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# Characteristic behaviors in an ultrathin Ising film with site- (or bond-) dilution at the surfaces

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ABSTRACT

The phase diagram, magnetization and Arrott plot of an ultrathin film with site or bond dilution at the surfaces are investigated by the use of the effective field theory with correlations (or the mean field theory for comparison). The system is consisted from the two Ising layers. A lot of characteristic phenomena can be found in them. In particular, the behaviors of them are completely different, depending on whether the site or bond dilution is performed at the surfaces. A lot of unexpected phenomena, such as a new type of frustration, have been obtained in the phase diagram and magnetization, when the strength of interlayer coupling between the two layers is changed.

## 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 perpendicular magnetized (Co/Pt) systems [1–3]. The magnetic properties are heavily depending on the topology of the substrate surface as well as the preparation procedure. These studies are motivated by numerous possibilities of their applications in nanotechnology [4]. In particular, when the size of a magnetic material decreases to a nanometer scale, magnetic properties of a simple magnetic material (such as Co) will be a complex function of finite-size, defects and surface effects. The physics of these effects governs the nanomagnetism of a material and points to the new way of finding important possible applications.

Theoretically, the study of Ising thin films has a long history, although the magnetic properties of an ultrathin Ising film consisting of a few atomic layers have not been examined so much. In a series of recent works [5–9], we have examined the phase diagrams and the magnetizations of nanoscaled Ising (or transverse Ising) thin films consisting of a few magnetic layers by the use of the effective-field theory with correlations (EFT) [10,11]. The EFT corresponds to the Zernike approximation (ZA) [12] and it is believed to give more exact results than those of the mean field approximation (MFA). In these works, some completely different results have been obtained in them, when the site or bond dilution is performed at the surfaces of the system. Many unexpected phenomena, 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 [6], have been found in them, even when the thickness $L$ has been increased from $L=3$ to $L=10$ [9]. 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 Ref. [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 $\beta$ in ultrathin Co films. In particular, an Arrott plot [13] ($M^2$ versus $H/M$ plot, where $H$ is an applied magnetic field) using $R_{Hall}$ in place of $M$ has been applied, in order to determine the $T_C$ value accurately. The Arrott plot based on the MFA is normally valid for the determination of $T_C$ in a bulk magnetic system. As far as we know, it has not been discussed theoretically whether the plot can be applied to an ultrathin magnetic film with site- (or bond-) dilution at the surfaces. In fact, it is not so easy to fabricate pure ultrathin 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 of site- or bond-dilution at the surfaces on the magnetic properties (phase diagram, the temperature dependence of magnetization, the variation of saturation magnetization as a function of concentration $p$ for magnetic atoms and the Arrott plot) in an ultrathin Ising film with $L=2$. As far as we know, such an examination has not been reported even within the theoretical framework of the MFA. Accordingly, some results of

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the MFA are also given, in order to compare with the results of the EFT. In Section 2, the model and formulation are given. In Section 3, the phase diagram (or the variation of $T_C$ as a function of $p$) is examined and the thermal variation of magnetization as well as the variation of saturation magnetization are given. Furthermore, the effects of site- and bond-dilutions at the surfaces on the Arrott plot in the system are examined in Section 3. In Section 4, the effects of interlayer exchange interaction $J_1$ on the $T_C$ are studied, like the previous works [5–9]. The characteristic phenomenon has also been obtained in the phase diagram, like the above mentioned result reported in [5–9]. Furthermore, when the transverse field is applied even to the present pure ($p=1.0$) system, unexpected phenomena due to a new type of frustration can be obtained. These results are presented in Section 5.

## 2. Models and formulation

In this work, we consider the two Ising films with bond and site dilutions at the surfaces. The thickness $L$ of the system is given by $L=2$. The each site (black circles) on the figure is occupied by the Ising spin. In Fig. 1(A), the surfaces are diluted by non-magnetic (white) atoms. In Fig. 1(B), the bond dilution is performed at the surfaces. The two layers, namely $L=2$, are coupled by the interlayer exchange interaction $J_1$.

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

$$H = -J_S\sum_{(ij)}\mu_i\mu_j\xi_i\xi_j - J_1\sum_{(in)}\mu_i\xi_i\mu_m\xi_m - H\left(\sum_i \mu_i\xi_i + \sum_m \mu_m\xi_m\right) \tag{1a}$$

where $\mu_i$ is the Ising spin operator with $\mu_i = \pm 1$. $J_S$ is the exchange interaction between two nearest-neighbor magnetic atoms at the surface layer. The first (ij) term in the Hamiltonian equation (1a) and (1b) represents the contribution from the two surface layers. The second term represents the contribution from interlayer coupling between the two layers. Since only the surface is diluted in the system with the Hamiltonian equation (1a), $\xi_i$ 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. $H$ is the applied magnetic field, so that the third and fourth terms represent the contribution from the two layers under the applied magnetic field.

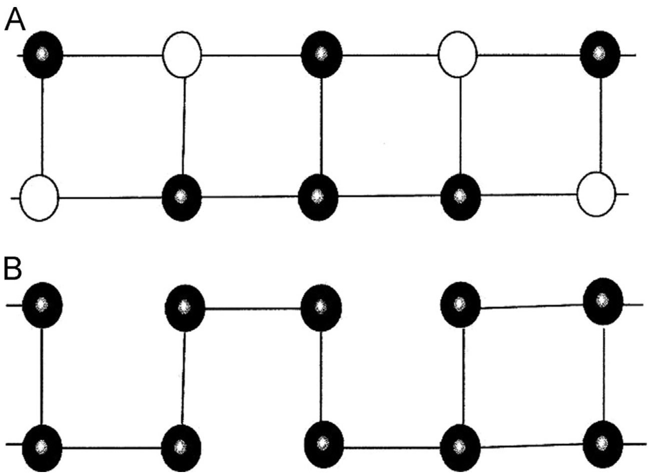

**Fig. 1.** Schematic representations of two nanoscaled thin films with a thickness $L=2$. The above (A) represents the thin film with site dilution at the surfaces and the down (B) is the thin film with bond dilution at the surfaces. The black circles are magnetic atoms. In (A), the white circles at 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 system in Fig. 1(B) is given by

$$H = -\sum_{(ij)}J_{ij}\mu_i\mu_j - J_1\sum_{(in)}\mu_i\mu_m - H\left(\sum_i \mu_i + \sum_m \mu_m\right) \tag{1b}$$

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

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

The surface exchange interaction $J_S$ is defined as

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

where the exchange interaction $J$ represents the corresponding interaction in the bulk system.

Within the theoretical framework of the EFT [10,11], we can easily obtain the magnetization $m$ of the two layers depicted in Fig. 1(A), namely for the site dilution. It is given by

$$m = [p\{\cosh(A) + m\sinh(A)\} + (1-p)]^4 \\ [p\{\cosh(B) + m\sinh(B)\} + (1-p)]f(x+H)|_{x=0,} \tag{4}$$

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

$$f(x) = \tanh(\beta x) \tag{5}$$

where $\beta = (1/k_BT)$ and $T$ is a temperature.

For the bond dilution depicted in Fig. 1(B), the magnetization is given by

$$m = [\langle \cosh(J_{ij}\triangledown)\rangle_r + m\langle \sinh(J_{ij}\triangledown)\rangle_r]^4 \\ [\cosh(B) + m\sinh(B)]f(x+H)|_{x=0}, \tag{6}$$

where $\langle F\rangle_r$ represents the random bond average.

Now, in order to obtain the transition temperature $T_C$ in each system, we must put $H=0.0$ into Eq. (4) or (6). By expanding the right-hand sides of Eqs. (4) and (6), the transition temperature can be determined from, for the site dilution,

$$1 = 4p^2[p^3a_1 + 3p^2(1-p)a_2 + 3p(1-p)^2a_3 + (1-p)^3a_4] \\ + p[p^4a_5 + 4p^3(1-p)a_6 + 6p^2(1-p)^2a_7 + 4p(1-p)^3a_8 + (1-p)^4a_9] \\ + 4p(1-p)[p^3a_{10} + 3p^2(1-p)a_{11} + 3p(1-p)^2a_{12} + (1-p)^3a_{13}], \tag{7}$$

and for the bond dilution,

$$1 = 4p[p^3b_1 + 3p^2(1-p)b_2 + 3p(1-p)^2b_3 + (1-p)^3b_4] \\ + p^4b_5 + 4p^3(1-p)b_6 + 6p^2(1-p)^2b_7 + 4p(1-p)^3b_8 + (1-p)^4b_9, \tag{8}$$

where the coefficients $a_n$ ($n=1$–13) in Eq. (7) and the coefficients $b_n$ ($n=1$–9) in Eq. (8) are given in Appendix. The coefficients $a_n$ and $b_n$ as well as Eqs. (4) and (6) can be easily calculated by applying a mathematical relation $\exp(a\nabla)F(x)=F(x+a)$.

For the following discussions, let us here define the three parameters $t$, $r$ and $h$ as

$$t = \frac{k_BT}{J}\ r = \frac{J_1}{J} \text{ and } h = \frac{H}{J} \tag{9}$$

## 3. Numerical results

In this section, let us examine the magnetic properties (phase diagram and magnetization) in the two ultrathin films with site- and bond-dilutions at the surfaces by solving the equations given in Section 2 numerically. In the following, we also fix the value of $\Delta_S$ in Eq. (3) at $\Delta_S=0.0$.