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Phase diagrams and magnetic properties of a superlattice with alternate layers

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ABSTRACT

The phase diagrams and magnetic properties of an Ising superlattice are investigated by means of Monte Carlo simulation based on Metropolis algorithm. The system is formed by alternate layers of spins $S = 1$ and $\sigma = 3/2$. The effects of the exchange coupling interactions and the crystal field on the phase diagrams and magnetic properties of the system are examined. A number of characteristic behaviors have been found. In particular, tricritical point, critical end point, and isolated critical point may occur in the present system.

1. Introduction

Since the discovery of the magnetic interlayer coupling and the giant magnetoresistance, much effort has been directed towards the study of the critical phenomena in various magnetic layered structures, super-lattices, bilayer and ultrathin-films [1–4]. This is because of the easiness of their preparation made possible by the recent advances of modern vacuum science and this is because of their potential technological importance in various fields [5]. Consequently, considerable effort has been focused on the understanding of layered structures and superlattices [6–10]. Wang et al. [11] have used the Ising model in a transverse field (IMTF) to describe the properties of ferroelectric–antiferroelectric superlattices that might be fabricated from order–disorder materials. They have found that the number of antiferroelectric layers plays a crucial role in the phase transition properties of the superlattices . The phase diagrams of a spin-1 Ising superlattice with alternating transverse field were studied by Saber et al. in Ref. [12]. The critical temperature can increase or decrease with the increasing thickness of the superlattice. In Refs. [13,14], Belmamoun et al. have investigated the magnetic properties of a finite superlattice with disordered interfaces. They have found that the existence and the number of compensation points depend strongly on the thickness of the film. The same results are found in Ref. [15] where Monte Carlo Simulation (MCS) has been used to study critical and compensation behaviors of a ferrimagnetic superlattice on a simple cubic lattice. In some recent work [16], the effect of the transverse crystal field on the magnetic properties of a superlattice with disordered interface has been investigated. A number of characteristic phenomena are found, such as the possibility of two compensation points. Experimentally, Ahlberg et al. [17] have explored the effect of the interlayer exchange coupling in Fe/V (001) superlattices on the temperature dependence of the magnetic properties. The temperature dependence of the remanent magnetization was proven to be significantly affected by the strength of the ferromagnetic coupling.

On the other hand, ferrimagnetic mixed spin system has attracted a lot of interest. In these systems, two different nearest-neighbor spins are coupled by anti-ferromagnetic exchange interaction. In Ref. [18], Monte Carlo simulation has been used to study the magnetic properties and the critical behaviors of a ferrimagnetic mixed spin (1/2, 1) Blume–Capel model with a four-spin plaquette interaction on two-dimensional square lattice. The critical behavior of the system shows the presence of reentrant and even double reentrant phenomenon for some value of the system parameters. In Ref. [19], the authors studied, within a mean-field approach, the stationary states of the kinetic mixed spin (3/2, 2) Ising systems. Interesting phenomena are found such as dynamic tricritical and dynamic critical end point. Recently, Feraoun et al. [20] have employed Monte Carlo simulation to investigate the magnetic behavior of a ferrimagnetic nanowire on a hexagonal lattice with a spin-3/2 core surrounded by a spin-1 shell. The results present rich critical behavior, which includes the

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first- and second-order phase transitions, the tricritical and critical end points. In Ref. [21], critical and compensation properties of a ferrimagnetic mixed spin (1, 3/2) Ising on a square lattice are investigated by standard and histogram Monte Carlo simulations. Some rich phenomena are found, such as the existence of a tricritical point and a re-entrant behavior. In Ref. [22], the effects of a bimodal random crystal field on the phase diagrams and magnetization curves of the ferrimagnetic mixed spin (1/2, 3/2) Blume–Capel model are examined by using the effective field theory with correlations on a honeycomb lattice. It was found that the model presents one or two compensation temperatures for appropriate values of the random crystal field.

As far as we know, however, the mixed spin (1, 3/2) Ising superlattice with alternate layers has not been studied. The purpose of the present work is to investigate the effect of the exchange interaction coupling and the crystal field on the phase diagrams and the compensation behavior of a superlattice composed of alternate layers of spins $S=1$ and $\sigma=3/2$ within the framework of Monte Carlo simulations. The outline of the present paper is organized as follows: in Section 2, we briefly present our model and the related formulation, 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 (see Fig. 1) of size $L \times L \times N$, with N being the number of layers in the system or its thickness and $L \times L$ represents the number of sites in each layer. The superlattice is made with alternate layers, σ-type of spin-3/2 and S-type of spin-1.

The Hamiltonian of the system is given by

$$\mathcal{H} = -J_S \sum_{\langle ij \rangle} S_i S_j - J_\sigma \sum_{\langle kl \rangle} \sigma_k \sigma_l - J_{Int} \sum_{\langle ik \rangle} S_i \sigma_k - D \sum_i S_i^2 - D \sum_k \sigma_k^2 \quad (1)$$

where J_S stands for the coupling constant between the spins S, whereas J_σ is the coupling constant between the spins σ. J_{Int} is the coupling constant between the spins S and σ. $S_i = \pm 1, 0$ and $\sigma_k = \pm 3/2, \pm 1/2$ are the usual Ising variables. The summation indices $\langle ij \rangle$, $\langle kl \rangle$ and $\langle ik \rangle$ denote the summations over all pairs of neighboring spins S–S, σ–σ, and S–σ, respectively, and we have fixed the value of J_S throughout the simulation ($J_S = 1$). D is the crystal field interaction acting on the spins S and σ. Using Monte Carlo simulation based on Metropolis algorithm [23], we apply periodic boundary conditions in the x and y directions. Data were generated over 20–40 realizations by using 30 000 Monte Carlo steps per site after discarding the first 15 000 steps. The results are reported for systems size $L=50$ and $N=4$. A number of additional simulations were performed for $L=70$ and $L=100$, but no significant differences were found from the results presented here. Our program calculates the following parameters, namely

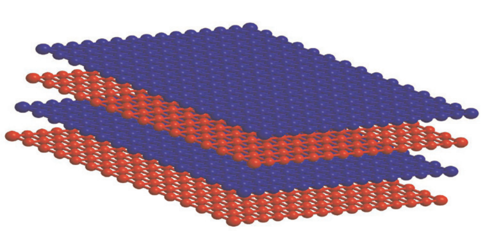

Fig. 1. Schematic representation of the superlattice formed by alternate S-layer type with $S = \pm 1, 0$ and σ-layer type with $\sigma = \pm 3/2, \pm 1/2$.

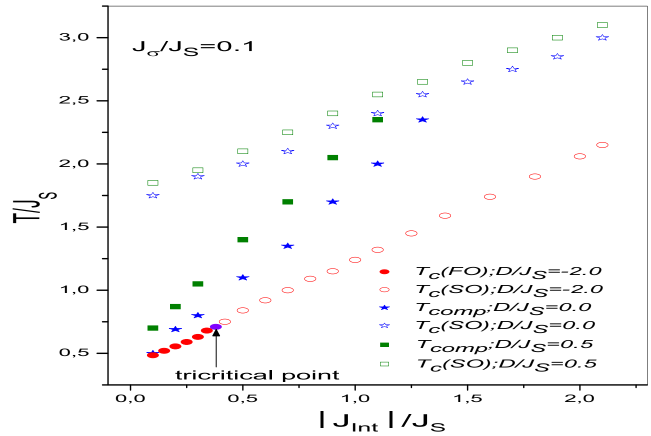

Fig. 2. The phase diagrams of the system in $(T/J_S, |J_{Int}|/J_S)$ plane for $J_\sigma/J_S = 0.1$ and for different values of D/J_S ($D/J_S = -2.0$, 0.0 and 0.5).

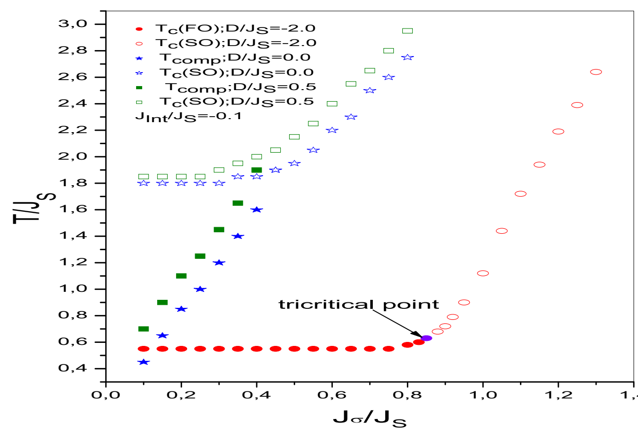

Fig. 3. The phase diagrams of the system in $(T/J_S, J_\sigma/J_S)$ plane for $J_{Int}/J_S = -0.1$ and for different values of D/J_S ($D/J_S = -2.0$, 0.0 and 0.5).

The sublattice magnetizations per site are defined by

$$M_S = \frac{1}{L \times L \times \frac{N}{2}} \left\langle \sum_i \left(S_i \right) \right\rangle \quad (2)$$

$$M_\sigma = \frac{1}{L \times L \times \frac{N}{2}} \left\langle \sum_i \left(\sigma_i \right) \right\rangle \quad (3)$$

The total magnetization per site is given by

$$M_T = \frac{M_S + M_\sigma}{2} \quad (4)$$

The internal energy of the superlattice is defined by

$$E = \frac{1}{L \times L \times N} \langle \mathcal{H} \rangle \quad (5)$$

The sublattice magnetic susceptibilities are given by

$$\chi_S = L \times L \times \frac{N}{2} \beta \left(\left\langle M_S^2 \right\rangle - \langle M_S \rangle^2 \right) \quad (6)$$

$$\chi_\sigma = L \times L \times \frac{N}{2} \beta \left(\left\langle M_\sigma^2 \right\rangle - \langle M_\sigma \rangle^2 \right) \quad (7)$$