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Monte Carlo simulated dynamical magnetization of single-chain magnets

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ABSTRACT

Here, a dynamical Monte-Carlo (DMC) method is used to study temperature-dependent dynamical magnetization of famous Mn_2Ni system as typical example of single-chain magnets with strong magnetic anisotropy. Simulated magnetization curves are in good agreement with experimental results under typical temperatures and sweeping rates, and simulated coercive fields as functions of temperature are also consistent with experimental curves. Further analysis indicates that the magnetization reversal is determined by both thermal-activated effects and quantum spin tunnelings. These can help explore basic properties and applications of such important magnetic systems.

1. Introduction

Various nanoscale spin chains have been attracting great attention because of their important properties and potential applications in information science and technology [1–5]. The single-chain magnet (SCM) is a new member of such nanoscale spin chains, and its basic spin unit comes from some transition-metal or rare-earth ions combined with appropriate organic molecules [2–14]. A famous SCM is the $[Mn_2Ni]$ system [3–7], with $C_{62}H_{64}N_{10}O_{14}Cl_2Mn_2Ni$ and $C_{60}H_{66}N_{12}O_{14}Cl_2Mn_2Ni$ as two typical formula units with spin $S=3$. A well-known Arrhenius law has been observed for their spin relaxation at high enough temperature [15,16]. On the other hand, at low enough temperature, quantum Landau–Zener (LZ) spin tunneling should play important roles in their spin reversal [17,18]. Such phenomena can be investigated by using some methods for single-molecule magnets [19–28]. As for SCM systems, inter-spin exchange interactions play important roles and thermal effects can cause Glauber spin dynamics [5,6], which was originally proposed for one-dimensional Ising spin model [29–31]. Furthermore, a systematical experimental study shows that quantum nucleation can become important to reverse single spins, create domains of reversed spins, and reverse the whole SCM [7]. Therefore, it is useful to elucidate what roles these play in determining dynamical magnetization of SCM systems.

Here, we use the hybrid DMC method and thereby investigate the $[Mn_2Ni]$ SCM system as a typical example of SCMs, taking both classical and quantum effects into account. Our results for typical temperatures and sweeping rates are consistent with corresponding experimental curves. It is very interesting that we can satisfactorily fit the simulated and experimental B_c–T curves by one simple function. These means that the DMC method and simulated results are both reasonable and reliable for such SCM systems. Furthermore, we explain magnetization reversal modes for different temperatures on the basis of our simulated results and analyses. More detailed results will be presented in the following.

2. Model and methods

Here, we use the hybrid DMC method and thereby investigate the $[Mn_2Ni]$ SCM system as a typical example of SCMs, taking both classical and quantum effects into account. Our results for typical temperatures and sweeping rates are consistent with corresponding experimental curves. It is very interesting that we can satisfactorily fit the simulated and experimental B_c–T curves by one simple function. These means that the DMC method and simulated results are both reasonable and reliable for such SCM systems. Furthermore, we explain magnetization reversal modes for different temperatures on the basis of our simulated results and analyses. More detailed results will be presented in the following.

The single-chain magnet can be considered a one-dimensional composite spin lattice whose spins can be constructed by repeating a basic unit of $[Mn_2Ni]$: Mn–Ni–Mn (or Mn^{3+}-Ni^{2+}–Mn^{3+}). The antiferromagentic Ni–Mn interaction is much stronger than

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the ferromagnetic Mn–Mn one so that the low-temperatures physics of this spin chain can be modelled by an effective ferromagnetic chain of the units of [Mn_2Ni] ($S=3$) with spin interaction only between the nearest units [3,4,6–12].

The ferromagnetic spin Hamiltonian can be expressed as [7,14,9]

$$\hat{H} = \hat{H}_0 - \sum_{i=1}^{N-1} J\hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1} - \sum_{i=1}^{N} g\mu_B B_z \hat{S}_i^z \tag{1}$$

where g is the Lande g factor ($g=2$ is used), μ_B is the Bohr magneton, J (>0) is the ferromagnetic exchange constant. $\hat{\vec{S}}_i = \{\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z\}$ is the spin vector operator for the i-th Mn_2Ni unit, and

$$\hat{H}_0 = \sum_{i=1}^{N} \{ -D(\hat{S}_i^z)^2 - E[(\hat{S}_i^x)^2 - (\hat{S}_i^y)^2]\} \tag{2}$$

is the Hamiltonian for the isolated ferromagnetic spin.

D and E are the anisotropic parameters. As for the parameters of the spin interaction and on-site anisotropy, we use $J/k_B = 1.56$ K and $D/k_B = 2.5$ K from thermodynamical measurements [7,14,9]. The transverse anisotropic parameter E is much smaller, but necessary to realize the Landau–Zener spin tunneling. We take $E/k_B = 0.1$ K by comparing our simulated results with experimental ones.

We use a dynamical Monte Carlo method to simulate the spin dynamics of the interacting spin system under sweeping magnetic field [32,33,28]. At the beginning, we set all of the spins at the state $S^z = -3$.

We divide the time t into small time steps with a step length Δt and describe the Monte Carlo time points with $t(n)$, where n takes 0, 1, 2, 3,…. The magnetic field starts from $-B_0$ and increases by an increment of $\Delta t \cdot \nu$ until B_0. The spin can be reversed within a Monte Carlo step (MCS) through the two reversal mechanisms.

For the classical thermal activation, we can obtain the following probability P_{th} that is within the time decrement Δt [15,16]:

$$P_{th} = 1 - \exp(-R_i \Delta t) \tag{3}$$

where $R_i = R_0 \exp(-\Delta E_i/k_B T)$ is the transition rate, k_B is the Boltzmann constant, T the temperature, and R_0 the characteristic frequency for the spin system ($3\times10^8\ s^{-1}$). ΔE_i is the potential barrier of the i-th spin between $S_i^z = -3$ and $S_i^z = 3$, as shown in Fig. 1.

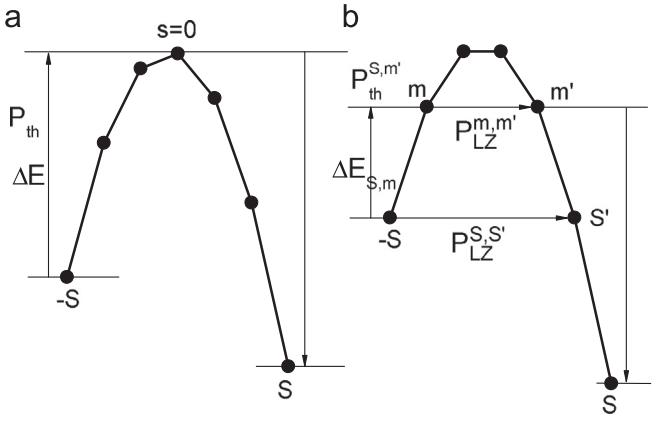

Fig. 1. A schematic of the three spin reversal mechanisms: thermal-activated barrier hurdling (a), direct and thermal-assisted LZ tunnelings (b). The horizontal solid line with arrow means that the two energy levels satisfy the resonance conditions. The probabilities, energy levels, barrier, and other symbols are defined in the text.

There is a necessary condition for a LZ tunneling of a spin to occur: one of the spin energy levels on the side must be equivalent to another, for example, $E_m(t) = E_{m'}(t)$, as shown in Fig. 1. With the neighboring spins taken into account, such conditions are satisfied at the given magnetic fields [28]. The corresponding LZ transition probability is given by

$$P_{LZ}^{m,m'} = 1 - \exp\left[-\frac{\pi(\Delta_{m,m'})^2}{2\hbar g\mu_B|m-m'|\nu}\right] \tag{4}$$

where the tunneling splitting $\Delta_{mm'}$ is the energy gap at the avoided crossing of states m and m', and ν denotes the sweeping rate of the magnetic field.

When m equals $S=-3$ and m' is S', we obtain a direct LZ tunneling with the probability $P_{LZ}^d = P_{LZ}^{S,S'}$. For other possible LZ tunneling to happen, the spin at first must be excited from $S^z=-3$ to the m values through some thermal activations, as shown in Fig. 1. Considering the thermal probability $P_{th}^{S,m}$ which can be obtained by using the expressions (3), the probability of spin reversal in this channel, P_{LZ}^m, is given by $P_{LZ}^m = P_{th}^{S,m}\cdot P_{LZ}^{m,m'}$. All the three spin-reversal channels are combined to give the total probability for a spin reversal [28]:

$$P^{tot} = 1 - \left(1 - P_{th}\right)\left(1 - P_{LZ}^d\right)\prod_m \left(1 - P_{LZ}^m\right) \tag{5}$$

In our simulations, we take $\Delta t = 0.1$ ms and use 100 units of Mn_2Ni with free boundary condition. The magnetization is calculated by averaging S_i^z over the 100 spin sites. Each data point is calculated by averaging 10,000 independent runs to reduce possible errors. The value of B_0 is made large enough to obtain complete hysteresis loops with the help of a symmetrization treatment.

3. Main results and analysis

Presented in Fig. 2 are our typical simulated magnetization curves for five different field sweeping rates ν (0.001, 0.004, 0.017, 0.07, and 0.28 T/s) at three different temperatures T: 2.5, 1.5, and 0.5 K. The simulated results show that the hysteresis loops are strongly dependent on both temperature T and field sweeping rate ν. Our simulation shows that there is no hysteresis loop for all the field sweeping rates when temperature reaches 3 K, and at 2.5 K, the thermal effects are dominant and spins can be easily reversed,

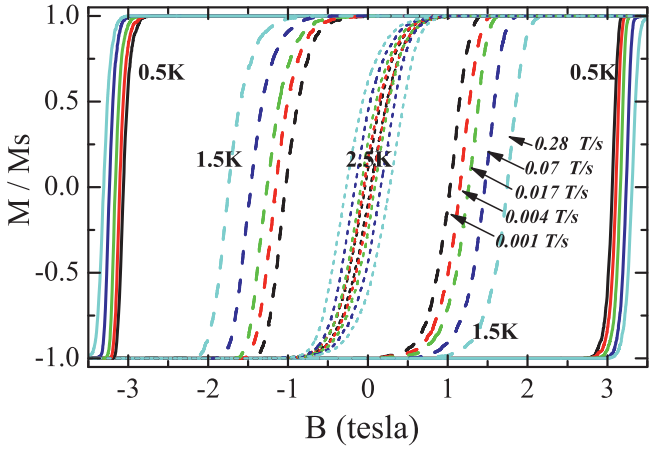

Fig. 2. Hysteresis loops (normalized magnetization (M/M_s) curves against the sweeping field B) for three temperatures: 0.5, 1.5, and 2.5 K. For every temperature, five magnetization curves are plotted with five field sweeping rates: 0.001, 0.004, 0.017, 0.07, and 0.28 T/s (from the innermost loop to the outermost for each temperature).