Physica B 454 (2014) 204–209

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Unconventional phase diagrams in an ultra-thin spin-1 Ising film with site (or bond) dilution at the surfaces

T. Kaneyoshi

Nagoya University, 1-510, Kurosawadai, Midoriku, Nagoya 458-0003, Japan

ARTICLE INFO

Article history:
Received 16 May 2014
Received in revised form
10 July 2014
Accepted 24 July 2014
Available online 6 August 2014

Keywords:
Nanoscaled thin film
Phase diagrams
Tricritical point
Effective field theory

ABSTRACT

The phase diagrams of two nanoscaled thin films with bond and site dilutions at the surfaces, described by the spin-1 Ising model with single-ion anisotropy (D), are investigated by the use of the effective field theory with correlations. They are consisted of two layers. A number of characteristic phenomena have been found in the behaviors of transition temperature and tricritical point, which are heavily dependent on the ratios ($r=J_1/J$ and $d=D/J$) and a concentration (p) of bond or site dilution at the surfaces, where J is the exchange interaction in inner layer and J_1 is the exchange interaction between the surface.

1. Introduction

Over several years, the bulk spin-1 Ising model with single-ion anisotropy (or Blume-Capel model) has been investigated in some detail using a number of methods, such as mean-field theory, effective-field theory, the high-temperature series expansion method and Monte-Carlo simulation. All of these methods indicate the existence of a tricritical point at which the system changes from the second-order phase transition to the first-order ones. They have also been applied to the various theoretical examinations of spin-1 Ising films. On the other hand, a lot of quasi-2D magnetic systems have been realized experimentally in recent years by growing a few atomic layers of a ferromagnetic material on the top of a nonmagnetic substrate, such perpendicularly magnetized (Co/Pt) systems [1–3]. The systems may be modeled by a kind of ultra-thin spin-1 Ising films with a positive single-ion anisotropy. Theoretically, the effective-field theory with correlations (EFT) [4–6] has been applied very recently to the examinations of various magnetic properties of ultra-thin spin-1 Ising (or spin-1 transverse Ising) films (for the references, see the works [7–10]). The EFT corresponds to the Zernike approximation [11] and it is believed to give more exact results than those of the mean-field theory. In these works [7–9] of ultra-thin films, nevertheless, the problems on the dilution have not been studied theoretically. Furthermore, most of theoretical works on these thin films, except [10], have been discussed for the case in which the interlayer coupling J_1 between the surface and the next inner layer is fixed at the value of the inner layer coupling J.

In a series works on ultra-thin spin-1/2 Ising (or transverse Ising) films with bond and site dilutions at the surfaces [12–16], we have examined the magnetic properties (phase diagram and magnetizations) by the use of the EFT. Some unconventional phenomena have been found in the magnetic properties of these systems, such as the appearance of a broad maximum in the variation of transition temperature (T_C) as a function of r ($r=J_1/J$) for the site dilution, while such a phenomenon has not been obtained for the bond dilution. Experimentally, 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 ultrathin Co films. From this point of view, it may be interesting theoretically to examine the phase diagram of an ultra-thin spin-1 Ising film with site (or bond) dilution at the surfaces, especially paying attention to the changes of r- and p-values, where p is a concentration of site (or bond) dilution. 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 affects seriously to their magnetic properties.

The aim of this work is, within the theoretical framework of the EFT, to investigate the effects on the phase diagram (T_C and tricritical point T_t) in an ultra-thin spin-1 Ising film with the site- or bond-dilution at the surfaces, especially paying attention to the

E-mail address: kaneyosi@is.nagoya-u.ac.jp

http://dx.doi.org/10.1016/j.physb.2014.07.065
0921-4526/

influences of r and p. In fact, such an examination has not been reported before. In Section 2, the models and formulation are given. In Section 3, the two formulations for obtaining the phase diagrams are given in the two parts A and B, since the calculations for site-dilution in the part A must be treated by the ways different from those for the bond-dilution in the part B. In the part C, the standard phase diagrams are obtained and they are compared between the two systems with site- and bond-dilutions. In Section 4, the effects of interlayer exchange interaction r on the T_C and T_t are studied, like the previous works [12–16,10]. A broad maximum in the T_C curve characteristic to the case of site dilution, the existence of T_t in the curve and some unconventional behaviors of a critical concentration at which the T_C curve reduces to zero are obtained in the phase diagram.

2. Models and formulation

In this work, we consider the two spin-1 Ising films with bond and site dilutions at the surfaces, as depicted in Fig. 1, in which they are consisted of the two disordered surfaces. The each site (black circles) on the figure is occupied by a Ising spin. In Fig. 1(A), the surfaces are diluted by non-magnetic atoms (white circles). In Fig. 1(B), the bond dilution is performed. The surface layer is coupled to the next center layer with an exchange interaction J_1. These models have been discussed in [16] for the spin-1/2 thin film with same disordered surfaces.

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

$$H=-J_S\sum_{(ij)}S_i^Z S_j^Z\xi_i\xi_j-J_1\sum_{(im)}S_i^Z\xi_i S_m^Z\xi_m-Js\sum_{(mn)}S_m^Z S_n^Z\xi_m\xi_n -D\sum_{(i)}\left(S_i^Z\right)^2\xi_i-D\sum_{(m)}\left(S_m^Z\right)^2\xi_m \quad (1,\mathrm{a})$$

where the spin-1 operators S_i^Z takes the values ±1, 0. J_S is the exchange interaction between two nearest-neighbor magnetic atoms at the surface layer. D represents the single-ion anisotropy at the surfaces. The first (ij) and third (mn) terms in the Hamiltonian (1,a) represent the contributions from the surface layers. Since only the surface 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 on the surface is occupied by a non-magnetic atom.

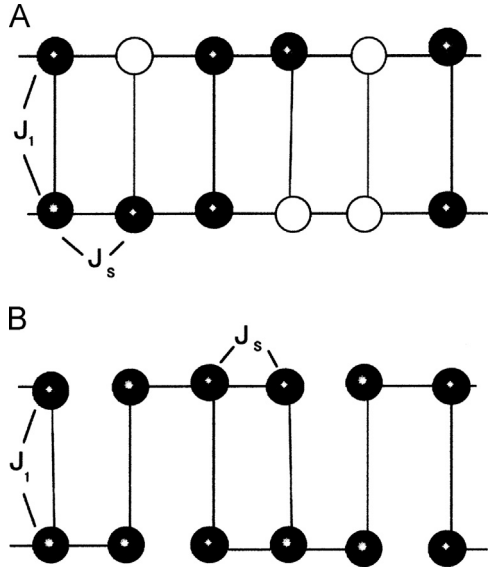

Fig. 1. Schematic representations of two nanoscaled thin films with two layer thickness. The above (A) represents the thin film with site dilution at the surfaces and the down (B) is the thin film with bond dilution at the surfaces. The black circles are magnetic atoms. In (A), the white circles at the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

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

$$H=-\sum_{(ij)}J_{ij}S_i^Z S_j^Z-\sum_{(mn)}J_{mn}S_m^Z S_n^Z-J_1\sum_{(im)}S_i^Z S_m^Z -D\sum_{(i)}\left(S_i^Z\right)^2-D\sum_{(m)}\left(S_m^Z\right)^2, \quad (1,\mathrm{b})$$

where the exchange interaction J_{ij} (or J_{mn}) at the surface 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 surface exchange interaction J_S is often defined as

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

in order to clarify the effect of surfaces on physical properties in the system, where J is the exchange interaction for the bulk.Within the theoretical framework of the EFT [4–6], we can easily obtain the magnetization m (or $m=\langle\langle S_i^Z\rangle\rangle_r$, where $\langle\langle\cdots\rangle\rangle_r$ expresses the random average) of the two layers depicted in Fig. 1(A), namely for the site dilution. It is given by

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

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

$$F(x)=\frac{2\sinh(\beta x)}{2\cosh(\beta x)+\exp(-\beta D)}, \quad (5)$$

where $\beta=1/k_BT$ and T is a temperature. Furthermore, the second moment q ($q=\langle\langle(S_i^Z)^2\rangle\rangle_r$) 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

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

with

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

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

$$m=[q\{<\cosh(J_{ij}\nabla)>_r-1\}+1+m<\sinh(J_{ij}\nabla)>_r]^4[q\{\cosh(B)-1\}+1+m\sinh(B)]F(x)|_{x=0} \quad (8)$$

$$q=[q\{<\cosh(J_{ij}\nabla)>_r-1\}+1+m<\sinh(J_{ij}\nabla)>_r]^4\left[q\{\cosh(B)-1\}+1+m\sinh(B)\right)]G(x)|_{x=0} \quad (9)$$

with

$$\left\langle\cosh(J_{ij}\nabla)\right\rangle_r=p\cosh(J_S\nabla)+(1-p) \text{ and } \left\langle\sinh(J_{ij}\nabla)\right\rangle_r=p\sinh(J_S\nabla).$$

3. Phase diagrams

In this section, let us discuss how to get the mathematical expressions for obtaining the second-order phase transition temperature and the tricritical point in the two ultra-thin films of the previous section. For the aim, the procedure is a little different between the site dilution and the bond dilution, while the general procedure is essentially similar to that in the bulk given in [6]. At first, let us