



# Magnetic and thermodynamic properties of a ferromagnetic mixed-spin (1/2, 1, 3/2) three-layer film superlattice



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## ARTICLE INFO

### Article history:

Received 11 February 2018

Received in revised form 20 April 2018

Accepted 23 April 2018

Available online 24 April 2018

### Keywords:

Three-layer film superlattice

Transition temperature

Magnetization

Exchange coupling

Layer thickness

Monte Carlo simulation

## ABSTRACT

Using the Monte Carlo simulation, we have studied the magnetic and thermodynamic properties of a ferromagnetic three-layer film mixed-spin (1/2, 1, 3/2) system. We have discussed the influence of intralayer and interfacial exchange couplings, film thickness, magnetic atom concentration and temperature on the magnetization of the superlattice system, magnetic susceptibility, internal energy and specific heat of the system. The phase diagrams in various parameters planes are obtained. Loads of interesting magnetic behaviors have been found, such as double-peak and triple-peak phenomena in the susceptibility and specific heat curves as well as obvious finite size effects for small layer thickness. Through a comparison, there is qualitatively a good agreement between our results and those of other theoretical and experimental studies.

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## 1. Introduction

In recent years, with the rapid development of modern science and technology, the technology and means of synthesizing thin film materials are more diverse, such as pulsed controlelectrodeposition [1], Sol-Gel [2], magnetron sputtering technology [3] and so on made magnetic thin film materials into the mainstream of development. Because of the complexity and diversity of multilayer superlattice structure, they are quite different from bulk material in structure, which can exhibit excellent magnetic and thermodynamic properties and attract a lot of theories and experimental scientists to conduct extensive and in-depth research on various film systems [4–8]. Many High-tech information storage products have emerged, such as the hard disk drive with reading heads made by a giant magnetoresistance film and magnetic memory storage devices with the advantages of low energy consumption, anti-radiation, fast reading and writing [9–13].

As a main content of the research on new composite materials nowadays, the physical properties of the three-layer superlattice structures have been extensively studied both experimentally and theoretically. In experiment, the researchers studied the properties of the magnetic multilayer materials such as interfacial anisotropy by means of the spin-wave resonance [14], light scattering [15] and other methods. On the other hand, the theoretical research of multilayer systems is of great significance for the guidance of experimental exploration. The studies of magnetic superlattice multilayer materials cover two-layer superlattice, three-layer superlattice and even multilayer superlattice materials. Much effort has

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been devoted to the various physical parameters on the magnetic properties of multilayer superlattice systems. Particular interests has directed to the effects of the thickness of magnetic film materials and material types and the magnetic properties. The energy spectra and thermodynamic properties of the magnetic superlattice have also been investigated by different methods such as the Monte Carlo (MC) simulation [16–18], the mean-field theory (MFT) [19], the effective-field theory (EFT) [20], the linear cluster mean-field approximation theory [21], etc. M. Abid et al. have focused on magnetic properties of Ni/V multilayers [22]. The influences of Ni layer thickness on the magnetization and the critical temperature ( $T_c$ ) have been studied. And other different structures of the three layers and multilayer film systems such as Au/FePt/Au [23], FePt/Pt/Cr [24], Fe/Cr/Fe [25], Fe/Si/Fe [26], Ni/Cu/Co [27], NiFe/Ru/NiFe [28], NiFe/NB/NiFe [29], Fe/ZnSe/Fe [30], GaGdN/GaN [31], Co/Nb/Co [32], Co/Ge/Co [33], CoFe/IrMn/NiFe [34], Co<sub>2</sub>MnSi/Al/Co<sub>2</sub>MnSi [35], Co/Pt multilayers [36] and Ni/Pd multilayers [37] have been studied experimentally. The booming of these experimental researches also inspires people to further understand the magnetic mechanism of magnetism in superlattices and multilayers. W. Jiang et al. used the EFT theory and Green's function method to study the energy spectrum, quantum fluctuations, specific heat and other physical quantities of the double layer magnetic multilayer films and find the changes of these physical quantities under different parameters [38,39]. R. K. Qiu et al. studied the double and triple layers of ferromagnetic resonance frequency of the superlattice materials as well as the influence of the interlayer exchange coupling and temperature on it, and developed the use of the method in improving the ferromagnetic resonance frequency [40]. J. Hu et al. focused on the exchange coupling effect on magnetic three-layer systems which contains a perpendicular anisotropic interlayer [41]. Using the MC method, E. Birsan et al. studied the triple-layer as well as the multilayer Heisenberg thin film with long range dipolar interactions [42,43]. A magnetization relaxation phenomenon and a spin-glass-like behavior were found by C. S. Xiong et al. in Ref. [44]. A. Moschel et al. used the Green function method to calculate the spin wave excitation spectrum and the sub-lattice magnetization of the system with ferromagnetic and anti-ferromagnetic layers [45]. A. Feraoun et al. studied the phase diagrams and magnetic properties of the mixed spin (1, 3/2) superlattice in MC simulation [46]. M. Ertas et al. used the EFT to study the related magnetic properties including the critical and compensation temperatures of the mixed spin (2, 5/2) bilayer simple cubic superlattice [47,48]. R. E. Camley et al. studied the spin spectrum of the double-layer ferromagnetic system with the MFT [49]. H. Puzkarski studied the interlayer exchange coupling and spin wave of double layer ferromagnetic films [50].

It should be mentioned that the Monte Carlo simulation is relatively rare for the study of three-layer and multilayer superlattice system. M. Žukovič et al. investigated the critical and compensation behaviors of a ferri-ferromagnet ternary mixed spin alloy by means of MC simulations. They confirmed and calculated the critical superexchange interaction ratio  $R_c$  and figured out the importance of  $R_c$  as well as atomic concentration in dominating the temperature dependence of magnetic and thermodynamic properties [51]. F. El. Hallani, using both MC simulation and MFT, studied the magnetic properties of spins-3/2 and 1/2 Blume–Capel model in the bilayer separated by a non-magnetic spacer of thickness [52]. The results show that the multilayer transition temperature strongly depends on the thickness and the crystal-field of the non-magnetic layer. W. Liu et al. used the EFT to examine the influences of the layer thickness, the diluted magnetic atom concentration and the exchange interaction on the magnetic properties of the Ising three-layer superlattice system [53]. In our previous studies, we have successfully applied the MC simulations to work out the magnetic and thermodynamic behaviors of the double-layer [54] and multilayer systems [55,56]. In this article, we established the three-layer superlattice ferromagnetic mixed-spin (1/2, 1, 3/2) Ising model. Using the MC simulation, we studied the influence of the temperature, film thickness, the exchange coupling and magnetic atomic concentration on the magnetization, magnetic susceptibility, internal energy, specific heat and the phase transition temperature. In addition, we believe that it is meaningful to make a comparison between our results with those with EFT, which can prove the study reliable. This article is organized as follows: in Section 2, we introduce the Ising model and the numerical method. The detailed results and discussion are presented in Section 3. Finally, a brief summary is given in Section 4 as a conclusion.

## 2. The model and method

We consider a three-layer film superlattice on a simple cubic lattice with the periodic boundary condition in all directions. Fig. 1 depicts the atomic distribution of a unit cell of the three-layer film superlattice. Different shapes and colors of the lattices represent different types of sublattices. We here adopt the classical Ising model to describe the present system.  $S_{ia}^z$ ,  $S_{jb}^z$ ,  $S_{kc}^z$  signify the spins of sublattices A, B, C.  $L_a$ ,  $L_b$ ,  $L_c$  are the thicknesses of A, B, C three layers, respectively. Thus, the total layer thickness of the cell in superlattice is  $L = L_a + L_b + L_c$ . The Hamiltonian of the system can be given by

$$H = -J_{aa} \sum_{\langle i,i' \rangle} \xi_i S_{ia}^z \xi_{i'} S_{i'a}^z - J_{bb} \sum_{\langle j,j' \rangle} \xi_j S_{jb}^z \xi_{j'} S_{j'b}^z - J_{cc} \sum_{\langle k,k' \rangle} \xi_k S_{kc}^z \xi_{k'} S_{k'c}^z - J_{ab} \sum_{\langle i,j \rangle} \xi_i S_{ia}^z \xi_j S_{jb}^z - J_{bc} \sum_{\langle j,k \rangle} \xi_j S_{jb}^z \xi_k S_{kc}^z - J_{ca} \sum_{\langle i,k \rangle} \xi_i S_{ic}^z \xi_k S_{ka}^z \quad (1)$$

where  $S_{ia}^z = \pm 1/2$ ,  $S_{jb}^z = \pm 1$ , 0 and  $S_{kc}^z = \pm 3/2$ ,  $\pm 1/2$ .  $J_{aa}$ ,  $J_{bb}$ ,  $J_{cc}$ , respectively represent the intralayer exchange couplings in sublattices A, B, C, and  $J_{aa} > 0$ ,  $J_{bb} > 0$ ,  $J_{cc} > 0$ . Meanwhile, the interfacial exchange couplings between two adjacent layers of different types atoms are denoted by  $J_{ab}$ ,  $J_{bc}$ ,  $J_{ca}$ , and  $J_{ab} > 0$ ,  $J_{bc} > 0$ ,  $J_{ca} > 0$ . In the simulation, we select  $J_{aa}$  as the reduced unit of energy and temperature and take  $J_{aa} = 1.0$ .

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