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Monte Carlo study of randomly diluted ferromagnetic thin films

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Using Monte Carlo simulations, we have studied the Ising model with random, nonmagnetic impurities on an $N \times N \times L$ simple cubic lattice. Systems with ferromagnetic nearest-neighbor coupling and periodic boundary conditions in the x-y plane are studied for $N=40$ and $1 \le L \le 40$ for several values of p, the concentration of magnetic ions. The average magnetization, susceptibility, and specific heat are calculated as a function of temperature for different values of L and p. The transition temperature T_c decreases monotically to zero as the concentration p decreases towards the percolation threshold for the width L. The shift of T_c is consistent with $L^{-\lambda}$, where λ is equal to 1.56 in the critical region.

I. INTRODUCTION

In the past few years, there has been considerable interest in the effects of impurities on phase transitions[1] and in the finite-size scaling of magnetic thin films.[2] From studies in the square[3-5] and cubic[1-6] Ising models with random site impurities, it is known that the transition temperature, T_c, decreases monotonically towards zero as the impurity concentration increases towards the percolation limit. (For the square lattice[7] $p_c=0.593$ for site percolation, while for the cubic lattice[7] $p_c=0.3113$.) It is also believed that the critical exponents of the random system are related to the pure-lattice exponents.[1] In particular, Harris[8] has suggested that the sharpness of the phase transition in a system with random quenched impurities is unchanged if the specific-heat exponent α of the pure system is negative. If α is positive, the asymptotic critical behavior is expected to change as T_c is approached. Monte Carlo simulations[3-5] for two-dimensional (2D) Ising models, where $\alpha=0$, find no evidence for changes in critical behavior. This is in agreement with the renormalization-group[9] analysis which suggests for $d=2$ pure system critical exponents with some sort of logarithmic corrections. Thin magnetic films[10] have always received great attention, since the ideas of finite-size scaling[2] can be checked. With the recent success of molecular-beam techniques in fabricating magnetic films of near atomic thickness,[11,12] the finite-size scaling ideas can be checked experimentally.

In this paper we will report new results using Monte Carlo simulations in randomly diluted thin films containing ferromagnetic Ising spins, where the combined effects of randomness and finite-size scaling on the transition temperature, T_c, and other thermodynamic properties will be examined. In Sec. II we describe the model and the numerical approach used. In Sec. III we present and discuss our results, and finally in Sec. IV we summarize our conclusions.

II. MODEL AND MONTE CARLO TECHNIQUE

We studied $N \times N \times L$ simple cubic Ising lattices containing random, nonmagnetic site impurities. The Hamiltonian of this model is

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

where the nearest-neighbor exchange constant $J_{ij}=J\epsilon_i\epsilon_j$ and $\epsilon_i=1$ if site i is occupied and zero otherwise, and $S_i=\pm 1$. Systems with ferromagnetic coupling $J>0$ and periodic boundary conditions in the x-y plane are studied for $N=40$ and $L=1$, 2, 4, 6, 8, 16, 40 for several values of p, the concentration of magnetic ions. We used the Monte Carlo method,[13] a standard procedure for the investigation of the statistical mechanics of finite systems, for obtaining the different thermodynamic properties. One Monte Carlo step (MCS) was defined as $(N \times N \times L)$ attempted spin moves, where $(N \times N \times L)$ is the total number of spins in the system. Between 1000 and 6000 MCS were used to obtain each data point. For $p \le 0.6$, the data were averaged over at least three different configurations of random impurities. For larger values of p, the results were essentially independent of the particular magnetic impurity configuration used for the system sizes studied here.

III. RESULTS

In this section we discuss the behavior of magnetization, susceptibility, and specific heat in the randomly diluted ferromagnetic thin films as a function of both the temperature, T and concentration, p, of the magnetic impurities. We emphasize particularly that the $T_c(p)$ for a given thickness L approaches zero at the percolation threshold for that width, which can be obtained from different methods.[7]

Figure 1 plots the magnetization in the ordered state (obtained upon cooling) as a function of temperature for four different film thicknesses $L=2$, 4, 8, 16. For each thickness L, the concentration of the magnetic impurities p shown equals 0.9, 0.7, and 0.5. Notice that for a given thickness L, a reliable estimate of the transition temperature T_c can be obtained. We defined $T_c(p)$ for a given L, as the value of the magnetization at its half maximum value. Note that for $L \leq 4$, the magnetization for $p=0.5$ is relatively low for the configuration of the random impurities shown in Fig. 1. By averaging different random configurations, we find there is no magnetization at $T=0$ for $p=0.4$ and $L \leq 4$. As can be seen by Fig. 1, by increasing the thickness to $L=8$, even films with $p=0.5$ have a nonzero magnetization, i.e., long-range order at a finite temperature.

In Fig. 2 we plot the magnetic susceptibility χ as a function T for different thin films thicknesses L and different concentrations of magnetic impurities p. For a given L, the susceptibility has a sharp peak for all magnetic impurity concentrations $p > p_c(L)$, in the percolation threshold for a given thickness.[7] In all of the cases, the susceptibility shows a peak near the location where the magnetization shows a rapid decrease. The data shown in Fig. 2 indicate that finite-size effects are important (i.e., we obtain finite susceptibilities at $T=T_c$) and the location of the peak shifts to lower temperatures with an increasing p. This behavior is true for every thickness L. The peak in the susceptibility is insensitive to the particular configuration of magnetic impurities used, provid-

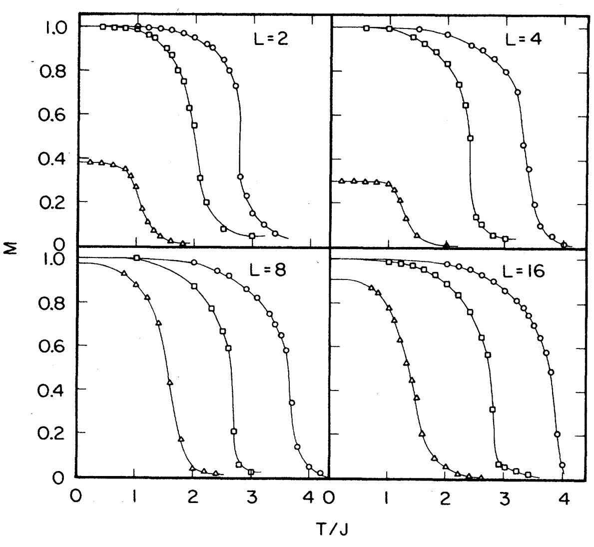

FIG. 1. Temperature dependence of the spontaneous magnetization M for various thickness $L=2$, 4, 8, 16. For every L the concentration of the magnetic impurities p is equal to (○) 0.90, (□) 0.70, and (△) 0.50, respectively.

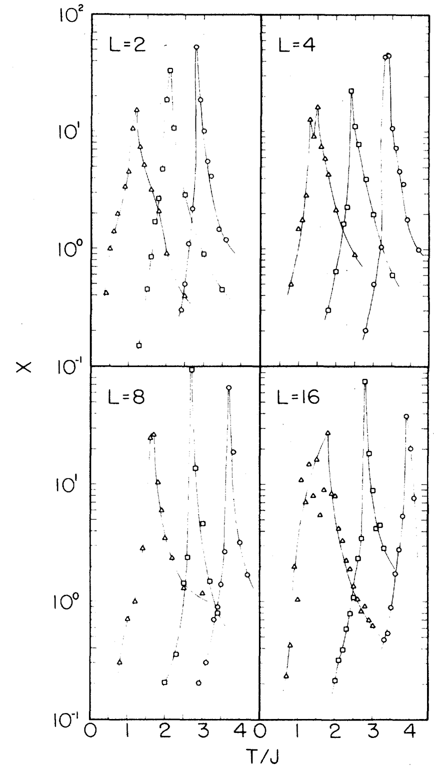

FIG. 2. Temperature dependence of the magnetic susceptibility χ for various thickness $L=2$, 4, 8, 16. For every L, p is equal to (○) 0.90, (□) 0.70, and (△) 0.50, respectively.

ed that $p \geq 0.6$. For $p \leq 0.5$, quite noticeable differences appear between the results of different configurations of magnetic impurities. In these cases, special care was taken to average the measured thermodynamic quantity over different random impurity configurations.

In Fig. 3, the specific heat is shown for several concentrations of magnetic impurities $p=0.9$, 0.7, and 0.5 for different thin-film thicknesses $L=2$, 4, 8, 16. The general characteristics for the specific-heat data are the same as for the susceptibility. In all of the cases we examined, the effect of decreasing p was to move the peak in a lower T. For a given value of L, the peak value decreases quite rapidly with decreasing concentration of magnetic impurities. As expected for low p the peak in the specific-heat data is not as sharp as for high p. In principle, one can extract for a given L and p the transition temperature, T_c, from the position of the peak in the specific-heat data. However, we find that the peaks in the susceptibility data are more pronounced and its position can be obtained easily. In addition, we systematically find for the same configuration of magnetic impurities that the position of the specific-heat peak is always lower than the susceptibility peak. Therefore, for the determination of the critical temperature, $T_c(p)$, we used the position of the susceptibility peak. The position of the specific-heat peak, as well as the behavior of the magnetization (Fig. 1), was used as a consistency check.

Our estimates for $T_c(p)$ for different thin film thickness L are shown in Fig. 4. For $L=1$, which is the 2D Ising

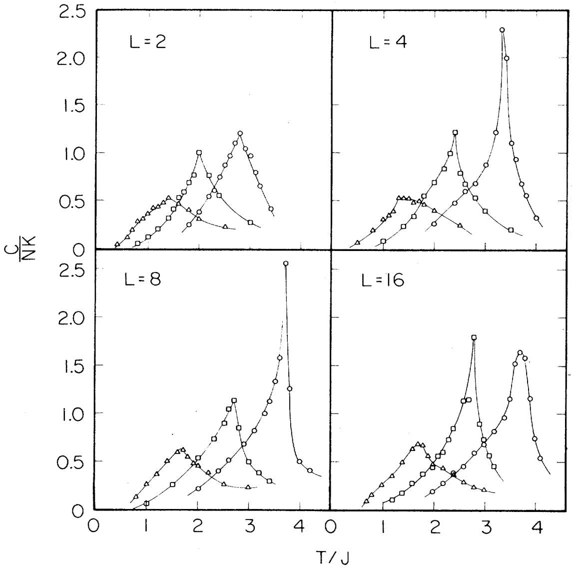

FIG. 3. Temperature dependence of the specific heat c for various thickness $L=2$, 4, 8, 16. For every L, p is equal to (○) 0.90, (□) 0.70, and (△) 0.50, respectively.

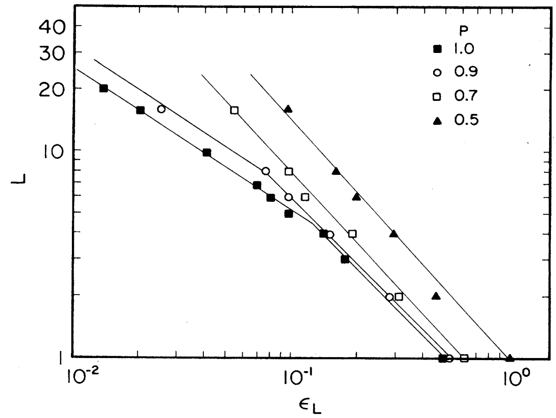

FIG. 5. log-log plot of the shift of the critical temperature ϵ_L vs L for different concentrations p of the magnetic ions. The straight lines indicate possible exponent estimates.

ferromagnet, our results agree reasonably well with previous Monte Carlo simulations for the same system.[3-5] For $p=1$ and $L=1$, $T_c(p=1)=2.269$, the 2D Ising result. As p decreases, $T_c(p)$ decreases and goes to zero at $p=0.59$, which is the 2D site percolation threshold for a square lattice. It has been shown,[3] and our results agree, that the critical exponent for the random $(p\neq1)$ 2D system are equal to the corresponding ones of the pure $(p=1)$ 2D Ising system. For $L=40$, which is the 3D diluted Ising ferromagnet, our results agree well with previous Monte Carlo simulations for the same system.[1] For $p=1$, we find that $T_c(p=1)=4.5$. For $L=40$, as p decreases, $T_c(p)$ decreases and approaches zero near $p=0.3113$, which is the 3D site percolation threshold for a cubic lattice. For the random 3D Ising ferromagnet, Landau argued[1] and our results support claims that there

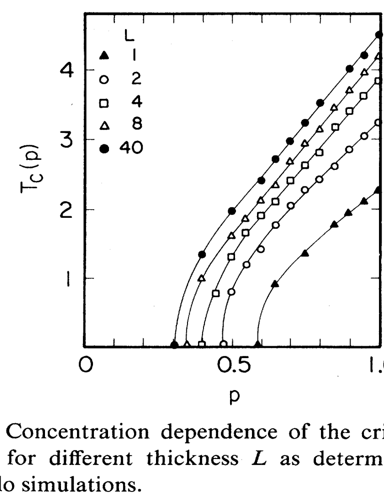

FIG. 4. Concentration dependence of the critical temperature $T_c(p)$ for different thickness L as determined from the Monte Carlo simulations.

is no change of the critical exponents away from the pure system values. For $p=1$, Binder[2] has systematically studied the crossover from two- to three-dimensional behavior. This crossover behavior will be examined below. Also in Fig. 4, we plot $T_c(p)$ as a function of p for three other thin-film thicknesses, $L=2,4,8$. For p fixed, as L increases from its $L=1$ value, $T_c(p)$ increases and very quickly approaches its 3D value, while for fixed L, $T_c(p)$ decreases and approaches zero as $p\to p_c(L)$. Notice from Fig. 4 for $p=0.4$ which is between the 3D and 2D percolation thresholds, there is no spontaneous magnetization for $L=1$. As the film thickness increases, long-range order does not develop until $L=8$. Clearly, the thickness L above which long-range order develops depends on the concentration of magnetic impurities p. For p close to the 2D percolation threshold, 0.59 $L\cong1$, while for close to the 3D percolation threshold, 0.3113, $L\to\infty$. For $p\leq0.35$, the critical thickness L for long-range order is $L\geq16$. To systematically check the thickness dependence of the transition temperature, $T_c(p)$, for a given p, we replotted our data shown in Fig. 1 to a form (Fig. 5) that is convenient to compare with the predictions of the finite-size scaling theory.[2] In Fig. 2 we plot on a log-log graph the shift of the critical temperature $\epsilon_L=1-T_c(L)/T_c(\infty)$ versus the thickness L. The results for $p=1$ shown in Fig. 2 agree with those of Binder.[10] Notice that for $p=1$ and small L, $\epsilon_L\sim L^{-1.0}$, while close to the critical region $\epsilon_L<0.1$, we have $\epsilon_L\sim L^{-\lambda}$, where $\lambda=1/\nu=1.56$ which agrees with the estimates of the simple finite scaling.[1,2] Notice that as p decreases, the critical region decreases[1,3] for strong dilution, i.e., $p\leq0.7$, we only see $\epsilon_L\sim L^{-1}$ as the critical region decreases significantly in size. Due to the decrease of the critical region with decreasing p, we were unable to draw any definite conclusions for the low p values on the effects of disorder on the critical exponents of the pure system.

IV. CONCLUSIONS

This paper represents a rather detailed Monte Carlo study of the behavior of randomly diluted Ising ferromagnetic thin films over a wide range of temperature, thin-film thickness, and concentration of magnetic impurities. We find that the addition of nonmagnetic impurities in a thin film of thickness L tends to decrease the position of the peak in the specific heat and susceptibility data. The decrease of the transition temperature, $T_c(p)$, with decreasing p and/or L can be understood by the finite-size scaling theory. Although we clearly see effects that are due to the addition of nonmagnetic impurities, such as the decrease of $T_c(p)$ with p for a given L, we find no evidence of a change in the critical exponents due to the randomness. It appears as though extensively larger lattices would probably be needed to approach the critical region more closely in order to measure critical exponents accurately. Recently, experiments have been performed[11,12] to check some of the finite-size scaling ideas for spin glass systems. It will be very interesting if similar experiments could be done on thin film of diluted Ising ferromagnets.

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