The Effect of Nano-Vacancy Defect on Ising Magnet in a Reduced Geometry

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ABSTRACT

Monte Carlo simulation was performed to observe the effect of nano-vacancy defects on the magnetic behavior of Ising spins in a reduced geometry, i.e., a porous ultra-thin-film. The magnetic properties were investigated as a function of the vacancy concentration and as a function of temperature, especially in the magnetic phase transition region. The fourth-order cumulant and finite-size-scaling via a double logarithmic plot were used to extract critical temperatures and effective critical exponents for each vacancy concentration. From the results, with increasing magnitude of the porosity, it was found that the Ising phase-transition-point shifted from its two-dimensional value, that the critical temperature $k_BT_C/J \approx 2.269$ to a lower temperature and towards zero temperature. Furthermore, in the phase transition region, the power law relation between the magnetic properties and the linear dimension of the system was found. Consequently, this supports the validity of the finite-size-scaling theory even in the porous structure. Additionally, the finite-size-scaling extraction of the effective critical exponents indicated that for small numbers of vacant defects, the considered nano-vacancy defects structure fell into the two-dimensional universality.

Key words: Nanostructure, Vacancy defect, Magnetic ultra-thin-film, Ising model, Monte Carlo simulation

INTRODUCTION

The magnetic system in a reduced geometry, i.e., thin-film or ultra-thin-film, has been known to be of technological and application importance, especially in the magnetic recording industries according to their exceptionally-high magnetic anisotropy (Murayama et al., 2000; Plumer et al., 2001; Johnson et al., 1996). However, it is also known that under the normal condition, vacancy defects in material frequently occur during the material processing. The vacancy defect, i.e., the porosity at nanometer size is often found to randomly distribute in the material structure. As a result, the magnetic properties of the material are altered from its ideal condition and any calculation based on this ideal condition will lead to an incorrect application design. On the other hand, inclusion with porosity, the porous magnetic media becomes a novel artificial structure with interesting properties such as enhanced coercivity. Furthermore, the porous magnetic structure is also a key factor to control the magnetic critical properties. Because of the smaller number of neighboring atomic sites, there is a reduction in the average ferromagnetic exchange coupling. As a result, this nano-defect can be used to control the magnetic phase transition and hence the Curie temperature. As can be seen, all of these draw a significant interest in using porous magnetic as a new medium for exploring novel magnetic phenomena and may lead to innovative industrial applications.

Consequently, there comes an interest to model how the nano-vacancy defect affects the properties of the magnetic materials. It is interesting to investigate how the defect alters the magnetic behavior, especially at the magnetic phase transition point. In this study, the magnetic system in a reduced structure, i.e., thin-film was considered in order to investigate the magnetic profiles and its phase transition under the influence of nano-vacancy defects by means of Monte Carlo simulations. As a prototype, the study was based on the ultra-thin structure, i.e., the planar square lattice, under an inclusion of nano-sized porosity, e.g., number of atoms missing. In the simulation, the Ising model was chosen to represent magnetic spins since strong magnetic anisotropies are common in ultra-thin ferromagnetic films, and there is evidence which suggests that Ising model is useful to model magnetic ultra-thin-film from both theoretical (Binder and Hohenberg, 1974; Bander and Mills, 1988) and experimental studies (Li and Baberschke, 1992; Elmers et al., 1994; Dunlavy and Venus, 2004). In a simulation update, a sophisticated Wolff algorithm (Wolff, 1989) was used to update the magnetic configurations. By varying the vacancy-defect concentrations and temperatures, the observables, i.e., the magnetization and the magnetic susceptibility were carefully taken at the interval of twice the correlation time to minimize the statistical errors (Müller-Krumbhaar and Binder, 1973). A careful attention was paid to the magnetic phase transition to extract the critical temperature. In addition, to go for another step beyond previous Monte Carlo studies in literatures, the finite size effect was carefully taken into account and critical exponents were extracted to investigate the universality.

In outline, the numerical calculations and the methods used were firstly described. Secondly, the evolution of the magnetic properties as a function of void (vacancy) concentration and temperatures was shown. Then, the critical properties in terms of the critical temperatures and the effective critical exponents were reported. After that, observations on how the exponents depend on the vacancy concentrations were made. Finally, the results were discussed and the characteristic effective critical exponents were compared with those found in literatures (where applicable).

MATERIALS AND METHODS

In this study, the Ising Hamiltonian was considered:

$$H = -J \sum_{<ij>} S_i S_j, \qquad (1)$$

where the spin S_i took on the values ±1 and the sum included only first nearest-neighbor (1nn) pairs. Helical (periodic) boundary conditions were used in this geometry. The units of J/k_B and J were for temperature and energies respectively. The simulations were carried out for square lattice with number of atomic sites $N = L \times L$ where L varied from 20 to 40 with a step of 4. The vacancy concentration c, indicating the magnitude of porosity, was varied from 1 to 20 percent of N. These non-magnetic sites, being equivalent to the vacancy-type defect, do not occupy the magnetic moment, i.e., $S_i = 0$, giving no contribution to the above Hamiltonian. Consequently, the total number of Ising spins is $N' = N(1-c)$.

In updating the spin configuration, the Wolff algorithm (Wolff, 1989) was used to minimize the effect from statistical errors arising from correlation time τ (Müller-Krumbhaar and Binder, 1973). From an initial state, each simulation was waited until it resided in equilibration before measuring any observable, i.e., the magnetization per spin

$$m = \frac{1}{N'} \sum_{i=1}^{N'} S_i, \qquad (2)$$

and the internal energy

$$E = -J \underset{<ij>}{\ } S_i S_j, \tag{3}$$

Each measurement was taken when the number of flipped spins in the Wolff update exceeded or equalled to $N' \, x \, \tau$. Then, the expectation of magnetization per spin

$$[m] = \frac{1}{N'} \overset{N'}{\underset{t=1}{\ }} \left| m_t \right|, \tag{4}$$

where n' referred to number of measurement used in the time average, and the magnetic susceptibility

$$\chi = \beta \mathrm{N} \left([m^2] - [m]^2 \right), \tag{5}$$

where $\beta \equiv J/k_B T$, were calculated. For the investigation of the critical behavior, the effective critical temperatures $T_C(c)$ for each vacancy concentration c were located via the fourth-order cumulant U_L (Binder, 1981), i.e.,

$$U_L = 1 - \frac{1}{3} \frac{[m^4]}{[m^2]^2} \ . \tag{6}$$

At $T = T_C(\mathrm{c})$, U_L's becomes L-independent, so differing sizes L and L' give $\left. \frac{U_{L'}}{U_L} \right|_{T = T_C(c)} = 1$. Owing to finite size effects, $T_C^{\,b}(L=bL')$ against $1n^{-1}b$ needs to be plotted and extrapolated the results to the infinite limit, i.e., $1n^{-1} b \rightarrow 0$ (Binder, 1981). To maximize the efficiency of this $T_C(c)$ extraction, a single long simulation was performed at a temperature T_0 and the histogram method (Ferrenberg and Swendsen, 1988; Ferrenberg and Landau, 1991) was used to extrapolate U_L to temperatures nearby in order to find the cumulant crossing point. This temperature T_0 was chosen from the temperature at the peak of the magnetic susceptibility curve for the $L = 40$ system. Then, around 1 to 4 million spin configurations were used to create the histograms. To exclude the data being obtained from temperatures too far from the simulated temperature T_0, the range of extrapolation $|T - T_0|$ was restricted by the criterion $|U(T)-U(T_0)| \quad \sigma_E$ (Newman and Barkema, 1999) where $U \equiv \langle E \rangle$ is the average of the energy E, and σ_E is a standard deviation of E at T_0.

To extract the critical exponents to the magnetic critical behavior from finite size results, an empirical finite-size-scaling form for this porous media was considered. The purpose is to find the magnetic properties m and χ scale with L at a particular concentration c of the systems. The basic finite-size-scaling ansatz (Fisher, 1974; Stanley, 1987) rests on an assumption that the magnetic properties in the critical region scales with the reduced temperature $t = \frac{T}{T_C(c)} - 1$ in a power-law form. Hence the empirical forms for how the magnetization and susceptibility scale with L, at a fixed c, can be written as

$$[m(T,c)] = L^{-(\beta'/\nu')} \, \tilde{m} \, (L^{1/\nu'} t, c), \tag{7}$$

and

$$\chi(T,c) = L^{(\gamma'/\nu')} \, \tilde{\chi} \, (L^{1/\nu'} t, c), \tag{8}$$

where γ', β' and ν' are the effective critical exponents associated with χ, m and the correlation length ξ respectively. Based on this finite-size-scaling theory, it is generally known that

$\xi \sim L^{1/\nu'}$. For $c = 0$, the effective exponents are the critical exponents for the two-dimensional (2D) system. The functions $\tilde{\chi}$ and $\tilde{m}$ are scaling functions for a given c and the reduced temperature t. These scaling functions for a range of L should collapse onto a single curve with the correct critical temperature and suitable effective critical exponents. Next, the effective exponent $1/\nu'$ can be extracted from the derivative of the cumulant with respect to L at T_C owing to its variation with system size as $L^{1/\nu'}$ i.e. $dU_L/d\beta \sim L^{1/\nu'}$ (Binder, 1981) where this β (=k_BT) is the inverse temperature. Note that if Eq. (7,8) correctly encapsulate the nature of magnetic critical behavior in porous structures, one can extract the effective exponents (β'/ν') and (γ'/ν') by making a log-log plot of m or χ against L at T_C. Hence, the validity of the empirical equations Eq. (7,8) in modeling results from our simulations, in the critical region, can be done by investigating if linearity from the double logarithmic plots of χ or m against L are found. In addition, based on the hyperscaling relation (Fisher, 1969), the test of universality can be performed by considering the effective dimension (Freire et al., 1994; Rouault et al., 1995) via

$$d_{\text{eff}} = \left(\frac{\gamma'}{\nu'}\right) + 2\left(\frac{\beta'}{\nu'}\right). \tag{9}$$

For $c \rightarrow 0$, a 2D-like behavior, i.e., $d_{\text{eff}} = 2$ is expected.

RESULTS AND DISCUSSION

From magnetization m and susceptibility χ profiles for various vacancy concentration c and system sizes L, a suggesting crossover of behavior from a 2D-like for the $c = 0.00$ to a 1D-like (where there is no phase transition) for $c = 0.20$ or smaller was found (see Figure. 1). The transition point moves from 2D to 1D values with increasing the vacancy concentration in a good agreement with previous prediction in diluted magnet under the framework of percolation studies (Stauffer and Aharony, 1994).

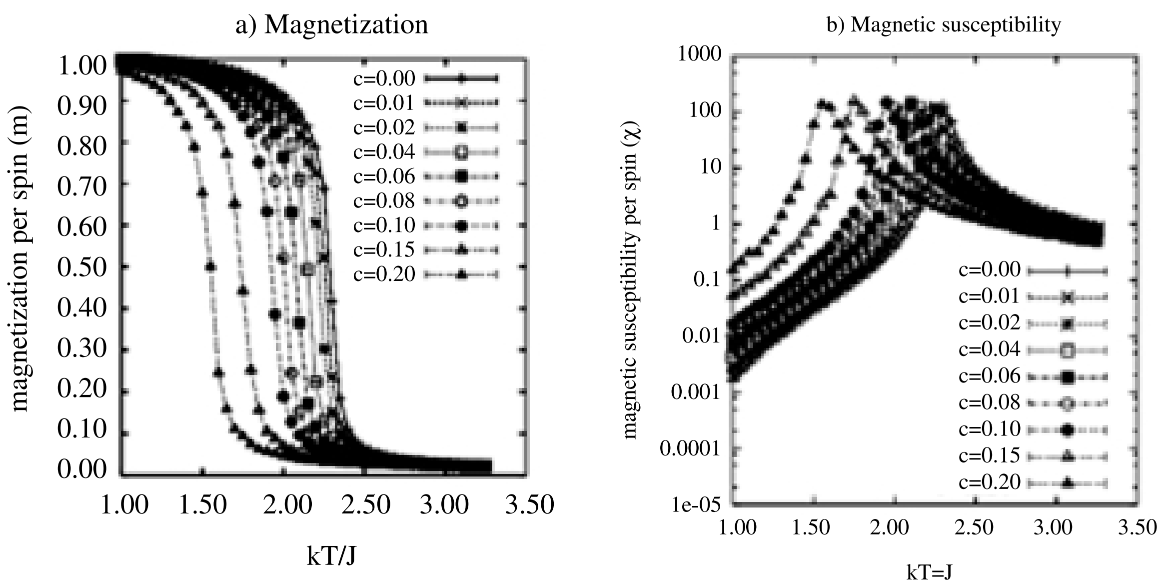

Figure 1. Magnetic properties of the porous 40(40 Ising spins, i.e. (a) the magnetization per spin m and (b) the magnetic susceptibility χ as a function of temperature, which present a reduction of the phase transition point with varying the concentration from $c = 0.00$ to $c = 0.20$. Lines are used to guide the eyes.

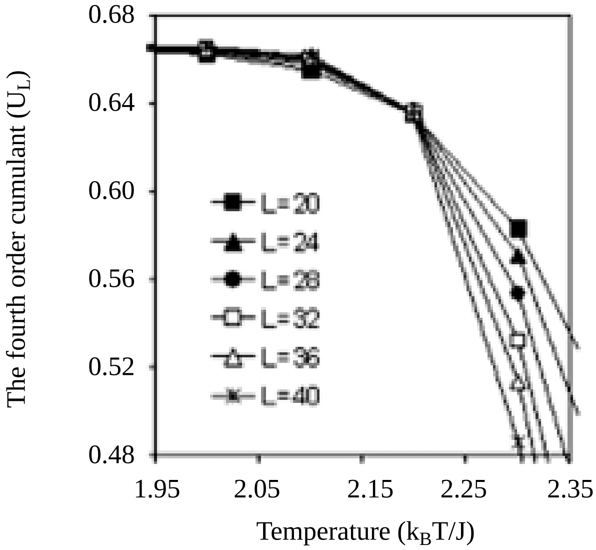

Figure 2. The fourth-order cumulant of the magnetization per spin U_L's for various linear dimension L as a function of temperature k_BT/J of the c = 0.02 system. Lines are used for a viewing aid. From the figure, the temperature at the middle of the crossing region suggests where the critical temperature T_C is.

Then, the critical temperatures T_C of the system at a particular c was calculated from the Monte Carlo simulations, using the cumulant crossing method, e.g., see Figure 2. From all the T_C's results, similarly, a change from 2D to 1D behavior was found as c was increased. This is because the number of vacancy sites has a strong effect on the averaged exchange coupling among the spins in the systems. Then, the more vacancies, the less magnitude of the average magnetic exchange coupling in the systems, and this strongly reduces the magnitude of the magnetization. Consequently, the transition from the ferromagnetic to the paramagnetic phase does not require as much thermal energy as it does in the ideal 2D system, and this results in smaller critical temperature T_C. The results of the critical temperature are presented in Figure 3 as a function of the effective thickness (1-c).

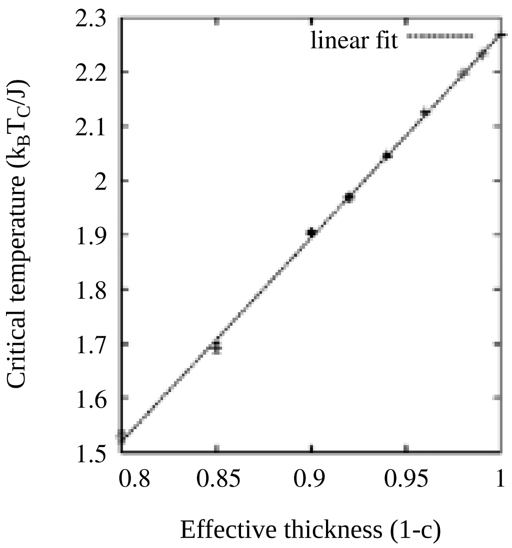

Figure 3. The critical temperatures k_BT_C/J as a function of effective thickness (1-$_c$) extracted from Monte Carlo simulations. Lines are added as a viewing aid. Best linear fit suggests an equation y = 3.76x – 1.48 and at y = 0 it is found that x = 0.39 ± 0.01.

As can be seen in Figure 3, a linear relation between effective thickness and critical temperature is found, providing a way to predict the critical temperature at any particular vacancy concentration. With the least-square linear fit, the critical temperature was found to cease down to zero at c = 0.39(0.01. This agrees well with the investigation of percolation in diluted magnet in 2D system (Stauffer and Aharony, 1994).

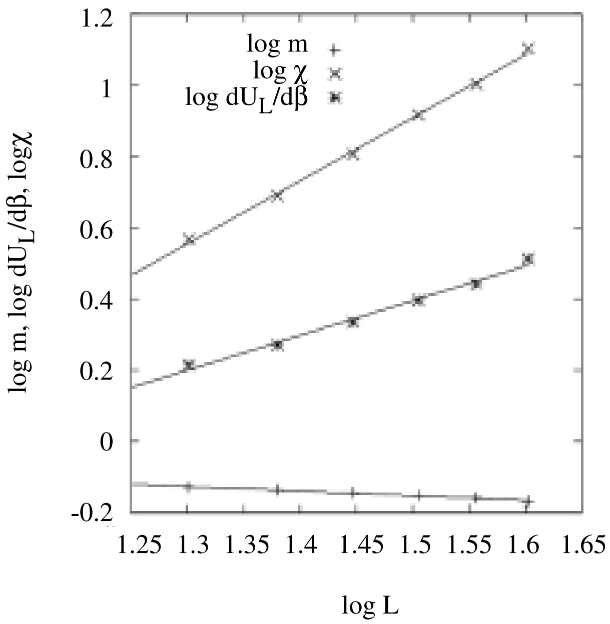

Figure 4. An example of the extraction of effective critical exponents β', γ/ν', and $1/\nu'$ from the slopes of least-square fits (see text) for c = 0.02 system. The apparent linear relations support Eq. (7,8).

On the other hand, in searching for the critical exponent to the magnetic behaviour, the effective critical exponents were extracted from Eq. (7,8) as well as the relation $dU_L/d\beta \sim L1/\nu'$ at T_C. As shown in Figure 4, results from the simulations, at T_C, indeed show very good linear relationships between log m (log χ, log $dU_L/d\beta$) and log L for all considered vacancy concentrations. The effective exponents β'/ν', γ/ν', and $1/\nu'$ were then extracted from the slopes of these linear least-squares fits. Then, the calculation of the effective dimension $d_{\mathrm{eff}} = \gamma/\nu' + 2\,\beta'/\nu'$ [see Eq. (9)] was performed. It was found that, for small c's, d_{eff} has a value of 2 within error bars (see Table 1) as expected. This confirms the 2D universality in ultra-thin-film with small number of the vacancy defects and ensures the possibility of using Eq. (7,8) to describe the critical behavior of the systems. However, for large number of the vacancy concentration, i.e., c 0.06, the ef fective critical exponent does not give any suggestive information. This is due to that the large number of vacancy sites randomly spread throughout the lattice giving rise to many random microstructures. As it is well-known that the microstructure has a strong effect on the magnetic properties, this may be such a case why the effective exponent and the effective dimension are not close to 2. To clarify this, more number of individual runs should be performed and the critical properties should be extracted from the average of the magnetic properties taken from those runs.

Table 1. Results of the critical temperatures, the critical exponents (extracted via finite-size-scaling functions) and the effective dimension d_{eff} for porous Ising spins with the vacancy concentration c ranging from 0.00 to 0.20.

c	$k_B T_C/J$	β'/ν'	ν'	γ'/ν'	d_{eff}
0	2.269 ± 0.001	0.124 ± 0.002	1.00 ± 0.01	1.75 ± 0.01	2.00 ± 0.01
0.01	2.233 ± 0.001	0.119 ± 0.005	1.00 ± 0.01	1.72 ± 0.02	1.96 ± 0.03
0.02	2.192 ± 0.001	0.123 ± 0.003	1.00 ± 0.01	1.76 ± 0.01	2.01 ± 0.01
0.04	2.129 ± 0.002	0.124 ± 0.001	0.99 ± 0.01	1.74 ± 0.02	1.99 ± 0.02
0.06	2.062 ± 0.004	0.102 ± 0.006	0.97 ± 0.02	1.65 ± 0.01	1.85 ±0.02
0.08	1.974 ± 0.006	0.083 ± 0.009	0.97 ± 0.01	1.49 ± 0.01	1.66 ± 0.02
0.1	1.898 ± 0.004	0.133 ± 0.005	0.99 ± 0.04	1.82 ± 0.09	2.10 ± 0.10
0.15	1.710 ± 0.010	0.075 ± 0.009	0.88 ± 0.07	1.44 ± 0.08	1.59 ± 0.09
0.2	1.530 ± 0.010	0.220 ± 0.008	0.92 ± 0.08	1.95 ± 0.03	2.39 ± 0.04

CONCLUSION

Monte Carlo studies on the Ising ultra-thin-film system were performed to investigate the effect of vacancy defect and its concentrations on the magnetic properties, i.e., the magnetization and the susceptibility per spins including its critical behavior in terms of the critical temperature and the effective critical exponent. The dimensional crossover of both m and χ from 2D- to 1D-like with increasing the vacancy concentration has been found. That the film T_C's evolve from 2D to 1D value with increasing the vacancy concentration is in good agreement with previous studies. From the results, at small concentration, i.e., c 0.04, the effective exponents and the effective dimensions are essentially the same as those in the ideal 2D structure, suggesting that the porosity does not affect the 2D universality. However, with large number of the vacancy concentration c, more number of individual runs needs to be taken to extract any informative results.

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