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Compensation behavior and magnetic properties of a ferrimagnetic mixed-spin (1/2, 1) Ising double layer superlattice

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ABSTRACT

The compensation behavior and magnetic properties of a ferrimagnetic mixed-spin (1/2, 1) Ising double layer superlattice have been investigated by Monte Carlo simulation. The effects of the exchange couplings and the layer thickness of the system on the compensation and transition temperatures, the magnetization, the susceptibility, the internal energy and the specific heat of the system have been examined in detail. In particular, we find some interesting phenomena such as various types of magnetization curves, originating from the competition between the exchange coupling and temperature. Our results can be compared with previous theoretical studies, and a good agreement has been obtained from a qualitative comparison.

1. Introduction

In recent years, due to the small size, the quantum effect and the interface effect, magnetic multilayer film materials have shown a great deal of fascinating properties different from the bulk materials , such as surface-enhanced magnetic moment , surface-enhanced magneto-crystalline anisotropy, enhanced interlayer coupling , giant magnetoresistance effect and magneto-optic effect, etc. [1–5]. These properties have attracted more and more theoretical and experimental scientists to carry out the extensive and deep studies for various kinds of magnetic multilayer film materials [6,7]. Multi-sublattice model has been made to describe and explain magnetic properties of rare-earth and transition metal compounds R_2Fe_{17} , $Ho_2Fe_{11}Ti$ and $TbMn_6Sn_6$ [8–10]. The compensation point of the ferrimagnetic material has a great application in magnetic recording field [11–13]. Therefore , when the theoretical study get a major breakthrough , a large number of outstanding experimental work are constantly emerging. M. Abid et al. have focused on magnetic properties of Ni/V multilayers [14]. The influences of Ni layer thickness on the magnetization and the critical temperature (T_c) have been studied. Ryazanov et al. have also studied the effects of thickness on T_c in the Nb-$Cu_{0.43}Ni_{0.57}$ bilayers by [15]. They have found the nonmontonic behavior of T_c with the increasing of ferrimagnetic interlayer thickness. It has been observed that the thickness of the AlO interlayer has a strong effect on the hysteresis loops for the FeCoSiN/AlO/FeCoSiN trilayers [16].

In theory , one of the most studied works for the layered magnetic materials mainly concentrated in the magnetic properties of magnetic bilayer. Jiang et al. have studied the variation of the energy spectra and specific heat of the bilayer for different physical parameters by linear spin-wave approximation and Green function method [17,18]. Qiu et al. have studied the spin-wave resonance frequency in a ferromagnetic bilayer or triple-layer film with single-ion anisotropy by using the linear spin-wave approximation and Green's function method [19]. The surface enhancement phenomenon and dynamic nature of the critical phenomena have been investigated by Aktaş et al. [20]. The effects of bimodal random crystal field have been studied on the phase diagrams and magnetization curves of ferrimagnetic mixed spin-1/2 and spin-3/2 Blume-Capel models with correlations for honeycomb lattice by using the effective field theory [21]. The critical properties of the mixed spin Ising model consisting of spin (−1/2, 3/2) have been investigated by Yigit et al. Using the effective-field theory (EFT), they have found that one or two temperatures for appropriate values of the random crystal fields [22]. Belmamoun et al. have studied the magnetic properties of a finite superlattice with disordered interfaces$(A)_L(A_pB_{1-p})(A_{1-p}B_p)(B)_L$ within the framework of an effective field theory [23]. M. Boughrara et al. have found that the existence of the compensation points depending strongly on the thickness of the film [24]. Using the mean-field theory and Glauber-type stochastic dynamics, the dynamic magnetic properties have been examined for the mixed spin (2, 5/2) Ising bilayer system with AFM/AFM interactions and crystal-field interactions in an oscillating field [25,26]. Feraoun et al. have employed MC simulation to study the magnetic properties of a ferrimagnetic nanowire on a hexagonal lattice with a spin-3/2 core surrounded by a spin-1 shell layer [27]. The phase diagrams and

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magnetic properties of the mixed spin (1, 3/2) Ising superlattice with alternate layers have been investigated by means of Monte Carlo (MC) simulation based on the Metropolis algorithm by Feraoun et al. [28]. In addition, Liu et al. have used the effective field theory to study the magnetic properties of a random diluted spin (1/2, 1, 3/2) superlattice which consists of three different ferromagnetic materials [29]. Recently, Kantar et al. have investigated the hysteresis and compensation behaviors of a spin-1 bilayer Ising model on a square lattice by the EFT [30]. It is worth mentioning that the dynamic phase transitions and dynamic phase diagrams of the kinetic spin-1/2 bilayer system have been studied within Glaube-type stochastic dynamics based on the EFT [31]. From the point of experiment, the effect of the layer thickness has become an attractive project in the research for the bilayers and the multilayers. The effects of Ti/TiN multilayers thickness on T_c have been studied in Cu/Nb/Cu trilayers [32]. The experimental observations of Cu/Nb/Cu trilayers have also shown the significance of the layer thickness on the superconducting T_c [33]. On the other hand, there are lots of theoretical efforts devoted to the study for the effect of layer thickness on the compensation behavior and magnetic properties of the multilayers. Using EFT, Oubelkacem et al. have investigated effects of layer thickness on the compensation temperature for an antiferromagnetic double layer superlattice by modeling a mixed spin-1/2 and spin-1 Ising system [34]. It is interesting that the T_c of the $Cu_{0.43}Ni_{0.57}$ ferrimagnetic bilayers increases with the layer thickness increasing [35]. All these results have illustrated that the layer thickness has played an important role in the magnetic properties of the multilayers.

Although previous valuable theoretical and experimental studies have been obtained, more research is still needed to further understand the magnetic and thermodynamic properties of the ferrimagnetic bilayer superlattice by using MC method. Therefore, in this paper , we will study the effects of the exchange couplings and the layer thickness on the compensation behavior and magnetic properties of the ferrimagnetic double layer superlattice. Moreover, it is significant to compare our results with those of the theoretical results by EFT and experimental work. The outline of the paper is composed as follows. In Section 2, we briefly describe our model and the method used. In Section 3, typical numerical results are presented and discussed. Section 4, some conclusions are drawn.

2. Model and Monte Carlo simulation

We consider a mixed layered ferrimagnetic spin-1/2 and spin-1 Ising double layer superlattice system consisting of two magnetic monolayers (A and B) on a cubic lattice. The system is shown in Fig. 1a and b. We define L_a and L_b denote the numbers of the atom layers for the upper layer (sublattice A) and the low layer (sublattice B), and L are the total layer thickness of a unit cell for the double layer superlattice, namely $L=L_a+L_b$. The red and blue balls represent the sublattices A and B, respectively. The Hamiltonian of the system is expressed as:

$$H = -J_{ab}\sum_{i,j}\sigma_{ia}^{z}S_{jb}^{z} - J_{aa}\sum_{i,i'}\sigma_{ia}^{z}\sigma_{i'a}^{z} - J_{bb}\sum_{j,j'}S_{jb}^{z}S_{j'b}^{z} \tag{1}$$

Among them, the J_{bb} (> 0) is the ferromagnetic exchange coupling between nearest neighbors between sublattices A (B) and A (B). J_{ab} represents ferrimagnetic exchange coupling between the nearest neighbors across the interface between sublattices A and B. σ_{ia}^{z} and S_{jb}^{z} denote the spin of magnetic atoms for sublattice A and B, respectively, where $\sigma_{ia}^{z} = \pm 1/2$ and $S_{jb}^{z} = 0, \pm 1$.

For simulation, we have adopted the standard importance sampling Monte Carlo method on the basis of the Metropolis algorithm [36] on an $N\times N\times L$ three-dimensional cubic lattice. $N\times N$ denote the number of the spins in each layer of the double layer superlattice cell. The periodic boundary conditions are used in three three-dimensional x, y, z-directions. It should be mentioned that additional simulations have been enforced to confirm the effect of the number of N on the results, but no significant difference has not been found from increasing N=20–100. Therefore, we select N=20 for simulation. In the single spin flip process, a possible new spin state was selected randomly before each spin flip trial. The flips can be accepted or rejected according to the Metropolis algorithm with the Eq. (2). The flow chart of Monte Carlo simulations is plotted in Diagram 1.

$$p = \exp(-\Delta H/k_B T) \tag{2}$$

where p denotes the probability of a successful spin flip, ΔH is the energy change involved in the variation of the spin states. k_B is the Boltzmann constant and T is the absolute temperature. For simplicity, we set k_B =1 in the simulation. Our results were achieved with the rest 15,000 Monte Carlo steps (MCS) per site after discarding the first 5000 MCS. The magnetization, susceptibility, internal energy and specific heat of the system are given as follows:

The sublattice magnetizations M_a and M_b for the sublattice A and B are

$$M_A = \frac{1}{N^2 L_a}\left\langle \sum_i S_{ia}^{z} \right\rangle$$
$$M_B = \frac{1}{N^2 L_b}\left\langle \sum_j S_{jb}^{z} \right\rangle \tag{3}$$

And the total magnetization M per site is

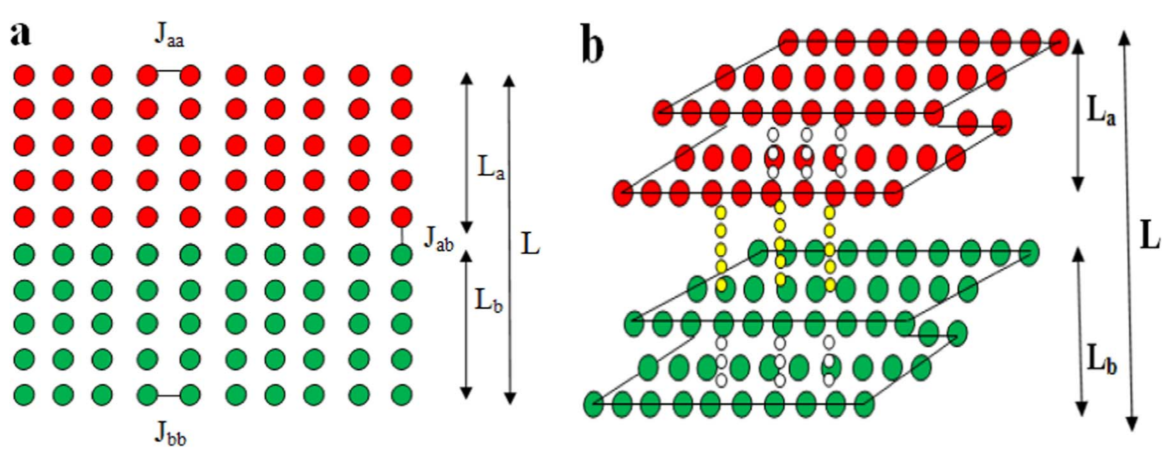

Fig. 1. Sketch of a unit cell of the ferrimagnetic double layer superlattice which is composed of two magnetic monolayers (A and B) on a cubic lattice: (a) cross-section and (b) three-dimensional. The red solid circles represent magnetic atoms for sublattice A (spin $\sigma = 1/2$) in the upper layer, and the green solid circles delegate magnetic atoms for sublattice B (spin $S = 1$) in the low layer. The dash lines connecting the red and green circles denote the nearest-neighbor exchange couplings (J_{aa}, J_{ab} and J_{bb}). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)