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Unexpected magnetic properties in an ultra-thin transverse Ising film with bond or site dilution at surfaces

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HIGHLIGHTS

- Phase diagrams in a ultra-thin transverse Ising film have been examined by the EFT.
- The thermal variations of magnetizations are examined.
- The effects of site and bond dilutions at the surfaces are clarified.
- Many unexpected results are obtained in the magnetic properties.

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ABSTRACT

The phase diagrams and magnetizations in a nanoscaled thin film with bond and site dilutions at the surfaces, described by the transverse Ising model, are investigated by the use of the effective field theory with correlations. We find a number of unexpected novel phenomena in them, when the ratio between the transverse field at the surfaces and the transverse field in the inner layer takes a large value; such as the increase of transition temperature, even when the dilution with nonmagnetic atoms at the surfaces is increased.

1. Introduction

Theoretically, the research on the bond or site dilution in a ferromagnet has a long history and has been studied by using a variety of approximations and mathematical techniques. At the present, we think that the problem has been examined in detail and any unknown phenomenon has not be left in the bulk problem. In recent years, on the other hand, magnetic nanoscaled systems have been attracting much attention not only to their fundamental importance, but also due to many technological applications [1–3]. But, it is not so easy to fabricate pure nanosystems. The existence of disorder in the nanoscaled magnetic systems, such as site and bond disorders especially at their surfaces, affects seriously to their magnetic properties, because of their finite sizes. It constitutes an important role in material science. In the nanoscaled magnetic systems, nevertheless, the problems on the dilution have not been studied theoretically so much [4–13]. Furthermore, most of theoretical works on the thin films 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.

Our recent works [14,15] have shown that the ferromagnetic phase transition in a ultra-thin film, described by the transverse Ising model (TIM), may differ markedly from that in the bulk, depending on the surface situations, namely the site and bond dilutions at the surfaces. In these works, the magnetic properties (phase diagram and magnetizations) have been examined by the use of the effective-field theory with correlations (EFT) [16,17]. The EFT corresponds to the Zernike approximation [18] and it is believed to give more exact results than those of the mean field theory. When the value of r ($r=J_1/J$) is taken as a very small or a very large value, some interesting phenomena have been found in the magnetic properties of the systems with thickness L ($L=3$ and $L=4$), such as the appearance of a broad maximum in the variation of transition temperature (T_C) as a function of r for the site dilution, while such a phenomenon has not been obtained for the bond dilution. Furthermore, the T_C of bond dilution in the system with $L=3$ is always larger than the corresponding one of site dilution. From this result, there exists a region in the phase diagram where the longitudinal magnetization m_T for the site dilution is always given by $m_T=0.0$ in the whole temperature region, while the m_T for the bond dilution takes a finite value

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below its T_C. In Ref. [19], the thickness dependences of T_C in the systems have been examined by changing the value of L from $L=3$ to $L=10$. We also found the same behaviors as those in Refs. [14,15] even for the system with $L=10$. In Ref. [20], the same phenomena as those in Refs. [14–18] have been found in the phase diagrams even for the spin-1 TIM thin film with $L=3$.

Here, one should notice that the characteristic phenomena found in Refs. [14,15] heavily depend on the restrictions of zero transverse fields ($\Omega_S=\Omega=0.0$) and uniformly applied transverse fields ($\Omega_S=\Omega\neq 0.0$), where Ω_S is the transverse field at the surfaces and Ω is the transverse field in the inner layer. As far as we know, any work has not clarified what phenomenon happens in the TIM ultra-thin film, when the ratio p ($p=\Omega_S/\Omega$) takes a large value ($p>1.0$). The aim of this work, therefore, is to examine the effects of $p>1.0$ on the fundamental magnetic properties (phase diagram and magnetizations), using the theoretical framework of the EFT. In particular, the temperature dependences of longitudinal and transverse total magnetizations are examined, in order to clarify whether the unexpected behaviors of phase diagrams are correct. We find that many unexpected new phenomena can be obtained in the magnetic properties, when $p>1.0$ and $h=\Omega/J\geq 1.0$. In Section 2, we define the models and give briefly the formulations of the two systems with a bond dilution and a site dilution at the surfaces, in order to examine whether they may show some different behaviors. The numerical results of the phase diagrams and the magnetizations in the two systems with disorders at the surfaces are discussed in Section 3.

2. Models and formulation

In the previous works [14,15], we have discussed the two 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 and the pure inner layer. The thickness L of the system is given by $L=3$. The each site (white circles) on the figure is occupied by a Ising spin. In Fig. 1(A), the surfaces are diluted by non-magnetic atoms. In Fig. 1(B), the bond dilution is performed at the surfaces. The surfaces are coupled to the inner layer with an exchange interaction J_1.

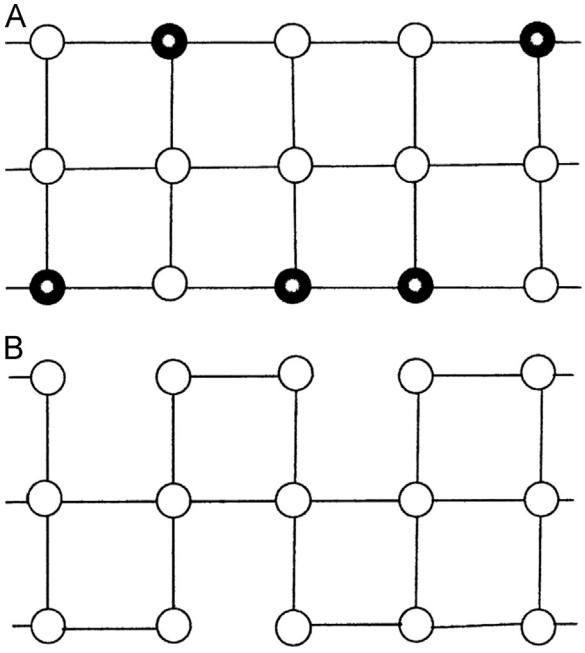

Fig. 1. Schematic representations of two nanoscaled thin films with a thickness $L=3$. The above (A) represents the thin film with site dilution at the surfaces and the down (B) is the thin film with bond dilution at the surfaces. The white circles are magnetic atoms. In (A), the black circles at the surfaces represent nonmagnetic atoms. The lines connecting the white circles represent the nearest-neighbor exchange interactions (J_S, J_1 and J).

The Hamiltonian of the system in Fig. 1(A) is given by

$$H=-J_S\sum_{ij}\sigma_i^Z\sigma_i^Z\xi_i\xi_j-J\sum_{nm}\sigma_m^Z\sigma_n^Z-J_1\sum_{im}\sigma_i^Z\xi_i\sigma_m^Z-\Omega_S\sum_i\sigma_i^X\xi_i-\Omega\sum_m\sigma_m^X, \tag{1a}$$

where σi^{α} ($\alpha=z$ and x) are the Pauli spin operator with $\sigma_i^Z=\pm 1$. J_S is the exchange interaction between two nearest-neighbor magnetic atoms at the surface layer and J is the exchange interaction in the inner layer. Ω_S and Ω represent the transverse fields at the surface and in the inner, respectively. The first (ij) and second (mn) terms in the Hamiltonian Eq. (1a) represent the contributions from the surface layer and the inner layer, respectively. Since only the surface is diluted in the system with the Hamiltonian Eq. (1a), ξ_i takes unity with a probability q when the site i is occupied by a magnetic atom and takes 0 with a probability $(1-q)$ when the site i on the surface is occupied by a non-magnetic atom.

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

$$H=-\sum_{ij}J_{ij}\sigma_i^Z\sigma_i^Z-J\sum_{nm}\sigma_m^Z\sigma_n^Z-J_1\sum_{im}\sigma_i^Z\sigma_m^Z-\Omega_S\sum_i|\sigma_i^X-\Omega\sum_m\sigma_m^X, \tag{1b}$$

where the exchange interaction J_{ij} at the surfaces is randomly distributed according to the probability distribution function

$$P(J_{ij})=q\delta(J_{ij}-J_S)+(1-q)\delta(J_{ij}) \tag{2}$$

The surface exchange interaction J_S is often defined as

$$J_S=J(1+\Delta_S), \tag{3}$$

in order to clarify the effect of surfaces on physical properties in the system.

As discussed in Refs. [14,15], within the theoretical framework of the EFT [16,17], the biggest difference between the bond and the site dilutions at the surfaces comes from the T_C versus r plot in the system with $q<q_0$, where $q_0=0.4284$ is the critical concentration for the bulk system with the coordination number $z=4$ [16,17]. The T_C plot for the bond dilution has not expressed any broad maximum, but also shown the monotonic increase with the increase of r. But, the T_C plot for the site dilution has shown a broad maximum. Furthermore, the broad maximum in the T_C versus r plot for the site dilution has been also found, even when a uniform transverse field (or $\Omega_S=\Omega$) has been applied to the thin film with $q<q_0$. As discussed in Ref. [15], for a uniformly applied transverse field, the transition temperature (T_C) of bond dilution is always larger than the corresponding one of site dilution. From this result, there exists a region in the phase diagram where the longitudinal magnetization m_T for the site dilution is always given by $m_T=0.0$ in the whole temperature region, while the m_T for the bond dilution takes a finite value below its T_C. The phenomenon has easily been understood by drawing the critical field h_C versus q curves for the bond and site dilutions. The critical value h_C is given by the value of h ($h=\Omega/J$) at which the T_C versus h curve reaches zero. As far as we know, these phenomena have not been reported in a lot of previous works for TIM thin films (for the references, see the recent works [8,13]). Here, the longitudinal magnetization $m_T=m_T^Z$ or the transverse magnetization m_T^X per site for the site dilution at the surfaces is defined by

$$m_T^{\alpha}=\left(\frac{2m_S^{\alpha}q+m_c^{\alpha}}{2q+1}\right) \tag{4a}$$