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Monte Carlo simulation of magnetic properties of a nano-graphene bilayer in a longitudinal magnetic field

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ABSTRACT

Monte Carlo simulation has been used to study the magnetic properties of a nano-graphene bilayer which consists of the upper layer A with spin-3/2 and the bottom layer B with spin-5/2. The effects of the single-ion anisotropy, the intralayer exchange coupling and the longitudinal magnetic field on the magnetization, the susceptibility, the blocking temperature and hysteresis loops of the mixed-spin nano-graphene bilayer system have been examined detailedly. In particular, the variations of the blocking temperature with different intralayer exchange couplings, single-ion anisotropies, and the longitudinal magnetic field are obtained for the present system. Many multiple hysteresis loop behaviors have also been found, depending on the combinations of both the upper and bottom layer magnetizations in the longitudinal magnetic field. Through a comparison, our results obtained are according well with other theoretical researches and experimental results.

1. Introduction

Over one decade, graphene has become the focus of carbon-based materials due to its remarkable physical and chemical properties. It sparkles with many performances, such as electrical energy storage, high mechanical stability, and low-intensity. With the development of nanotechnology, it is likely to make graphene become one of the lightest and thinnest two-dimensional materials, which results from its unique structure of benzene's six-membered rings. Furthermore, the discovery of nano-graphene's original magnetic behaviors has broadened its potential prospect in many fields, such as biosensor [1], solar cells [2], linear magneto resistance [3], environmental science [4], chemical engineering [5] ect.

On one hand, the exploration of graphene in experiment has received great interests. Graphene has been manufactured by diverse methods at present, which advances the process in the preparation of nano-graphene. Zhong et al. applied the method of high concentration of carbon source under low pressure and cool slowly to prepare double-layer graphene with homogeneous layers [6]. Graphene has also been synthesized by the process of graphite's ultrasonic treatment in water or sodium dodecyl benzene sulfonate. The results illustrate that the majority of graphene under five layers possess high electrical conductivity [7]. Moreover, light transmittance of nano-graphene has been improved through the technique of exfoliation-inserting layers again-inflation [8].

On the other hand, theoretical explanations can lay the foundation for experimental evidences. In recent years, a number of theoretical models and methods have been devoted to exploring the physical properties of nano-graphene. The density-

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functional theory is employed to study electronic and magnetic properties of cobalt-vacancy defect complexes in graphene [9]. The results show that both the vacancycobalt separation and the sub-lattice of the vacancy relative to cobalt can determine the magnetization induced on the cobalt atom. The mean-field theory has been applied to study the magnetic properties of graphene nanostructures [10]. It is found that the magnetic field and the external in-plane electric play important roles in the ground phase diagram. What is noticeable is that the edge-state spins arranged parallel to one another in a zigzag edge express a very strong ferromagnetic interaction, which makes the nano-graphene become the excellent ferromagnet with a higher Curie temperature [11]. A Boumali has studied the mean energy, the free energy and the specific heat of graphene structure [12]. L. Xu et al. have probed into the topological phases in biased ferromagnetic bilayer graphene with an external ferromagnetic exchange coupling under the magnetic field [13]. Besides, Peres et al. have analyzed the variations of magnetic susceptibility of graphene with temperature [14]. The effect of nono-magnetic defects on the magnetization in graphene has also been examined by V.V. Nelayev et al. with ab-initio simulation [15]. By Green's functional method and density functional theory, X. Zhong et al. have studied transport properties and the stacking dependent electronic structure of bi-layer graphene nano-ribbons suspended between gold electrodes [16]. Using effective-field theory (EFT) with correlations, the magnetic properties of a nano-graphene bilayer described by a transverse Ising model have been investigated in an external magnetic field [17]. The results revealed that the exchange coupling, the single-ion anisotropy, the transverse field and the external magnetic field have profound impacts on the magnetization, the susceptibility and the blocking temperature of the nano-graphene bilayer.

It is well known that Monte Carlo simulation is a successful method for mixed-spin Ising models, which can provide proper evidences for the analysis of the physical origin of magnetism. By modeling the single-layer and double-layer nano-graphene mixed-spin Ising systems, Monte Carlo simulation has been used to investigate the effects of the defects, the size effect, the crystal field and the external magnetic field on the magnetization, the blocking temperature and hysteresis loops of the nano-graphene system with mixed spin $\sigma = 3/2$ and spin $S = 5/2$ [18–20]. It has been discovered that the double hysteresis loop behaviors exist for some certain physical parameters. In our previous work, the thermodynamic properties, such as internal energy and the specific heat of a nano-graphene bilayer in the external magnetic field have been discussed by Monte Carlo simulation [21]. Although many efforts have been devoted to understanding the physical properties of the nano-graphene bilayer, less attention has been paid to the magnetic properties of the nano-graphene bilayer subjected to the external magnetic field by using Monte Carlo simulation. In particular, the blocking temperature dependences of different physical parameters have not been further clarified. Thus, we intend to explore whether the nano-graphene bilayer system can express richer hysteresis loop behaviors. Therefore, our intention of this paper is to study the effects the exchange coupling, the single-ion anisotropy and the external magnetic field on the magnetization, the susceptibility, the blocking temperature and hysteresis loops of the nano-graphene bilayer.

The outline of this paper is classified as follows. The model, the Hamiltonian of the system and the calculation procedure of Monte Carlo simulation have been discussed detailedly in Section 2. In Section 3, we shall show typical simulation results for the magnetization, the susceptibility, the blocking temperature and the hysteresis loops. The summary and conclusions are obtained finally in Section 4.

2. Model and Monte Carlo simulation

The structure of the nano-graphene bilayer is depicted in Fig. 1. It consists of different spins with the antiferromagnetic intralayer exchange coupling in the upper layer ($\uparrow\downarrow, \sigma = 3/2$) and with the ferromagnetic intralayer exchange coupling in the bottom layer ($\uparrow\uparrow, S = 5/2$). Similar three-dimensional structures have also been described in Refs. [17,21]. Then we shall present the Hamiltonian of the system as follows:

$$H = -J_A \sum_{i,j} \sigma_{iA}^z \sigma_{jA}^z - J_B \sum_{i,j} S_{iB}^z S_{jB}^z - J_{AB} \sum_{i,j} \sigma_{iA}^z S_{jB}^z - D_A \sum_i \left(\sigma_{iA}^z\right)^2 - D_B \sum_j \left(S_{jB}^z\right)^2 - h\left(\sum_i \sigma_{iA}^z + \sum_j S_{jB}^z\right) \quad (1)$$

where the first three sums only operate the nearest-neighbours, $\sigma_{i(j)A}^z$ represents the spin operator on the upper layer ($\sigma_{iA}^z = \pm 3/2, \pm 1/2$), and $S_{i(j)B}^z$ represents the spin operator on the bottom layer ($S_{jB}^z = \pm 5/2, \pm 3/2, \pm 1/2$).Both J_A (<0) and J_B (>0) denote the exchange couplings in the upper and bottom layer, respectively. J_{AB} stands for the interlayer exchange coupling between the upper and bottom layer. D_A and D_B are the single-ion anisotropies in the upper and bottom layer, respectively. h denotes the external magnetic field.

For our simulation, the method used is the standard single-spin-flip importance method on the basis of the Metropolis algorithm [22], which is constructed on the $N \times L$ three-dimensional honeycomb lattice. We define N and L as the number of spins in each layer and the thinness of the bilayer ($L = 2$), respectively. Further simulations have also been carried out for the choice of the size of system. For the variations of N from 48 to 108, we have not found obvious differences. Therefore, such is the case with $N = 48$ for the selection of our simulation, shown in Fig. 1. As a guarantee, not less than 5000 Monte Carlo steps (MCS) per site were eliminated to balance the system before averaging thermal quantities over the next 15000 MCS. The physical quantities are calculated as follows:

The upper and bottom layer magnetizations M_A, M_B are expressed by: