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Phase diagrams of a finite superlattice with two disordered interfaces: Monte Carlo simulation

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ABSTRACT

The phase diagrams and the magnetic properties of an Ising finite superlattice with two disordered interfaces are investigated using Monte Carlo simulations based on Metropolis algorithm. The superlattice consists of k unit cells, where the unit cell contains L layers of spin-1/2 (A atoms), L layers of spin-1 (B atoms), and a disordered interface, with two layers in between, which is characterized by a random arrangement of A and B atoms $A_pB_{1-p}A_{1-p}B_p$ with a negative A–B coupling. The A–A and B–B exchange coupling are considered ferromagnetic. We have investigated the effects of the thickness of the film, the crystal field interactions and the surface exchanges coupling on the magnetic properties. The obtained results show that the number of compensation points and the number of first-order phase transition lines depend strongly on the thickness, the probability p and the exchange interactions in the surfaces.

1. Introduction

The investigation of magnetic superlattices has attracted more attention because of their important applications in various fields [1]. Consequently, considerable effort has been devoted on the understanding of layered structures and superlattices [2–6]. The study of the relation between the composition and the structure of these systems on the one hand, and their magnetic properties on the other hand, has become an active field of research [7,8].

The majority of works have been devoted to the multilayers with disordered interface of the type A_pB_{1-p} [9–14]. Jascur et al. [15] have examined a multilayer system with disordered interface and they have found many characteristic behaviors, especially the dependence of the compensation behavior on the thickness of the bulk layers. Veiller et al. [16] have studied the phase diagrams of a multilayer system with disordered interface by the use of Monte Carlo simulations. The results indicate that the magnetic ordering is driven by the disordered interfaces. Therefore, it is reasonable to assume that the existence of a disordered interface and different anisotropies can modify the magnetic properties of multilayer systems. In Ref. [17], Moutie et al. have also studied the same system by using the effective field theory, and have shown that the system exhibits one or two compensation points. In an other paper [18], Belmamoun et al. have investigated the critical and compensation behaviors of a finite superlattice with two disordered interfaces using effective field theory. They have found that the critical temperature is not influenced by the change of the thickness of the superlattice (number of unit cell). In contrast, the existence and the number of compensation points depend strongly on the number of unit cells in the superlattice. In Ref. [19], the disorder and layer transitions in the interface between an Ising spin-1/2 film denoted (n), and an Ising spin-1 film denoted (m), have been studied using Monte Carlo simulations. It has been found that, for low values of the coupling J_p between the two films, the layers of the film (n) undergo a first order layering transition. These transitions have also been found in the film (m) for higher values of the coupling J_p. Boughrara et al. have applied Monte Carlo Simulations to study a ferrimagnetic superlattice with a disordered interface on a simple cubic lattice [20]. They have examined the effect of the thickness of the superlattice on its critical behavior. They have found that the existence and the number of compensation points depend strongly on the thickness of the film.

In this work, we are going to study the magnetic properties of a superlattice with two disordered interfaces. In particular, we investigate the effects of the thickness of the film and the crystal field interactions on the critical and compensation behaviors.

The outline of this paper is as follows: in Section 2, we describe our model and review the basic of Monte Carlo simulations. The results and discussions are presented in Section 3, and finally Section 4 is devoted to our conclusions.

2. Model and formalism

We consider an Ising superlattice consisting of k unit cells, each of which consists of L layers of spin-1/2 A atoms, L layers of spin-1

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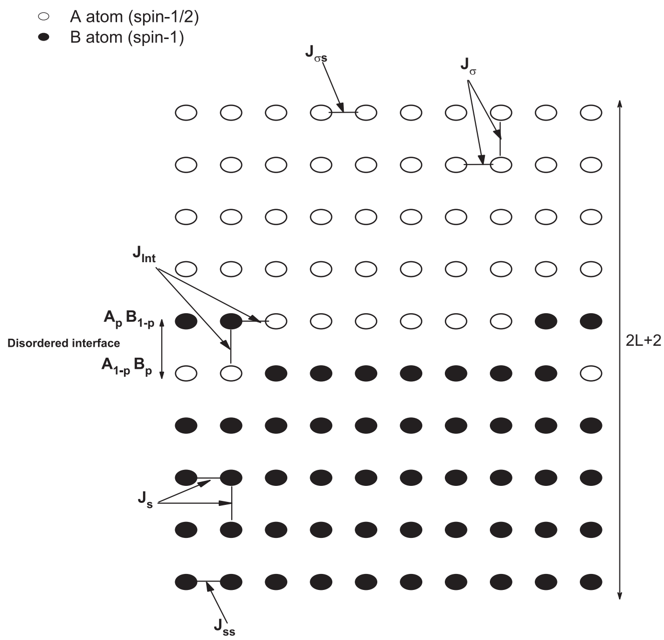

Fig. 1. A schematic cross-section of the $(A)_L(A_pB_{1-p})(A_{1-p}B_p)(B)_L$ unit cell of the magnetic superlattice.

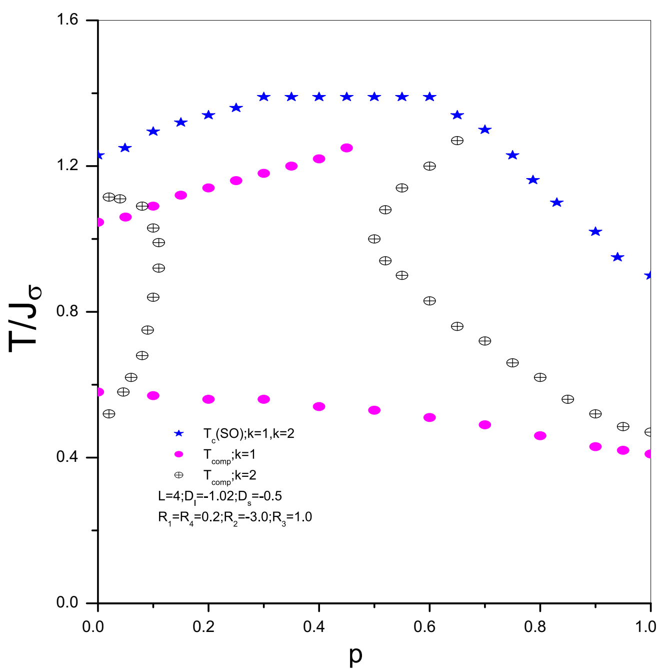

Fig. 2. The phase diagram in $(T/J_\sigma, p)$ plane for $L = 4$, $D_I = -1.02$, $D_s = -0.5$, $R_1 = 0.2$, $R_2 = -3.0$, $R_3 = 1.0$ and $R_4 = 0.2$.

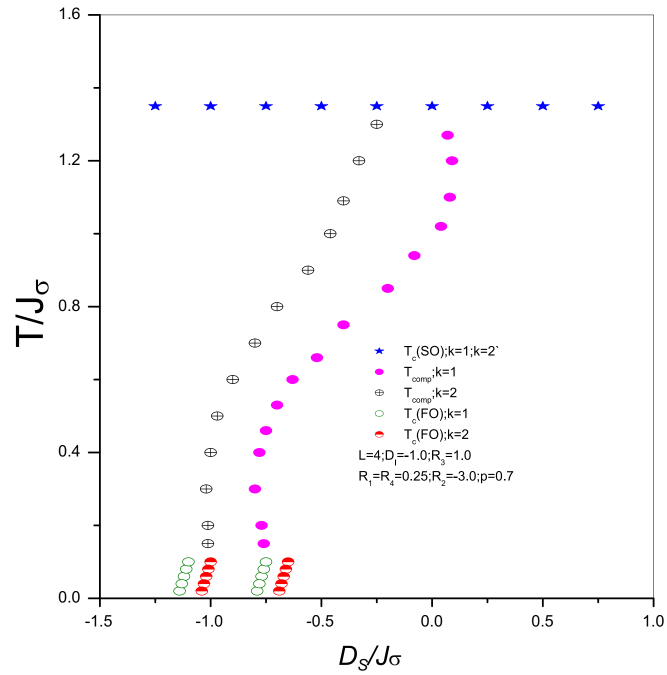

Fig. 3. The phase diagram in $(T/J_\sigma, D_S/J_\sigma)$ plane for $L = 4$, $D_I = -1.0$, $R_4 = 0.25$, $R_1 = 0.25$, $R_2 = -3.0$, $R_3 = 1.0$ and $p = 0.7$.

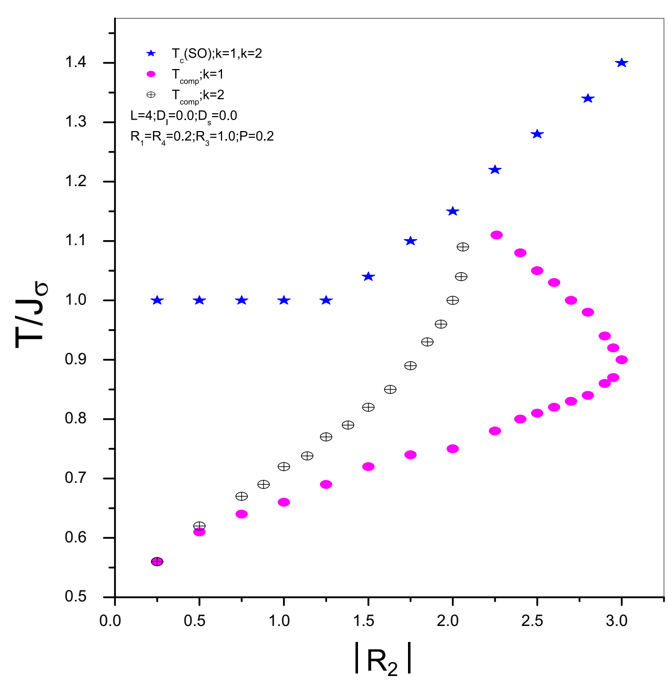

Fig. 4. The phase diagram in $(T/J_\sigma, |R_2|/J_\sigma)$ plane for $L = 4$, $D_I = D_s = 0.0$, $R_1 = 0.2$, $R_3 = 1.0$, $R_4 = 0.2$ and $p = 0.5$.

B atoms and a disordered interface layer $(A_pB_{1-p})(A_{1-p}B_p)$ of A and B atoms randomly mixed. A cross section of the unit cell of the superlattice is depicted in Fig. 1.

The Hamiltonian of the system is expressed as follows:

$$\mathcal{H} = -\sum_{\langle ij\rangle}\left\{J_{ij}\sigma_i\sigma_j\xi_i\xi_j + J'_{ij}S_iS_j(1-\xi_i)(1-\xi_j) + J_{Int}(\sigma_iS_j\xi_i(1-\xi_j))\right\} - D_s\sum_i S_i^2 - D_I\sum_i S_i^2\delta_{ib}(1-\xi_i) \tag{1}$$

where the first sum runs over all pairs of nearest neighbors. $J_{ij} = J_\sigma$, $J'_{ij} = J_s$, and J_{Int}, are the exchange interactions between $A-A$, $B-B$, and $A-B$ pairs of atoms in the bulk. $J_{ij} = J_{\sigma s}$ and $J'_{ij} = J_{ss}$ are the exchange interactions if both spins σ_i and S_i are in the surface of A and B layers, respectively. D_s and D_I are the crystal fields acting on the B layers and on the disordered interfaces, respectively. σ_i is the spin-1/2 operator on the A atoms, S_i is the spin-1 operator on the B atoms and the random variable ξ_i takes the average $\langle\xi_i\rangle_A = 1$ in the A-layers, $\langle\xi_i\rangle_B = 0$ in the B layers, and $\langle\xi_i\rangle_{Int} = p$ in the first interface layer and $\langle\xi_i\rangle_{Int} = 1-p$ in the second one.

We take an initial configuration with the spins σ in the $-1/2$ state, and the spins S in the 1 state. Our system consists of k unit