponding to these phases are shown in figure 2.

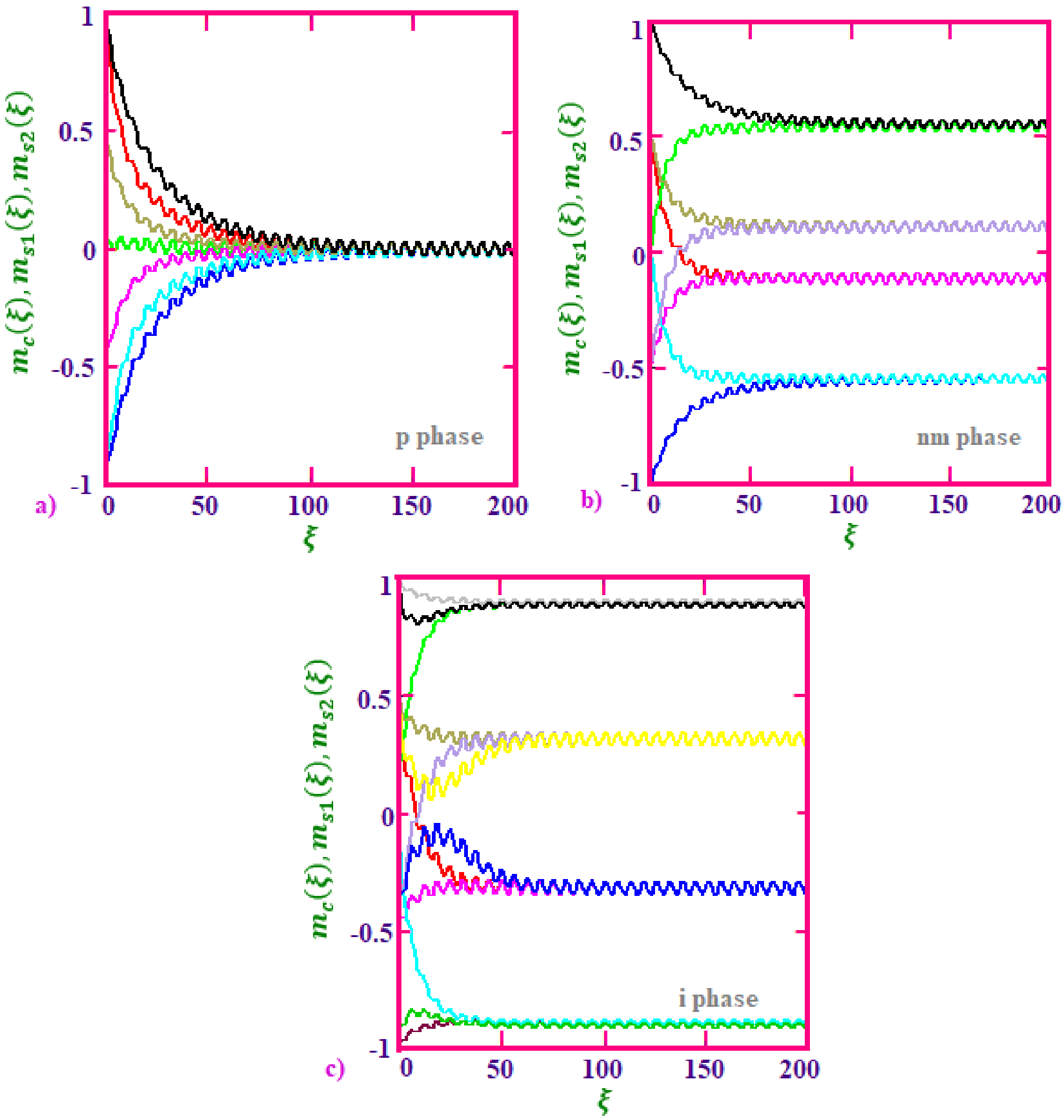

Fig. 2. Time variations of the core and shell magnetizations:
a) paramagnetic phase $k_BT/J = 5.8$, $h_0/J = 1.6$, $J_s/J = 1.8$, $D/J = -1$;
b) nonmagnetic phase $k_BT/J = 5.2$, $h_0/J = 1.6$, $J_s/J = 2.4$, $D/J = -1$;
c) ferrimagnetic phase $k_BT/J = 2.4$, $h_0/J = 1.6$, $J_s/J = 1.8$, $D/J = -1$;

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