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Unique phase diagrams in ultra-thin Ising films with dilutions

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ABSTRACT

The phase diagrams of two nanoscaled thin films with site (or bond) dilution, described by the spin-1 (or spin-1/2) Ising model, are investigated by the use of the effective field theory with correlations. They are consisted of two layers. Some unique features have been found in the phase diagrams, while they show many similar behaviors for both the spin-1/2 films and the spin-1 films with a positive single-ion anisotropy. It is clarified that the unique behavior of critical concentration in the spin-1 system with site dilution and a positive single-ion anisotropy at which the transition temperature reduces to zero is completely equivalent to that in the spin-1/2 system with site dilution.

1. Introduction

Nowadays, a lot of quasi-2D magnetic systems have been realized experimentally by growing a few atomic layers of a ferromagnet on the top of a nonmagnetic substrate, such perpendicularly magnetized (Co/Pt) systems [1–3]. The hysteresis is normally examined in a variety of nanoscaled magnetic thin films, since the shape of hysteresis loop is very important for the manufacture of magnetic recording media. In [3], on the other hand, the anomalous Hall effect, where the Hall resistance (R_{Hall}) is proportional to the perpendicular component of magnetizations, has been used to obtain the T_C, the temperature dependence of magnetization M and the critical exponent β in ultra-thin Co films. The systems seem to be a kind of ultra-thin spin-one Ising films with a positive single-ion anisotropy. From this point of view, it may be interesting theoretically to examine the phase diagram of an ultra-thin spin-one Ising film with a positive single-ion anisotropy, especially when the surfaces are disordered by site (or bond) dilution. In the previous work [4], the phase diagrams of an ultra-thin spin-1 Ising film with a negative single-ion anisotropy have been investigated, in order to clarify how the tricitical behavior can be obtained in such an ultra-thin film with dilutions. In fact, it is not so easy to fabricate pure ultra-thin films experimentally. The existence of disorder, such as site- (or bond-) dilution at the surfaces, may affect seriously to their magnetic properties.

In a series of recent works [5–11], we have examined the phase diagrams and the magnetizations of nanoscaled spin-1/2 and spin-1 Ising (or transverse Ising) thin films consisting of a few magnetic layers by the use of the effective-field theory with correlations (EFT) [12,13]. The EFT corresponds to the Zernike approximation [14] and it is believed to give more exact results than those of the mean field approximation. For a variety of nanoscaled magnetic systems, furthermore, the Monte Carlo simulations [15–17] also show the same topologies for the magnetic properties as those obtained from the EFT. In the previous works [5–11], many unexpected phenomena have been found, such as the appearance of a broad maximum in the variation of transition temperature (T_C) for the site dilution at the surfaces, while such a phenomenon has not been obtained for the bond dilution at the surfaces, while the T_C is plotted as a function of interlayer coupling J_1 between the surface and the next inner layer. The different results between the site and bond dilution problems in ultra-thin films come from the differences of theoretical formulations between the two nanoscaled systems, as discussed in [5,6], while such differences could not be found in the bulk dilution problems. The unexpected phenomena have also been obtained, even when the thickness L of a film has been increased from $L=3$ to $L=10$ [9]. In [11], the phase diagrams and the magnetizations of ultra-thin spin-1/2 Ising (or transverse Ising) thin film with $L=2$ and dilutions have been discussed. The unexpected phenomena found in these films are just dependent on the sizes of the systems and the strength of coupling J_1. In other words, these phenomena come from the competion between the size of the system and the strength of coupling J_1, namely a kind of novel type of frustration. In fact, as has been discussed in the work [9], such phenomena become rapidly small with the increase of L. From these results, one may think that the phenomena come from the finite size effects peculiar to nanosystems. As is obtained in [10], however, the reentrant phenomena can be found only for the thin film with $L=4$, when a finite transverse field is applied to the system. Furthermore, these types

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of similar behaviors have been obtained in a lot of magnetic nanosystems described by the transverse Ising models, such as nanowire, nanotube and nanoislands [21–25]. From these facts, the phenomena come from a kind of novel type of frustration.

The aim of this work is, within the theoretical framework of the EFT, to investigate the effects of J_1 on the phase diagram in an ultra-thin spin-1 (or spin-1/2) Ising film with the site- (or bond-) dilution, when the single-ion anisotropy is taken as a positive value and the value of L is fixed at $L=2$. The main physical reasons to select the value of L as $L=2$ and the single-ion anisotropy as a positive value are based on the results of [9] and the experimental works [1–3]. As far as we know, however, such a problem has not been discussed. Theoretically, when a value of single-ion anisotropy is taken as a positive value, it is expected in the bulk dilution problems that the results of the spin-1 dilution problems are essentially similar to those of the spin-1/2 dilution problems. It is also interesting to investigate theoretically whether such a phenomenon can be obtained in a diluted ultra-thin film, although, as far as we know, such a problem has not been discussed. In Section 2, the models and the formulation are given and the two formulations for obtaining the phase diagrams in the two systems with site- and bond-dilutions are given. In Section 3, the effects of interlayer exchange interaction J_1 on the T_C are studied, like the previous works [5–11]. A broad maximum in the T_C curve and the unique features of critical concentration at which the T_C curve reduces to zero are found for the spin-1 and spin-1/2 Ising systems with site- and bond-dilutions.

2. Models and formulation

In this work, we consider the two spin-1 Ising films with bond and site dilutions, as depicted in Fig. 1, in which they are consisted of the two disordered layers. The each site (black circles) on the figure is occupied by a Ising spin. In Fig. 1(A), the layers are diluted by non-magnetic atoms (white circles). In Fig. 1(B), the bond dilution is presented. Each layer is coupled to the next layer with an exchange interaction J_1. These models have been discussed in [10] for the spin-1/2 thin film with same disordered layers. The aim of this work is, accordingly, to compare the characteristic results of phase diagrams obtained from the theoretical formulations in [10] with the present ones obtained for the spin-1 Ising film, while the present formulations are essentially equivalent to those in [4].

The Hamiltonian of the spin-1 system with site dilution like Fig. 1(A) is given by

$$H = -J_S\sum_{(ij)} S_i^Z S_j^Z \xi_i \xi_j - J_1 \sum_{(im)} S_i^Z S_m^Z \xi_i \xi_m - J\sum_{(mn)} S_m^Z S_n^Z \xi_m \xi_n - D\sum_i (S_i^Z)^2 \xi_i - D\sum_m (S_m^Z)^2 \xi_m, \quad (1,a)$$

where the spin-1 operator S_i^Z takes the values ±1 and 0. J_S is the exchange interaction between two nearest-neighbor magnetic atoms at the layer. D represents the single-ion anisotropy at the layer. The first (ij) and the third (mn) terms in the Hamiltonian (1,a) represent the contributions from the two layers. Since each layer is diluted in the system with the Hamiltonian (1,a), ξ_i takes unity with a probability p when the site i is occupied by a magnetic atom and takes 0 with a probability $(1-p)$ when the site i is occupied by a non-magnetic atom.

On the other hand, the Hamiltonian of the spin-1 system in Fig. 1(B) is given by

$$H = -\sum_{(ij)} J_{ij} S_i^Z S_j^Z - J_1 \sum_{(im)} S_i^Z S_m^Z - \sum_{(mn)} J_{mn} S_m^Z S_n^Z, \qquad - D\sum_i (S_i^Z)^2 - D\sum_m (S_m^Z)^2 \quad (1,b)$$

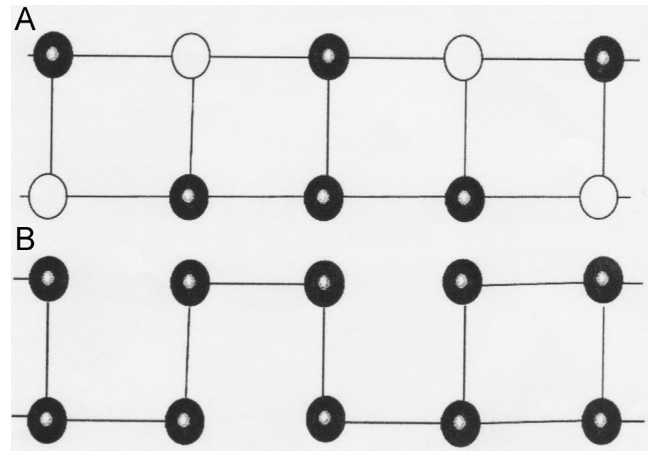

Fig. 1. Schematic representations of two nanoscaled thin films with two layer thickness. The above (A) represents the thin film with site dilution and the down (B) is the thin film with bond dilution. The black circles are magnetic atoms. In (A), the white circles at each layer represent nonmagnetic atoms. The lines connecting the black circles represent the nearest-neighbor exchange interactions (J_S and J_1).

where the exchange interaction J_{ij} (or J_{mn}) at each layer is randomly distributed according to the probability distribution function

$$P(J_{ij}) = p\delta(J_{ij} - J_S) + (1-p)\delta(J_{ij}), \quad (2)$$

The J_S is defined as

$$J_S = J(1 + \Delta_S), \quad (3)$$

in order to compare with the previous results in [5–11], where J is the exchange interaction in the bulk.

Within the framework of the EFT, the magnetization m (or $m=\langle S_i^Z\rangle_R$, where $\langle A\rangle_R$ expresses the random average of (A) of the two layers depicted in Fig. 1(A), namely for the site dilution, is given by

$$m = [pq\cos h(A) + (1-pq) + pm\sin h(A)]^4 \, [pq\cos h(B) + (1-pq) + pm\sin h(B)]F(x)|_{x=0} \quad (4)$$

where $A = J_S\nabla$, $B = J_1\nabla$ and $\nabla = \partial/\partial x$ expresses the differential operator. The function $F(x)$ is given by

$$F(x) = \frac{2\sin h(\beta x)}{2\cos h(\beta x) + \exp(-\beta D)}, \quad (5)$$

where $\beta = 1/k_B T$ and T is a temperature. Furthermore, the second moment q ($q=\langle (S_i^Z)^2\rangle_R$) in (4) is also given by the same equation as that of (4) only by replacing the function $F(x)$ with the new function $G(x)$. They are given by

$$q = [pq\cos h(A) + (1-pq) + pm\sin h(A)]^4 \, [pq\cos h(B) + (1-pq) + pm\sin h(B)]G(x)|_{x=0} \quad (6)$$

with

$$G(x) = \frac{2\cos h(\beta x)}{2\cos h(\beta x) + \exp(-\beta D)} \quad (7)$$

For the bond dilution in Fig. 1(B), the magnetization m and the second moment q are given by

$$m = [q\{\langle\cos h(J_{ij}\nabla)\rangle_R - 1\} + 1 + m\langle\sin h(J_{ij}\nabla)\rangle_R]^4 \, [q\{\cos h(B) - 1\} + 1 + m\sin h(B)]F(x)|_{x=0} \quad (8)$$