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The fractional magnetization plateaus of synthetic triangular heterostructures: Monte Carlo simulation

W.Z. Zhuo [a], J. Chen [a], M.H. Qin [a,*], M. Zeng [a], X.B. Lu [a], X.S. Gao [a], J.-M. Liu [b,*]

[a] Institute for Advanced Materials and Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, South China Normal University, Guangzhou 510006, China
[b] Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

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ABSTRACT

In this work, we study the magnetization process of triangular heterostructures formed by a number of multilayers which are coupled antiferromagnetically by Monte Carlo simulation of an Ising model. The antiferromagnetic in-layer and ferromagnetic inter-layer couplings are considered in each stack. Interestingly, it is observed that several additional magnetization plateaus can be stabilized by the consideration of the inter-stack coupling, in addition to the main 1/3 plateau observed in bulk system. Furthermore, the widths of these plateaus are mainly determined by the lattice structure and inter-stack coupling, and the heights are only dependent on the lattice structure. Thus, our work suggests a possible method of modulating the spin orders and magnetization plateaus in synthetic triangular heterostructures through detailed tuning the lattice structure.

1. Introduction

During the past several years, fascinating step-like magnetization behaviors observed in a number of frustrated spin systems such as triangular Ising spin-chain system $Ca_3Co_2O_6$ and $Sr_5Rh_4O_{12}$ have attracted widespread interest for their rich physics and potential applications [1–4]. For example, a four-step magnetization pattern has been observed at low temperatures (T) in bulk form of $Ca_3Co_2O_6$. Theoretically, the two-dimensional triangular rigid-chain model is well accepted for studying the magnetic properties of such triangular spin-chain system [5–7]. It has been proved that the equilibrium state of this model only produces the two-step (at $M = 1/3$ and $M = 1$, where M is the magnetization density) magnetization curve, and the experimentally observed multi-step magnetization behavior probably be due to the non-equilibrium magnetization [8–12]. In some extent, there is still an urgent need to find some other methods of modulating more stable plateaus in frustrated triangular systems, in order to speed up their application process. Thus, we draw our eyes on layered triangular heterostructures.

The study on the phase competitions in layered heterostructures becomes attractive from the following two viewpoints. On one hand, magnetic heterostructures can be potentially used in high-density storage technology and spintronic devices which are generally designed by building on thin films [13]. On the other hand, novel phases may be developed in this specific geometry, and rich physics responsible for their stabilizations are also very interesting. For example, [Co/Pt]/Ru heterostructures with ferromagnetic (FM) [Co/Pt] multilayers which are coupled through an antiferromagnetic (AFM) inter-stack interaction have been experimentally designed, which exhibits interesting magnetization plateaus [14–18]. Theoretical works suggest that additional intermediate phase is stabilized in certain magnetic field (h) region in the synthetic layered square heterostructures, leading to the generation of the additional plateau [19]. Furthermore, the intermediate state is proved to be resulted from the competition between the inter-stack interaction and Zeeman energy. Thus, one may question that if more stable plateaus can be stabilized in frustrated layered triangular heterostructures in which strong energy competitions are available. In fact, the magnetization behaviors in $Ca_3Co_2O_6$ thin film have been experimentally investigated, and only the 1/3 magnetization plateau is observed at low T [20–23]. Technically, it is possible to tune the inter-layer FM coupling into AFM coupling in $Ca_3Co_2O_6$ heterostructures by detailed modulating the distances between different layers and/or stacks. However, a detailed lattice structure design may not be well controlled in laboratory so far, while relevant theoretical progress is under the way.

* Corresponding authors.
E-mail addresses: qinmh@scnu.edu.cn (M.H. Qin), liujm@nju.edu.cn (J.-M. Liu).

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In this work, we study the magnetization process of layered triangular heterostructures formed by a certain number of stacks which are AFM coupled via spacers. In every stack, the AFM in-layer nearest neighbor (NN) and the FM inter-layer NN couplings are considered [24]. The phase diagram for systems with stacks of different sizes obtained by means of Monte Carlo (MC) simulations exhibits two intermediate phases over an extended h window. Thus, two additional nonzero magnetization plateaus can be stabilized in such a heterostructures model, in addition to those at $M = 1/3$ and 1 observed in bulk system. Furthermore, our work suggests that the widths (h-region) of the plateaus can be modulated by the inter-stack coupling and the lattice structure, while the heights (value of M) of the plateaus are only dependent on the lattice structure.

The remainder of this paper is organized as follows: in Section 2 the model and the simulation method will be described, Section 3 attributes to the simulation results and discussion, and finally the conclusion is presented in Section 4.

2. Model and method

For simplicity, we consider the heterostructures as a three-dimensional layered triangular lattice. The periodic boundary conditions are applied in the x- and y-axis directions, and the free boundary condition is applied in the z-axis direction. The system with L_z layers along the z direction are considered to be composed of stacks that contain a certain number (l_z) of layers (Fig. 1 shows the case of $L_z = 4$ and $l_z = 2$, as an example). Thus, the model Hamiltonian can be given by:

$$H = J \sum_{\text{in-layer}} S_i \cdot S_j + J_I \sum_{\text{inter-stacks}} S_i \cdot S_j + J_s \sum_{\text{in-stack}} S_i \cdot S_j - h \sum_i S_i, \qquad (1)$$

where the first term is the AFM in-layer NN coupling with $J > 0$, S_i is the Ising spin with unit length on site i. The second term denotes the AFM coupling between stacks with $J_I > 0$, while the third one is the FM coupling between layers in the same stack with $J_s < 0$, as shown in Fig. 1. The last term is the Zeeman energy with h applied along the $+z$ axis. Unless stated elsewhere, we set $J = 1$ as energy unit, and take other couplings and h as variables to study the magnetization behaviors.

The simulation is performed on a $L \times L \times L_z$ layered triangular lattice using the standard Metropolis algorithm and temperature exchange method [25,26]. It is well known that the temperature exchange method can be utilized to prevent the system from trapping in metastable free-energy minima due to the frustration. We take an exchange sampling after every 25 standard MC steps. Typically, the initial 5×10^4 MC steps are discarded for thermal equilibrium and another 5×10^4 MC steps are retained for statistic averaging of the simulation. In this work, the average magnetization M and the exchange energies are calculated. Generally, $L = 24$ is chosen, and other choice of L will be proved never affect our conclusions.

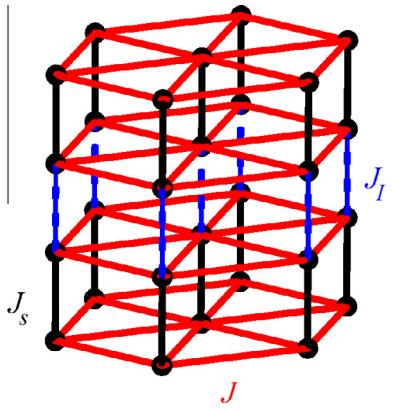

Fig. 1. Effective model of the layered heterostructures for $(L_z, l_z) = (4, 2)$ with in-layer coupling J, inter-stake coupling J_I, and inter-layer coupling in the same stack J_s.

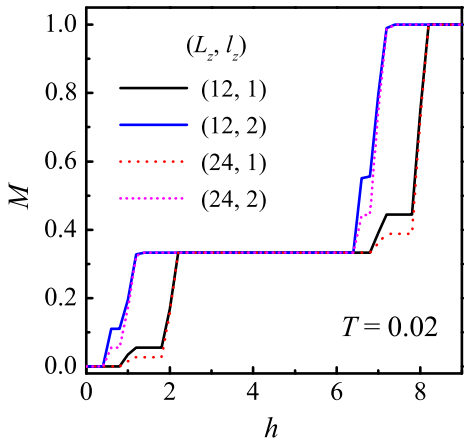

Fig. 2. Magnetization M as a function of h for systems with even numbers of L_z/l_z at $T = 0.02$ for $J_I = 1$ and $J_s = -1$.

3. Simulation results and discussion

For the bulk system with strong FM intra-chain coupling, the equilibrium states generating only two magnetization plateaus at $M = 1/3$ and $M = 1$ have been strictly confirmed. The former plateau is resulted from the so-called UUD state in which each triangle contains two up-spins and one down-spin. The magnetic properties in heterostructures are significantly dependent on the number of stacks (L_z/l_z), and the cases of even and odd number of L_z/l_z will be separately discussed below.

3.1. The case of even number of L_z/l_z

First, we study the magnetization behaviors of the model with even number of stacks. Fig. 2 shows the simulated M as a function of h at $T = 0.02$ for $J_I = 1$ and $J_s = -1$ for various (L_z, l_z) with even numbers of L_z/l_z. Interestingly, three additional plateaus (at $M = 0$, 1/18 and 4/9 for $L_z = 12$ and $l_z = 1$, as an example) are observed, in addition to the main plateaus at $M = 1/3$ and $M = 1$. Furthermore, the positions (transition h) and the widths of the additional plateaus are dependent on the value of l_z, and the heights of these plateaus are modulated by L_z and l_z, as shown in Fig. 2.

The physics underlying our simulations can be uncovered through the analysis of energy competitions and spin configurations. We calculate the h-dependence of the in-layer spin-exchange energy $E_{\text{in-layer}}$, the inter-stack coupling energy E_I, the FM coupling energy between layers in the same stack E_S, the Zeeman energy E_{zee} and the total energy E, respectively. The calculated results for $L_z = 12$ and $l_z = 1$ at $T = 0.02$ are shown in Fig. 3(a), and the corresponding magnetization curve is also presented in Fig. 3 (b). It is clearly shown that the inter-stack interaction plays an important role in the stabilization of the three additional plateaus. At $h = 0$, an in-layer disordered state in which the spin configurations UUD and DDU exist with the same probability in a triangular sub-lattice is developed. At the same time, the NN spins along the z direction in the same stack parallel with each other to satisfy E_S, while those between the stacks antiparallel with each other to satisfy E_I, leading to zero M. When h is increased to the first critical field h_1, the spins in surface stacks form the in-layer UUD spin