Critical behavior of an $Fe_xMg_{1-x}Cl_2$ model: Pure metamagnetic to random-field behavior

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A Monte Carlo study of a *quite realistic* model of $Fe_xMg_{1-x}Cl_2$ (a diluted anisotropic antiferromagnet in a field) has been performed in the strong concentration limit ($x=0.9$, 0.8, and 0.7). Simulations of field cooling (FC) and heating (FH) processes as well as isothermal field cycles are presented. A modification to the standard Metropolis algorithm to deal with layered systems has been introduced in the spirit of cluster-flip algorithms. Our results show that dilution does not destroy the tricritical point at least until $x=0.7$. We also show that the equilibrium temperature loops are reversible and the antiferromagnetic long-range order is established in a FC process for values of the applied field lower than the threshold field for the metamagnetic transition at zero temperature. On the other hand, irreversibilities found when performing rapid FH+FC loops in the same region of the phase diagram are studied.

I. INTRODUCTION

Critical behavior of diluted anisotropic antiferromagnets in a field (DAFF) which is a physical realization of the random-field Ising model (RFIM),[1] is still a subject of discussion. Some mean-field works exist for the simplest models[2–5] as the complexity of the system makes it extremely difficult to find analytical solutions for more realistic ones. Monte Carlo simulations then become a useful tool for the understanding of these systems. Until now this technique has been applied to the simplest models. For instance, Soukoulis *et al.* and Grest, Soukoulis, and Levin have tested the equivalence between DAFFs and RFIM in 2D and 3D (Refs. 3 and 5) considering simple square and simple cubic lattices with isotropic nearest-neighbor(NN) interactions. Diep, Galam, and Azaria[6] and Galam, Azaria, and Diep[7] have analyzed the existence of a tricritical point (TCP) in a DAFF consisting of a simple cubic lattice with isotropic interactions between nearest and next-nearest neighbors (NNN). Recently, a simulation on a highly diluted (50%) simple cubic lattice with isotropic nearest-neighbor antiferromagnetic interactions was performed by Nowak and Usadel,[8] paying special attention to the high-field region.

In spite of all this effort, many questions remain still open. For instance, the existence of a long-range order (LRO) is admitted for a 3D RFIM,[9,10] but it is under discussion for some DAFF's because of the long relaxation times involved.[2,11,12]

Experimental studies show, in general, that the state of the system at a particular point of the temperature-field (T,H) space depends on the process used to take the system to that point. It seems reasonable to suppose that some of the unclear aspects found when comparing theoretical with experimental results may depend on the particularities of the real system. For instance, the expected LRO as well as the shape of the magnetic domains (if any) formed while this LRO is being established, must be related to the kind of lattice considered, its spatial anisotropy, the existence of frustrated or competing interactions, its percolation threshold, etc.

In a previous work,[13] we have presented a Monte Carlo study of phase transitions on an $FeCl_2$ model. This model, though quite simple, kept the outstanding features of the system: highly spatial anisotropy (triangular lattice planes stacked along **c** axis), superexchange paths for the interplane interaction, competition and frustration in the plane. The results we have obtained with such a model are in excellent qualitative and quantitative agreement with experimental ones. Based on such a good description of the pure system, this work aims to reproduce some of the experimental results on the diluted system that are still unclear. In particular, we addressed our attention to the existence of a TCP and its behavior with dilution. We also studied the character of equilibrium temperature loops in constant field (whether they are reversible or not) and the existence of a LRO for a field cooling (FC) process. As mentioned above, irreversibilities in temperature loops have been experimentally reported. We have analyzed this fact by performing short simulations on our finite systems, showing that such irreversibilities correspond to a nonequilibrium effect. We have also investigated the experimental result stating that the magnetization issued from a FC process (m_{FC}) is

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greater than that issued from a field heating (FH) one (m_{FH}).[11,12] We have determined the irreversibility line from the first temperature where $m_{FC} > m_{FH}$ in a FC process and we tried to elucidate the kind of magnetic domains formed in this irreversibility region that are responsible for that result.

The paper is organized as follows. In Sec. II we describe the system and the studied quantities. In Sec. III we give some technical details of the simulated processes along with a description of a modification of the Glauber dynamics to adapt the algorithm to the study of layered systems. In Sec. IV we analyze our results and compare them with experimental ones. Finally, in Sec. V we present our conclusions and discuss possible future work.

II. DESCRIPTION OF THE SYSTEM

The Hamiltonian of the system may be written as follows:[13]

$$\mathcal{H} = -J_1 \sum_{\langle NN \rangle} \eta_i \eta_j s_i s_j - J_2 \sum_{\langle NNN \rangle} \eta_i \eta_k s_i s_k - J' \sum_{\langle NN' \rangle} \eta_i \eta_l s_i s_l - g\mu_B H \sum_i \eta_i s_i \ , \quad (1)$$

where $s_i = \pm 1$ is an Ising spin, $\langle NN \rangle$ and $\langle NNN \rangle$ denote the sum over the nearest and next-nearest neighbors in the plane, respectively, and $\langle NN' \rangle$ indicates the sum over the interacting spins belonging to adjacent planes. As the last interaction is a superexchange one, we have taken into account all the equivalent magnetic paths for the coupling of iron planes via the chlorine ones. Following Anderson's rule, this leads to 12 neighbors in each one of the neighboring planes.[13]

In order to simulate a given quenched disorder, we chose the sites at random and assigned to each site i one of the values of the corresponding occupation variable $\eta_i = 0, 1$, with a probability $\mathcal{P}(\eta_i = 0) = p$, until we got $N_p = p \times N$ "vacancies" (N being the total number of sites and $p = 1 - x$, the desired amount of dilution).

The values of the interaction constants have been taken, as in (Ref. 13), from Vettier's work.[14] As we have discussed in (Ref. 13), those values have been obtained fitting experimental data to a Hamiltonian which is different from Eq. (1). Thus, the relevant quantities are the ratios of the interaction constants and not their absolute values. To simplify comparison with experimental results, we have normalized these constants in the following way. We have performed simulations on the pure system varying the values of the interaction constants but keeping their ratios fixed, until we reproduced the value of T_N given by Vettier.[14] Hence, we have a ferromagnetic (NN) interaction $J_1/k_B = 6.74$ K, in competition with a frustrated antiferromagnetic (NNN) one $J_2/k_B = -1.01$ K and a superexchange antiferromagnetic interplane interaction $J'/k_B = -0.07$ K.

In the following we will use the notation,

$$h = \frac{g\mu_B H}{k_B} \ .$$

The studied quantities are global magnetization per site m, staggered magnetization along the **c** axis m_{st}, energy per site E, specific heat c, susceptibility χ, staggered susceptibility χ_{st}, and the Edwards-Anderson order parameter q. We also keep the last configuration of the lattice obtained at each point of the (T,h,x) space for further analysis.

III. TECHNICAL DETAILS

According to the $FeCl_2$ structure,[15] we have studied a system consisting of N_k triangular lattice planes of $N_i \times N_j$ sites each, stacked along the **c** axis, with full periodic boundary conditions. We have taken, in general, $N_i = N_j = 18$ and we have increased N_k with dilution; 12, 18, and 24 planes were considered for $x = 0.9$, 0.8, and 0.7, respectively. For the diluted system, the threshold field value of the antiferromagnetic to saturated paramagnetic phase transition at zero temperature cannot be calculated exactly, but it may be estimated in a mean-field approach by $h_0(x) = x h_0(x = 1)$.

To study the irreversibilities that have been experimentally found we have simulated different kinds of processes. To simulate a FH (FC) process, for low fields compared to $h_0(x)$, we start the simulation with antiferromagnetic (random) initial conditions and we raise (lower) temperature T, always taking the output at T as the input for $T + \Delta T$ ($T - \Delta T$). For values of the applied field comparable to or higher than $h_0(x)$, it is not obvious that the right initial condition is the antiferromagnetic one. In those cases, a zero-field-cooled (ZFC) process was simulated, to obtain the initial condition for the FH process at such a field.

From previous results on the pure system,[13,14] we know that FH and FC processes are not suitable to study critical phenomena in the low-T region, as the critical line $h_c(T)$ is expected to be more or less parallel to the T axis. We have verified that large fluctuations prevent a correct determination of the critical line. Hence, to study this region, we have performed isothermal processes, raising ($h \uparrow$) and lowering ($h \downarrow$) the applied field.

To study equilibrium properties we have used, in general, 5000 Monte Carlo steps per site (MCS/s) to compute averages after equilibrating over 5000 MCS/s. To test equilibration, some longer runs have been made for the biggest system in the critical region.

On the other hand, when investigating nonequilibrium effects, shorter runs to avoid rapid equilibration due to finite size,[5] have been made.

A. The "plane-flip" algorithm

We have observed that, while performing simulations of FC or $h \downarrow$ processes, the system may get trapped in a spurious state. The open and solid circle curves of Fig. 1 show the staggered magnetization obtained in a FC+FH cycle, for a value of field comparable to $h_0(x = 0.9)$. It is clear that the system cannot reach the antiferromagnetic state in FC, but gets frozen in a state having $|m_{st}| \neq 1$. On the other hand, during the FH process (solid circles), as soon as the thermal energy is high enough, the system goes into the antiferromagnetic state before the transition

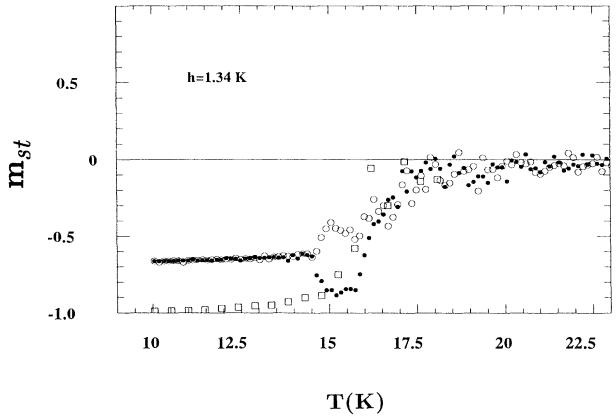

FIG. 1. $x=0.9$; m_{st} vs T curves in a constant field near $h_0(x=0.9)$. (○) FC and (●) FH curves obtained with standard Glauber dynamics. (□) FC curve obtained with plan-flip algorithm. In this case the antiferromagnetic state is reached.

to the paramagnetic state occurs.

Looking at the configurations corresponding to the FC frozen state, we observed that the low absolute value of m_{st} does not correspond to a domain state. On the contrary, ferromagnetic ordering was established in the plane but a stacking fault effect in the magnetic ordering along the **c** axis was observed.

The explanation of such a phenomenon is quite simple. As a FC process starts from high temperatures, we start the simulation from random initial conditions. Due to the high anisotropy of the system, the ferromagnetic in-plane order is the first to develop and so the system must choose which plane is going to be ordered parallel (+ plane) and which one antiparallel (− plane) to the applied field. Provided that during the Monte Carlo process a statistical mistake occurs, giving two neighboring planes parallel to the field, it will be very difficult to overcome in the following run (note that it costs a lot of energy to turn a single spin belonging to a ferromagnetically ordered + plane). This fact becomes enhanced as the temperature is lowered.

This kind of effect had also been observed in the pure system during a $h\downarrow$ process,[13] but in that case it could be avoided by taking smaller Δh steps. This is not the case for the diluted system. We have then modified the standard Glauber dynamics in the spirit of cluster algorithms.[16] As we are concerned with a layered system, we took the whole plane as the cluster to flip. Thus, during the equilibration process the flipping of a whole plane is proposed as a local change every t MCS/s (t being a parameter to determine in each case) and it is accepted or not according to standard Monte Carlo rules. The squares curve of Fig. 1 corresponds to a FC process obtained with the plan-flip algorithm. It is clear that the antiferromagnetic state is reached, even though the ΔT step is bigger than the one considered for standard Glauber dynamics. Notice that the plan-flip algorithm allows for changes of a plane as a whole; then the intra-plane exchange energy need not be raised to overcome an eventual statistical mistake.

IV. ANALYSIS OF RESULTS

We start discussing the results obtained for the lowest studied concentration of magnetic ions, $x=0.7$. Then, we will analyze the changes observed as the concentration varies from the pure system to $x=0.7$. In general, the lines shown in the figures are only a guide to the eye.

A. Concentration $x=0.7$

For this system we have studied three samples with a different distribution of quenched disorder so as to be sure that our results are not affected by a particular anomalous distribution of vacancies. Averaging over a number n_s of samples has been intentionally avoided so as not to wash out fluctuations that might be revealing, as we will see later, of the behavior of the system.

The approximated threshold magnetic field for the antiferromagnetic to saturated paramagnetic transition at $T=0$ K is $h_0(x=0.7)=1.17$ K and, Neél temperature, determined by a FH process in zero field, is $T_N=14$ K.

Compared to these values we have divided the (T,h) plane into two regions: low fields and high temperatures and high fields and low temperatures. As explained above, to avoid large critical fluctuations, different processes were used in each region.

1. High-temperature region

To determine the critical line in this region we performed equilibrated FH+FC cycles. Figure 2 shows the cycle of the staggered magnetization as a function of T, for two values of the applied field. We can clearly see that the transition is continuous and that the critical temperature obtained in FH is equal to that determined by a FC process. It is also interesting to note that for very low fields [Fig. 2(a)] the system chooses the antiferromagnetic state with a staggered magnetization of opposite sign to the one we have chosen as the initial condition of the FH process. The reason for this is that the coupling between the global magnetization (due to a possible statistical unbalance of vacancies in each sublattice) and the applied field is too weak to break the symmetry of the antiferromagnetic state. This is not the case for higher fields [Fig. 2(b)] where the system chooses, in this case, the same sign of m_{st} we have chosen as the initial antiferromagnetic condition. We confirmed this behavior while studying other samples: the system always chooses (except for the lowest fields) to establish an antiferromagnetic ordering in FC with the sublattice having the smallest number of vacancies parallel to the field.

We have found that the energy of the FC state is equal to the energy of the FH state, confirming that antiferromagnetic state is the LRO issued from a FC process.

As the applied field approaches $h_0(x=0.7)$, large fluctuations are observed while cycling at constant field. Then, to study this region of the phase diagram we have performed isothermal field cycles.

2. Low-temperature region

One of the topics still under discussion is the existence of a tricritical point once dilution has been considered.

Our results show that in this region the transition stays first order down to at least $x=0.7$.

Figure 3 shows the evolution of the hysteresis cycle with temperature. For low T [Fig. 3(a)] we can observe that, while the $h\uparrow$ curve has a continuous aspect with some plateaus, the $h\downarrow$ one is clearly discontinuous. This continuous aspect is a clear consequence of dilution. In the $h\uparrow$ process, the spins in the $-$ planes that are surrounded by vacancies may easily follow the applied field, giving rise to a soft rearrangement of the system. On the other hand, in a $h\downarrow$ process we start with a ferromagnetic initial condition and though dilution is always present, there is no random-field effect.[17] The transition takes place by inversion of the whole plane as was the case for the pure system.

As the cycle is performed at higher T, saturation in $h\uparrow$ processes is obtained as expected, for lower fields. For $T=7$ K the curves corresponding to $h\uparrow$ and $h\downarrow$ processes start crossing, showing the disappearance of hysteresis.

Figure 4 shows the cycle of energy corresponding to the isothermal loop at $T=5$ K of Fig. 3(a). It is clear that the parts of the $h\uparrow$ magnetization curves showing a continuous aspect at low T correspond to unstable states;

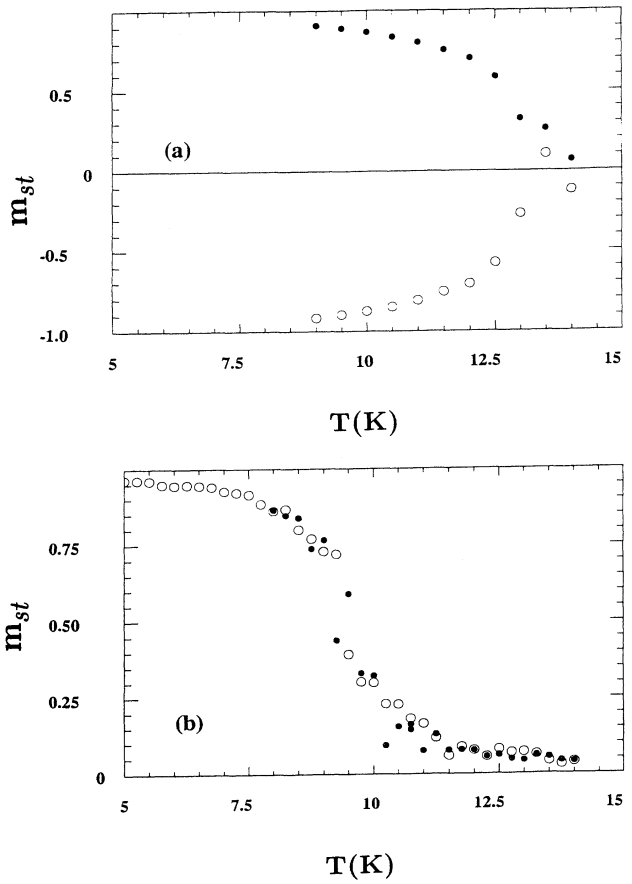

FIG. 2. Equilibrated FH (●) + FC (○) cycles of the order parameter for two values of the field $h<h_0(x=0.7)=1.17$ K. (a) $h=0.25$ K and (b) $h=1$ K. The critical temperature obtained in FH is the same as the one obtained in FC.

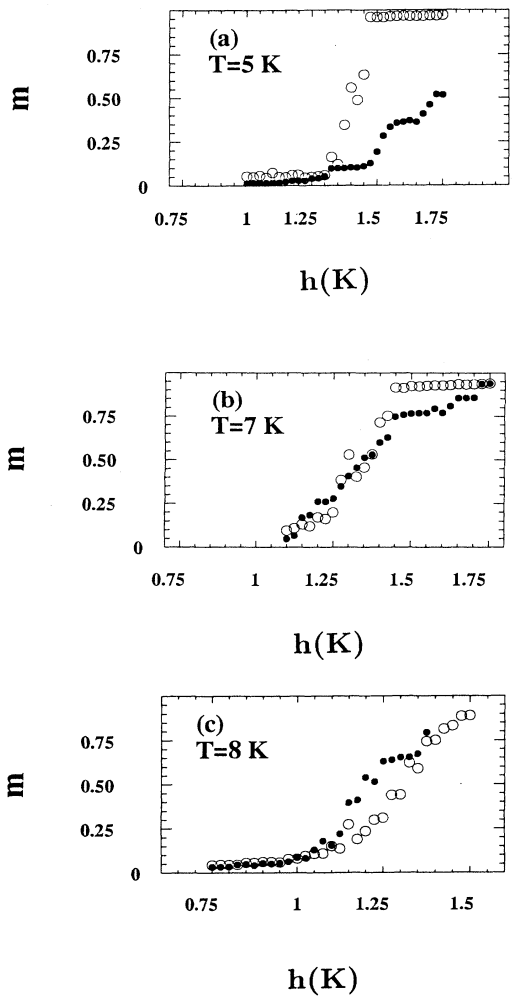

FIG. 3. $x=0.7$. Hysteresis loops for different values of $T\rightarrow T_t^-$. (●) $h\uparrow$, (○) $h\downarrow$. The $h\uparrow$ curve looks continuous for low T and difficult to saturate. (a) $T=5$ K, (b) $T=7$ K, (c) $T=8$ K.

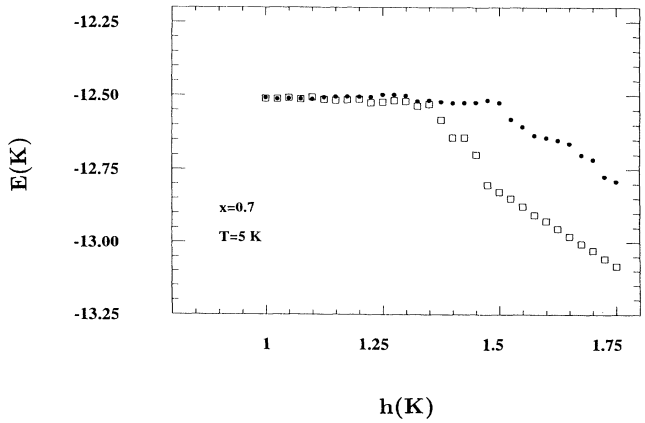

FIG. 4. $x=0.7$. $E(h)|_T$ loop for $T=5$ K corresponding to the magnetization loop of Fig. 3. It is clearly seen that the $h\uparrow$ branch of the hysteresis loop is unstable for $h>1.35$ K.

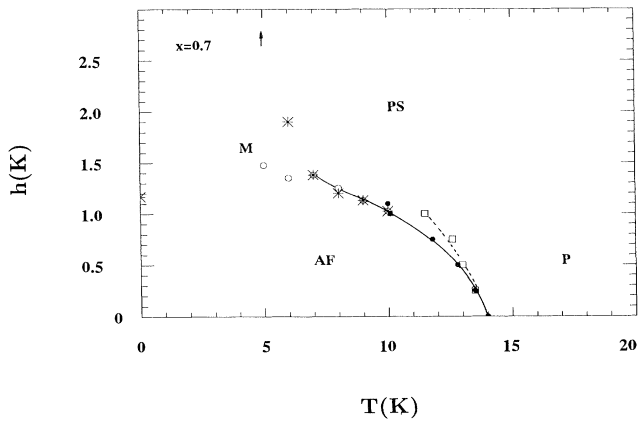

FIG. 5. Phase diagram for $x=0.7$, AF: antiferromagnetic phase, PS: saturated paramagnetic phase, P: paramagnetic phase, M: mixed region. (●) FH, (□) irreversibility line $T_{irr}(h)$ found in FC, (*) $h\uparrow$,(○) $h\downarrow$. The arrow indicates that saturation is found at higher fields.

the curve corresponding to the $h\uparrow$ process at $T=5$ K becomes unstable for $h>1.35$ K.

As for the pure case, we have determined the TCP as the point where hysteresis fades away. We obtain $T_t\approx 7$ K and a ratio $T_t/T_N\approx 0.5$.

We have also examined some of the configurations obtained in this region. We have found, as expected for a first-order transition, a coexistence of the two phases entering the transition; some planes are arranged antiferromagnetically and others in the saturated paramagnetic phase.

Figure 5 shows the phase diagram corresponding to $x=0.7$; the squares correspond to the irreversibility line that is discussed in the following paragraph.

3. *Study of irreversibilities in FH+FC cycles*

To search for the irreversibilities experimentally observed in FH+FC cycles on a finite system, we have performed shorter runs; 100 MCS/s for averaging after equilibrating over other 100 MCS/s.

Our results show that the cycle is completely reversible for low fields [Fig. 6(a)], but as it approaches the corresponding $h_0(x)$ value, irreversible phenomena appear [see Figs. 6(b) and 6(c)]. Calling T_{irr} the temperature where m_{FC} becomes different from m_{FH}, we obtain a line of irreversibilities that lies on the critical line $T_c(h)$ for low values of the applied field, but lies above it as the field increases. This result is in excellent agreement with experiments.[12] A similar $T_{irr}(h)$ line had been obtained by Monte Carlo simulation on a completely spatially isotropic model containing only NN interactions, but in this case there was no coincidence of both lines at low fields.[8]

We have studied the shape of the magnetic domains formed in the irreversibility region. As expected, the domains here are antiferromagnetic along the **c** axis but are ferromagnetically ordered in the plane. These

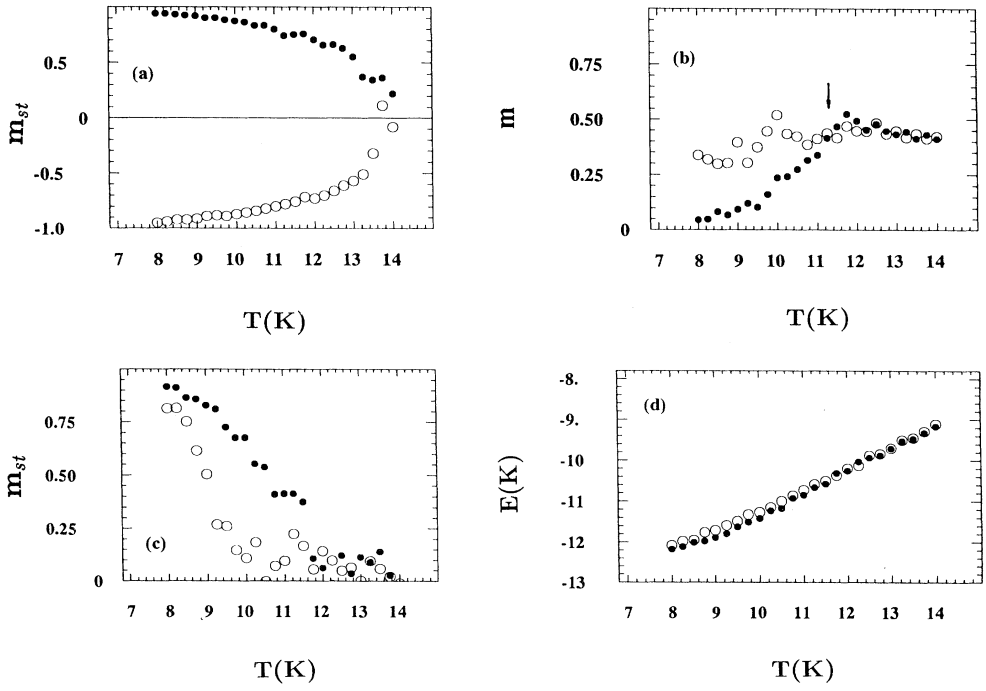

FIG. 6. Study of irreversibilities in a FH (●)+FC (○) process. (a) Low-field region: $h=0.25$ K. Order parameter as a function of temperature. (b) $m(T)|_h$ curve for $h=1$ K $\approx h_0(x=0.7)$. The arrow shows the point where $m_{FC}>m_{FH}$. (c) $m_{st}(T)|_h$ curve for $h=1$ K $\approx h_0(x=0.7)$. The antiferromagnetic LRO starts to develop in FC at a temperature which is lower than $T_c(h)$ obtained in FH. (d) $E(T)|_h$ curves for $h=1$ K. The energy per spin obtained in FC is not much higher than the one corresponding to the FH process due to the fact that the systems take advantage of the vacancies to establish the domain walls.

domains with their sublattices oriented in the opposite sense, are situated one beside the other as shown in Fig. 7. The explanation for this is that + clusters appear in − planes taking advantage of vacancies so as to lower energy, increasing the Zeeman term without losing exchange energy in the plane (in fact, there is also a small gain in second-neighbor exchange energy). Complementarily, as thermal energy is important in this region, some − clusters may appear, in the same way, in the + planes, compensating for the lost Zeeman term by the interplane exchange gain. The example shown in Fig. 7 has been obtained from a FC run at $T=11.25$ K and $h=1$ K. In this case there is an excess of + clusters caused by the orientation of the system with the sublattice having the highest concentration of spins parallel to the field and the existence of bigger + clusters in − planes (compared to the smaller − clusters in + planes) caused by the joint action of the field and the thermal energy. This effect may explain the experimental result $m_{FC} > m_{FH}$.[12]

Figure 6(d) shows that the fact of breaking into domains does not cause a great increase in the energy per spin. The reason for this is that the system takes advantage of vacancies to create the domain walls in the plane.

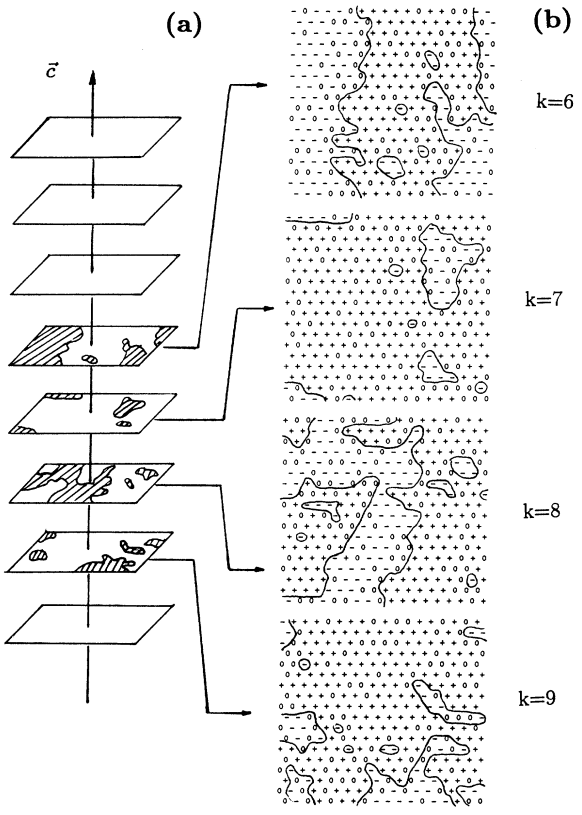

FIG. 7. Antiferromagnetic domains formed in the irreversibility region of the phase diagram. (a) shows schematically the 3D arrangement of the domains. (b) shows four adjacent planes (k is the index of the planes) issued from a FC run at $T=11.25$ K, $h=1$ K. Notice how the domain walls take advantage of vacancies to avoid losing too much intraplan exchange energy.

B. From pure system to $x=0.7$

We have performed the same kind of study we have just described for $x=0.8$ and for $x=0.9$. We will only discuss here the changes observed in the phase diagram and in the studied physical quantities as a function of dilution.

It is well known that for the RFIM, the specific-heat peak tends to disappear as the applied field increases.[18,19] Our results show, as expected, the same kind of behavior (Fig. 8). Notice that this is not the case for the pure system [Fig. 8(a)]. In addition, the same effect can be observed looking at a given value of the field and increasing dilution; the specific-heat peak also tends to disappear because of the smaller relative distance to the corresponding $h_0(x)$ value.

Another important difference with the pure case is found in the way to approach the TCP. In the pure system, we observed (Ref. 20) a clear difference in isothermal magnetization or staggered magnetization curves as a function of the field [$m(h)|_T$ or $m_{st}(h)|_T$] according to the region where the $h\uparrow$ process is performed. For instance, the fall of the $m_{st}(h)|_T$ curve becomes sharper as the process is performed at $T\rightarrow T_t^+$, and no difference is found as the process is performed at $T\rightarrow T_t^-$. Dilution modifies this kind of behavior, as has already been discussed for $x=0.7$. Figure 9 shows the evolution of hysteresis cycles in the low-temperature region as a function of dilution. We can see that the $h\uparrow$ curves look much more continuous as dilution increases. We have explained this in terms of clusters of spins surrounded by vacancies that can easily follow the rising field, giving start to a soft rearrangement of the system until saturation. In the case of $x=0.9$ [Fig. 9(b)] the small amount of vacancies in the system prevents this soft rearrangement from taking place and the system keeps its antiferromagnetic state until h is very near the transition value, similar to what happens in the pure case. However, the existence of some vacancies is responsible for the steps observed in the $h\uparrow$ curve.

On the other hand, the $h\downarrow$ curves are always discontinuous as, because of the ferromagnetic initial condition, no random-field effect is present, regardless of the amount of dilution.

Figure 10 shows cuts of the phase diagram (T,h,x) with planes $x=1,0.9,0.8$. The decrease of hysteresis width with dilution may be observed. The region between the hysteresis branches, denoted by M (mixed region), corresponds to the coexistence of the antiferromagnetic and ferromagnetic phases. The FC equilibrium line is coincident with the FH critical line.

We can also observe that T_t as well as T_N are shifted to lower temperatures as dilution is increased. This result is in quantitative agreement with experimental measurements of $T_t(x)$ (Ref. 21) and $T_N(x)$ (Ref. 23) as is shown in Table I. Recall that the values of the interaction constants correspond to Vettier's work[14] so an exact agreement in the values of absolute quantities cannot be expected. There are a few systematic measurements of the shift of T_t (Ref. 21) and T_N (Ref. 23) with dilution and, as each one has been performed on a different sample, calcu-

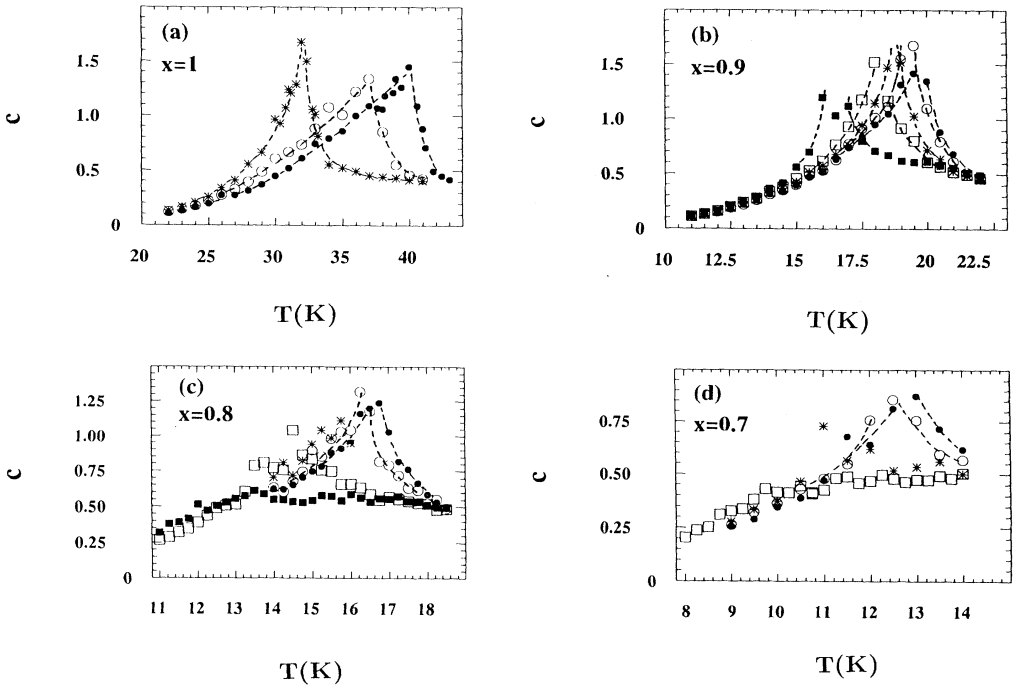

FIG. 8. Evolution of the specific-heat peak with dilution and field. (a) $x=1$, (●) $h=9$ K, (○) $h=10$ K, (*) $h=11$ K. Data issued from $h\uparrow$ using non-normalized interaction constants: $J_1/k_B=10$ K, $J_2/k_B=-1.5$ K, $J'/k_B=-0.5$ K (Ref. 13). (b) $x=0.9$; (●) $h=0.25$ K, (○) $h=0.5$ K, (*) $h=0.75$ K, (□) $h=1$ K (■) $h=1.25$ K. (c) $x=0.8$, (●) $h=0.25$ K, (○) $h=0.5$ K, (*) $h=0.75$ K, (□) $h=1$ K, (■) $h=1.25$ K. (d) $x=0.7$, (●) $h=0.25$ K, (○) $h=0.5$ K, (*) $h=0.75$ K, (□)$h=1$ K.

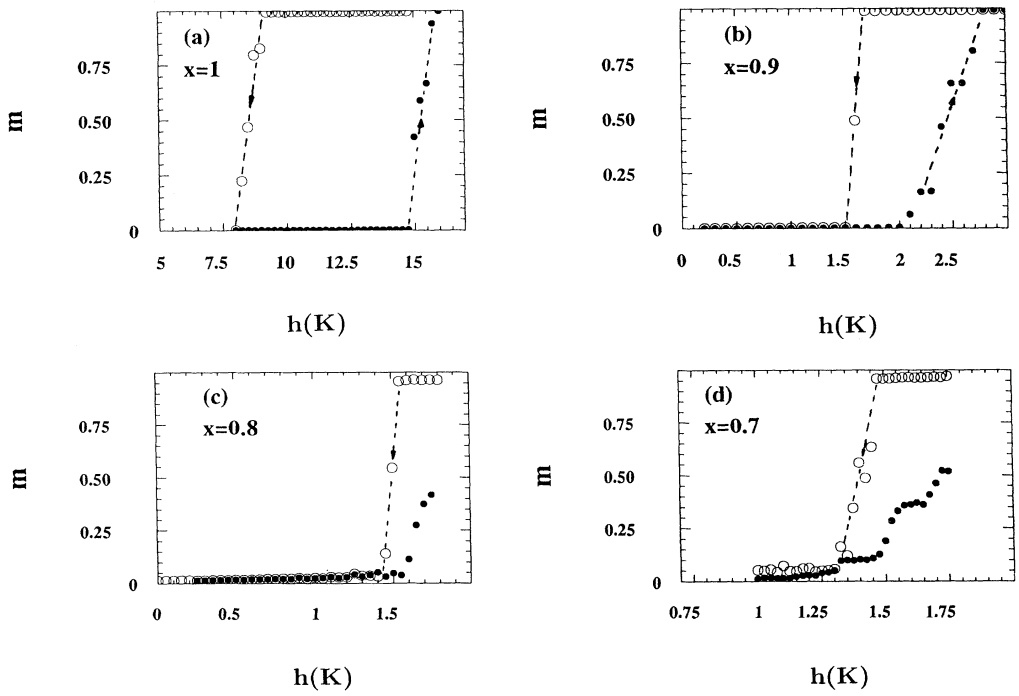

FIG. 9. Evolution of hysteresis loops with dilution in the low-T region. (●) $h\uparrow$ curves become continuous as dilution increases; (○) $h\downarrow$ curves are always discontinuous. (a) $x=1$; data corresponding to the interaction constants indicated in Fig. 8, (b) $x=0.9$, (c) $x=0.8$, (d) $x=0.7$.

lating the ratios of these two temperatures may be misleading.

Finally, Fig. 11 shows the 3D equilibrium phase diagrams. For the sake of clarity, we have split this figure into two parts: (a) corresponds to $h\uparrow$ and FH data in the low- and high-temperature region, respectively, and (b) corresponds to $h\downarrow$ and FH data. Again, to compare this phase diagram with experimental results, we have to consider different works. The experimental determination of the TCP has been performed in a different way to the one chosen in this work. Induced light scattering is used to study the first-order region. The values of the field H_1 and H_2, where scattering begins and ends when varying the field isothermally, are taken as the limit of the mixed phase region. The gap between these fields decreases with increasing temperature, and the TCP is determined as the point where these two values collapse. On the other hand, hysteresis effects have been measured, overimposed to the described scattering, for very low temperatures ($T<4$ K) (Ref. 24). As far as we know, no systematic measurement of hysteresis loops have been done as $T\rightarrow T_t^-$. It would be very interesting to perform such experiments to test whether hysteresis disappears at the same point found by Wood and Day for the collapse of $H_1(T)$ and $H_2(T)$. The comparison between T_t values found in that work and the T_t values found here seems to suggest that this may be the case.

TABLE I. Variation of T_t and T_N as a function of dilution. Comparison with experimental values (a) Wood *et al.* (Ref. 22) and (b) Bertrand *et al.* (Ref. 23).

X	T_t^{expt} (K)[a]	T_t^{MC} (K)	T_N^{expt} (K)[(b)]	T_N^{MC} (K)
1	20.5	19.9	24	22.9
0.9	16.5	15	20.5	20
0.8	13	12	17.6	16.75
0.7	8	7	13.6	14

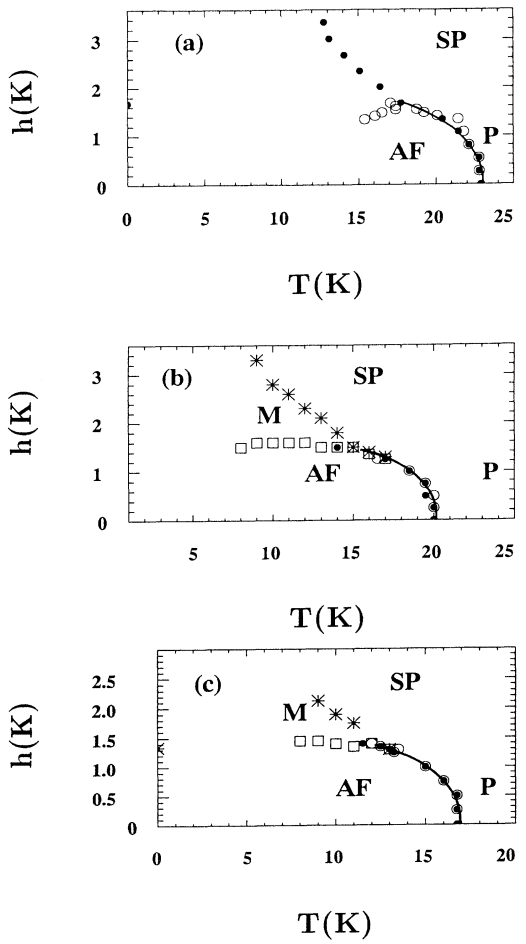

FIG. 10. Detailed cuts of the phase diagram along planes $x=cte$. **AF**: antiferromagnetic phase, **SP**: saturated paramagnetic phase, P: paramagnetic phase, M: mixed region. (a) $x=1$, (●) $h\uparrow$, (○) $h\downarrow$. (b) $x=0.9$, (●) FH, (○) FC, (□) $h\downarrow$, (*) $h\uparrow$, (□) $h\downarrow$. (c) $x=0.8$, (●) FH, (○) FC, (*) $h\uparrow$.

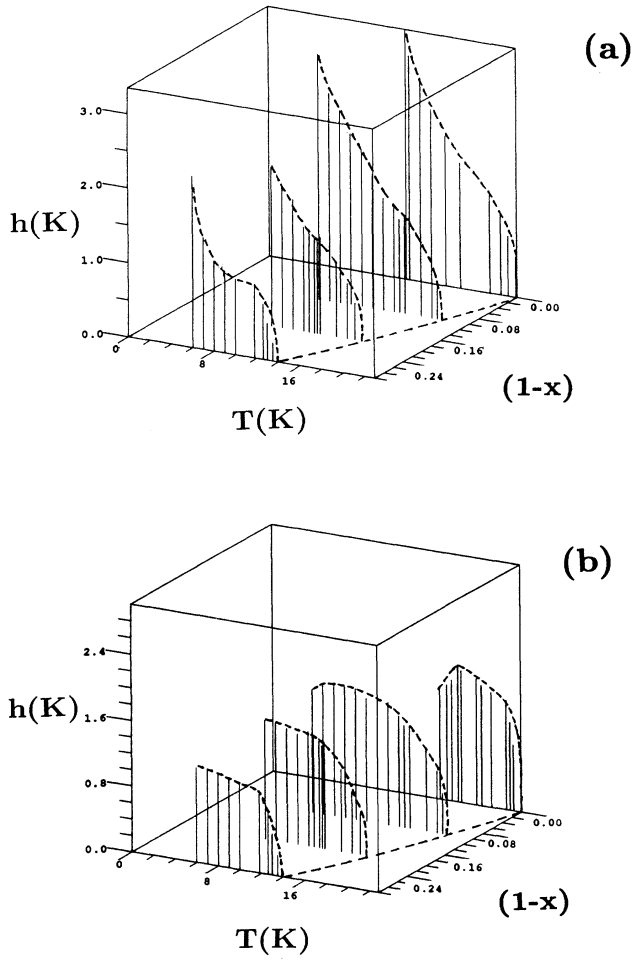

FIG. 11. 3D phase diagram. For the sake of clarity, only FH and $h\uparrow$ lines are drawn in (a) and FC and $h\downarrow$ lines in (b). Recall that FC and FH equilibrium processes give the same value of $T_c(h)$ for $h<h_0(x)$. This diagram may be compared with results given in Refs. 22, 23, and 24.

V. CONCLUSIONS

We have performed a Monte Carlo study of critical behavior of a quite realistic model of $Fe_xMg_{1-x}Cl_2$.

We have determined the phase diagram of the system in the space (T,h,x) with $x=0.9,0.8,0.7$. Our results show the existence of a TCP that is shifted to low temperatures as dilution increases. The values obtained for T_t as well as those obtained for T_N compare quite well with experimental ones.[21,23] The width of the hysteresis cycle is also found to decrease with dilution.

We have found that the stable LRO at low T and $h<h_0(x)$ is the antiferromagnetic phase and that the equilibrium cycles FH+FC are reversible for all values of $h<h_0(x)$. For $h>h_0(x)$, LRO is not reached in a FC process.

On the other hand, while studying fast FH+FC cycles to simulate, on a finite system, the long relaxation times observed experimentally, we have found that for low fields, the cycle is still reversible, while for $h\sim h_0(x)$, irreversibilities appear giving rise to $m_{FC}>m_{FH}$, in agreement with experimental results.[12] The irreversibility line T_{irr}, defined as the lowest temperature where $m_{FC}=m_{FH}$, is coincident with $T_c(h)$ for low fields, lies above it as the field approaches $h_0(x)$, in agreement again with experimental measurements.

We have also investigated the shape of the magnetic domains formed in the irreversible region. The microscopic description obtained seems consistent with results issued from Faraday microscopy.[24]

Recent Faraday rotation measurements on $Fe_xMg_{1-x}Cl_2$, have shown different domain patterns at a given point of the phase diagram, according to the process used to carry the system to that point. Simulation of this experiment would prove very interesting as it would allow us to study, simultaneously, the 2D Faraday rotation pattern along with the 3D structure of such domains. This simulation will need an increase in the system size in the directions perpendicular to the **c** axis, as it is necessary to change to a mesoscopic scale to observe such patterns.

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