# Interface roughening and domain growth in the dilute Ising model

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We have studied domain growth in the two-dimensional dilute Ising model following an instantaneous quench from a very high temperature to a temperature below the critical point. We have carried out Monte Carlo simulations of system sizes up to $600^2$ out to a maximum of 20 000 Monte Carlo steps per spin. We have interpreted the crossover from the curvature-driven regime to a new growth regime in the light of a phenomenological theory that describes the impurity roughening of the interface between the two phases.

The static equilibrium properties of the dilute Ising model have been studied extensively for several years.[1] The site-diluted Ising model is defined as

$$\mathcal{H}=-J\sum_i c_i c_j S_i S_j \ , \tag{1}$$

where $S_i$ and $S_j$ are the Ising spins at the lattice sites $\mathbf{r}_i$ and $\mathbf{r}_j$ and the random occupation variables take the values $c_i=1$ if the site $\mathbf{r}_i$ is occupied by a spin and zero otherwise. Therefore, the average concentration of the spins in the system is given by

$$p=\lim_{\mathcal{N}\to\infty}(1/\mathcal{N})\sum_{i=1}^{\mathcal{N}} c_i \ .$$

Note that the randomness in the site-diluted model lies in the local occupation, in contrast to bond randomness which leads to the bond-diluted Ising model. Recently, the dynamics of the dilute Ising models (DIM) have attracted attention. Both analytical arguments[2–5] and computer simulation[6–11] have shown the breakdown of dynamical scaling in the DIM. We note here that the latter scaling is dynamical scaling in the usual sense of the term used in equilibrium critical phenomena.[12]

The randomness in the DIM, albeit local, is quite different from that in the random-field Ising model[13–15] because the random field in the latter model is conjugate to the corresponding order parameter. Monte Carlo simulation of the early-time domain growth of the latter model[16,17] following a rapid quench from a high-temperature equilibrium state to a low-temperature unstable state established the breakdown of the so-called self-similar dynamical scaling[18,19] in agreement with the theoretical prediction of Grant and Gunton.[20,21] (The latter dynamical scaling describes the dynamical evolution in a system far from equilibrium with a time-dependent characteristic length scale, and should not be confused with the dynamical scaling in critical phenomena where the correlation length is time independent.) The dynamical scaling in nonequilibrium systems is associated with a power-law growth of the domains following a quench from a very high temperature $T_i$ to a low temperature $T_f$ below the critical point, i.e.,

$$R(t)\sim t^n \ , \tag{2}$$

where $R(t)$ is a length scale characterizing the average size of the domains at time $t$.

Stimulated by these interesting recent developments, we have investigated the phenomenon of the early-time domain growth in the DIM following an instantaneous quench from a high-temperature equilibrium state. Some aspects of the latter problem has been addressed earlier by Huse and Henley[22] and by Grest and Srolovitz.[23] Huse and Henley numerically investigated the roughening of the interfaces between the two phases in the DIM and concluded that in $d=2$ the transverse deviation from a straight line of a segment of interface of length $L$ scales as $L^{2/3}$. Moreover, arguing that the late-stage growth is a thermally activated process, they also predicted logarithmically slow growth, in contrast to the usual power-law growth (2). This prediction is in qualitative agreement with the Monte Carlo (MC) data of Grest and Srolovitz. In this paper we investigate the domain-growth law in the two-dimensional site-diluted Ising model in the early and intermediate time regimes by MC simulation. Then, from phenomenological arguments we predict the dependence of the crossover time $t^*$ on the concentration $c$ of the spins in the system. We find that this prediction is in reasonable qualitative agreement with our MC data.

There is no unique definition of the "characteristic length scale" in the literature. However, if scaling holds, any physically sensible length scale is acceptable as long as one is interested only in the universal properties. Grest and Srolovitz used the definition

$$R_E(t)=-E_0/[E(t)-E_0] \ ,$$

where $E(t)$ is the average energy of the system at time $t$ and $E_0$ is the equilibrium energy at $T=T_f$. However, it has been observed recently that using the ground-state energy instead of the equilibrium energy, as has often been done in the past, leads to large errors. On the other hand, Sadiq and Binder[24] prescribed a length scale in terms of the fluctuations of the order parameter in an $N$-spin system, viz.,

$$R_m^2(t)=N\left\langle\left[(1/N)\sum_i S_i\right]^2\right\rangle \ . \tag{3}$$

It is now well established that in the scaling regime the large sample-to-sample fluctuations[25] are equally severe

 

for $R_m(t)$ and $R_E(t)$, though less severe for $E(t)$ itself. However, $R_m(t)$ has the advantage over $R_E$ in that the former can be compared directly with the experimental data on the maximum peak height obtained from scattering experiments. Therefore, we have computed $R_m$ for the DIM.

For most of the simulations up to 1000 MC steps (MCS) we have used a modified version of the algorithm developed by Chowdhury and Stauffer[10,11] for the simulation of large samples of the dilute Ising model. Some runs up to 20 000 MCS were carried out with FPS 264 computers at the Center for Advanced Computational Science at the Temple University. In order to avoid any unwanted correlation in the dynamical evolution of the spins, we have picked up the spins randomly for updating rather than using sequential updating. The size of the

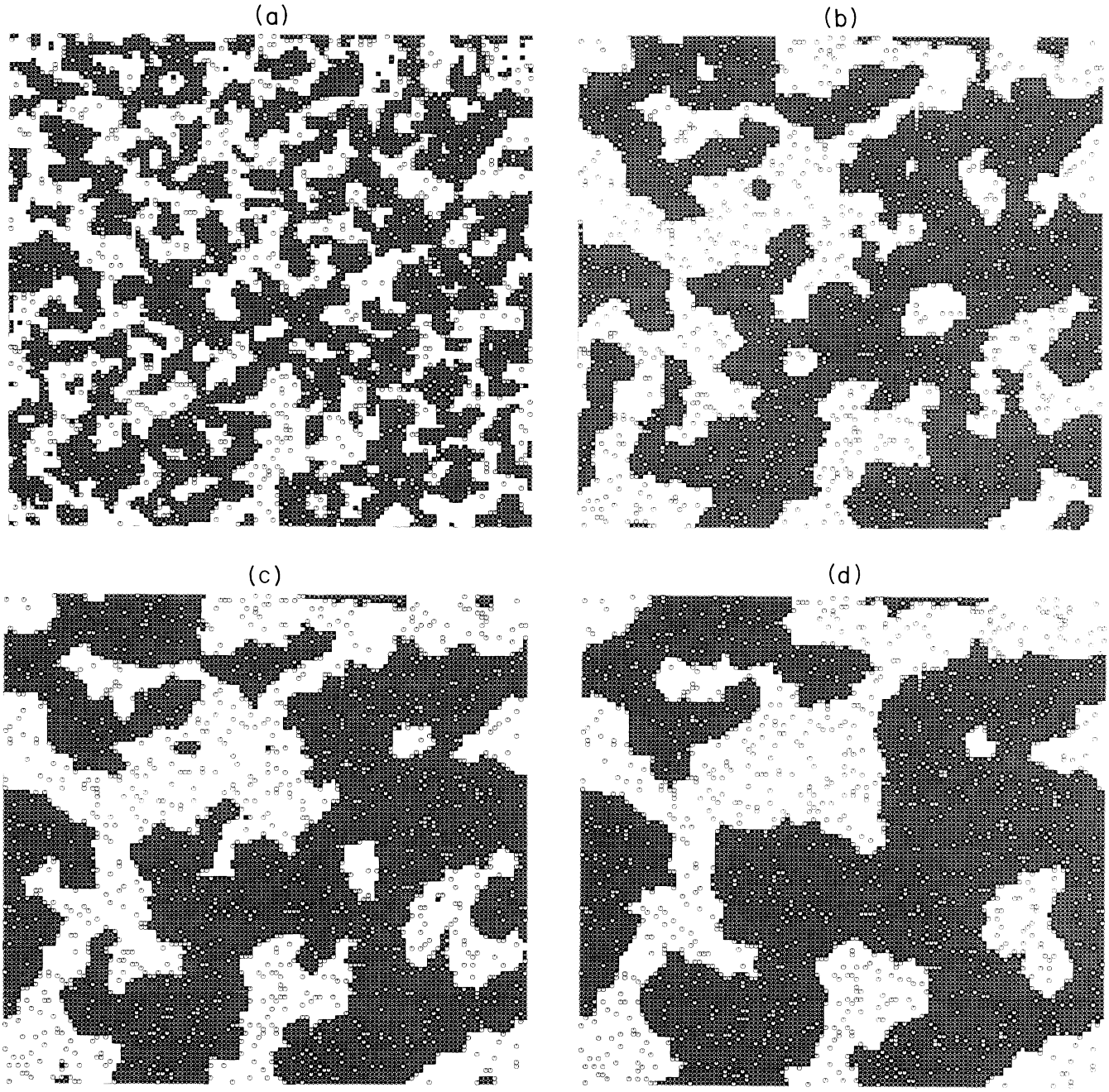


FIG. 1. Four typical configurations of a $120\times120$ sample of the DIM for $p=0.90$ at $T_f 0.35T_c$ ($p=1$) are shown at (a) $t=5$ MCS, (b) $t=50$ MCS, (c) $t=100$ MCS, and (d) $t=250$ MCS. The empty circles correspond to the vacant sites, the symbols * represent the "up" spins and the white portion of the figure correspond to the down spins.

samples of the DIM studied were $600 \times 600$. The samples were quenched from infinitely high temperatures (corresponding to random orientations of the spins) to a temperature $T \simeq T_c/2$. The time evolution of a typical configuration of the DIM is shown in Fig. 1. We computed the quantity $R_m^2$ at every MCS following the quench for a given dilution. We have averaged our data over a large number, $N_q$, of quenches, as shown in Fig. 2. The corresponding data are shown in Figs. 2 and 3. Note that the growth is (approximately) linear over an initial period of time and then crosses over to a different behavior at a time $t^*$ which depends on the concentration of the spins $p$. Also note that $t^*$ decreases with decreasing $p$. At a mean-field level one can understand the $p$ dependence of $t^*$ in the following way. The greater is the dilution, the smaller is the average interimpurity separation and, hence, the hindrance due to the impurities is felt at an earlier stage of evolution. However, such an argument ignores the most crucial feature of the problem, namely, fluctuation of the exchange interaction, as we discuss next.

In order to interpret our Monte Carlo data we present a phenomenological argument based on the roughening of the interface of the domains by the impurities,[22,26,27] taking the fluctuation of the exchange bonds into account. To do this we first discuss the case for the random-bond (rather than our random site-dilution) Ising model. Consider a situation shown in Fig. 4, in which a segment of the surface of a domain of characteristic radius $R$ has

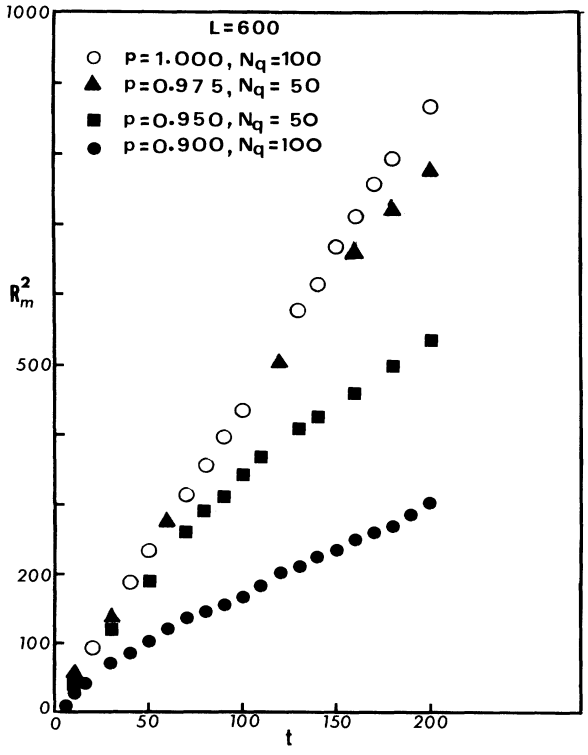


FIG. 2. $R_m^2$ for various $p$ in the DIM are shown as function of $t$.

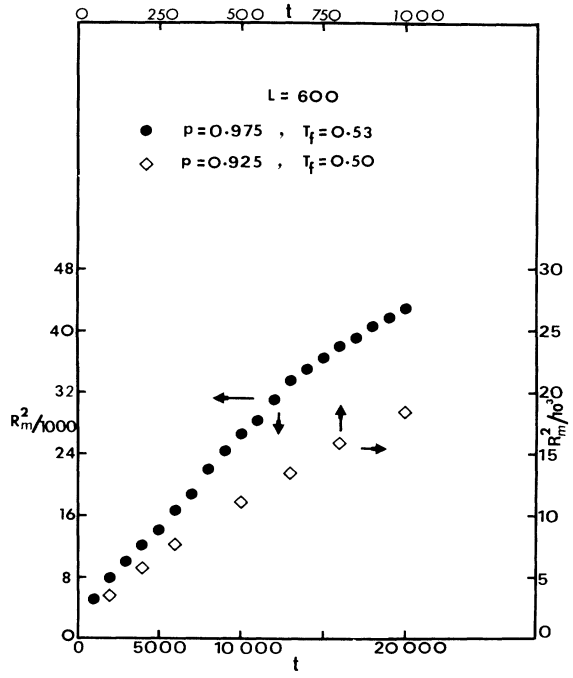


FIG. 3. Same as Fig. 2, but for different $p$ values and up to a longer time.

been roughened. The thermally induced roughening becomes significant when[28]

$$g(w^2/b) \sim 1 , \tag{4}$$

with $g$ proportional to the exchange constant $J$, i.e., when

$$w \sim b^{1/2}/g^{1/2} . \tag{4a}$$

On the other hand, impurity-induced roughening becomes dominant when[22,26,27]

$$g(w^2/b) \sim \sigma w^{1/2} , \tag{5}$$

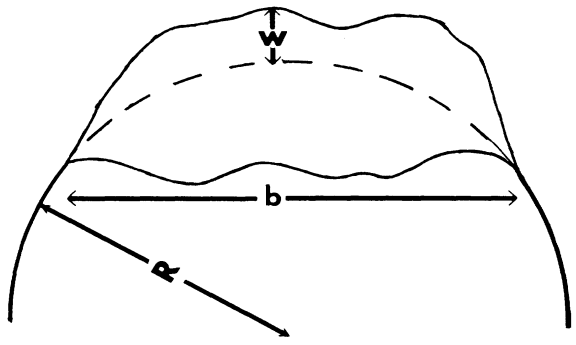


FIG. 4. Schematic representation of the interface roughening in the DIM in continuum. The dashed curve represents a smooth interface of a circular domain of radius $R$, whereas the complete curve describes a rough interface. The width and the breadth of the interface are $w$ and $b$, respectively.

i.e., when

$$w \sim (\sigma^{2/3}/g^{2/3})b^{2/3} \tag{5a}$$

where $\sigma$ is the variance of the random exchange bonds. In order to describe the crossover from the thermally induced roughening to the impurity-induced roughening, we propose the scaling form

$$w \sim (1/g^{1/2})b^{1/2} f(b/\xi) \tag{6}$$

where $\xi$ is a crossover length which will be determined below. In the limit $x \to 0$, $f(x) \to$ const, so that (6) reduces to (4a) for $b \ll \xi$. In order to recover (5a) from (6) in the limit $b \gg \xi$ we must have

$$\lim_{b \gg \xi} f(b/\xi) \sim b^{1/6}/\xi^{1/6} . \tag{7}$$

Substituting (7) into (6) we get

$$w \sim b^{2/3}/(g^{1/2}\xi^{1/6}) \quad \text{for } b \gg \xi . \tag{8}$$

Comparing (8) with (5a), we obtain

$$\xi \sim g^3/\sigma^4 . \tag{9}$$

The argument given above for the random-bond model can be taken over completely for our problem with the understanding that the variance $\sigma$ now arises from the site dilution and depends on the concentration $p$. In the concentration regime we are interested in, the impurity concentration is very small and hence, on the average, the impurity sites can be assumed to be effectively isolated from each other. Under such circumstances removing one site is equivalent to removing the four bonds attached to that site. Therefore, if $x$ is the event that in the random-site model a bond is occupied, then the probability distribution of the bond occupation in the site-diluted Ising model, in the extreme dilution limit, can be approximated by

$$P(x) = (1/4)[p\delta((x/4)-1) + (1-p)\delta(x/4)] .$$

This distribution leads to

$$\sigma \sim [p(1-p)]^{1/2}$$

for the variance of the bond distribution in the site diluted random Ising model. Hence, finally, we obtain

$$\xi \sim g^3/[p(1-p)]^2 . \tag{10}$$

Note that $\xi \to \infty$ as $p \to 1$, which implies that the impurity roughening vanishes in the limit $p \to 1$. This is consistent with the underlying physics of the problem. Also note that Eq. (10) does not hold for large concentration of impurities. Since $\sigma$ increases with increasing dilution, $\xi$ decreases with increasing dilution. Therefore, the higher is the dilution, the smaller is the time $t^*$ when the crossover from the Allen-Cahn law to the new regime begins to take place. This result is in qualitative agreement with our MC data presented in Figs. 2 and 3. However, a more direct quantitative comparison of this phenomenological theory with the estimates of $t^*$ from our MC data requires the relation between $\xi$ and $R$ and that between $R$ and $t$ in the crossover regime. Unfortunately, we have not yet been able to carry out this last step.

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