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Domain Growth in the Three-Dimensional Dilute Ising Model

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We investigate the kinetics of domain growth in the three-dimensional Ising model with quenched random site dilution, using Monte Carlo simulation technique. A crossover from the power law growth regime to a much slower growth observed in our simulation is interpreted through the roughening of the interfaces by the quenched impurities. The results are also compared with the corresponding results in two dimensions.

KEY WORDS: Dilute Ising model; interface roughening.

The growth of the ordered domains following an instantaneous quench of an Ising spin system from a high temperature T_h to a low temperature T_l below the coexistence curve is the prototype of growth processes in systems equilibrating freely from highly unstable initial states. Very recently, the effect of quenched random impurities on such growth processes has been investigated by Monte Carlo (MC) simulation in two dimensions.(1,2) The crossover from power law growth to logarithmic growth law has been argued(2) to be a consequence of the impurity-induced roughening of the interfaces,(3-7) which dominates over the thermal roughening on longer time scales. Since thermal roughening of the interface exists at all temperatures $T > 0$ for all dimensions $d \leqslant 3$ and since impurity roughening exists for $5/3 < d < 5$, it would be, in principle, possible to observe the interplay between these two roughening phenomena also in $d = 3$. Therefore, the main aim of this communication is to investigate the domain growth in the

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three-dimensional dilute Ising model (DIM) and to compare our results with the corresponding results in $d=2$ reported in Ref. 2.

Before describing our results, let us briefly summarize the concepts involved in the underlying physical phenomena. It is well known that during growth from highly unstable initial states in the pure Ising model, the local velocity of the interface is proportional to the local curvature of the interface. Hence, simple dimensional arguments lead to the well-known Allen–Cahn growth law $R(t) \sim \sqrt{t}$ for such curvature-driven growth. Note that the interface growing according to this law must be rough at all nonzero temperatures due to thermal roughening. However, this simple physical picture changes drastically in the presence of quenched random impurities. The interface must have sufficient thermal energy E_b to overcome the energy barrier arising from the pinning effect of the fluctuations in the local impurity configurations. For a domain of average linear size R, the time scale associated with such thermally activated process is $t \sim \exp[E_b(R)/k_B T]$. If $E_b(R) \sim R^x$ for large R, then $R(t) \sim (\log t)^{1/x}$. Since on long length scales this impurity-induced roughening dominates over the thermal roughening (see Ref. 2 for details), one observes a crossover from the initial $R(t) \sim t^{1/2}$ regime to a much slower "logarithmic" regime when the impurity-induced roughening dominates over the thermal roughening. Such crossover has already been observed in the simulation of the DIM for $d=2$.(2)

In this communication we focus our attention only on the DIM where the quenched randomness arises from random site dilution. The quenched nonmagnetic impurities occupy the sites on a cubic lattice randomly with probability $1-p$, where p is the concentration of the magnetic constituents (from now onward, we represent these magnetic constituents by *Ising spins*). The spin system is cooled instantaneously from an infinitely high temperature to a temperature T far below the corresponding transition temperature T_c. Since such a spin configuration is far from the equilibrium configuration at temperature T, ordered domains of *up* (or *down*) spins start growing with time. We let the system evolve temporally following the Glauber dynamics. A measure of the characteristic size of the domains is given by(8)

$$R^3 = \left\{ N \left\langle \left[(1/N) \sum_{i=1}^{N} S_i \right]^2 \right\rangle \right\}^{3/2}$$

where $\langle \cdot \rangle$ denotes average over a large number of quenches. We have computed R^3 for a three-dimensional DIM by MC simulation of simple cubic lattices 60^3 in size with periodic boundary conditions as a function of time t, where the time t is measured in units of Monte Carlo steps per spin

(MCS/spin). The computations were carried out on the FPS 264 array processors at the Center for Advanced Computational Science of Temple University.

Since $R \sim t^{1/2}$ according to the Allen–Cahn law for the curvature-driven growth of domains in the pure kinetic Ising model,⁽⁹⁾ we have plotted R^3 against $t^{3/2}$ in Fig. 1. Note that for each of the impurity concentrations p, R^3 can be fitted to $t^{3/2}$ up to a certain time t_c, beyond which the growth law crosses over to a much slower, possibly logarithmic, regime. Moreover, the smaller is the spin concentration p (i.e., the larger is the impurity concentration), the smaller is the crossover time t_c. These features of R are in qualitative agreement with the corresponding results in $d=2$ as reported in Ref. 2. However, there are some important quantitative differences; for the same impurity concentration, t_c is larger in $d=3$ than that

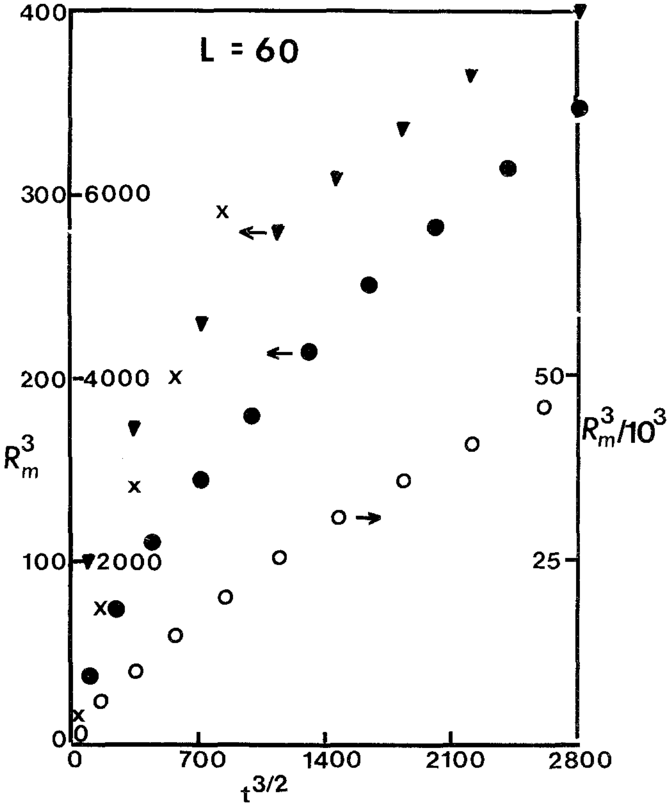

Fig. 1. Plot of R^3 for a 60^3 system of DIM as a function of $t^{3/2}$, for $p=$ (×) 1.0, (▼) 0.5, (●) 0.75, and (○) 0.9. Each datum is obtained by averaging over 100 quenches.

in $d = 2$. This is consistent with general physical intuition; the higher the dimensionality of space, the greater are the number of possible directions in which the domains can grow. Since the impurities tend to hinder the growth of the domains, their effect is much weaker if the number of ways to overcome this hindrance is larger. Therefore, in $d = 3$ a higher concentration of impurities is required for the crossover to take place.

Finally, we conclude that there is a crossover from curvature-driven power law growth to logarithmic growth of the domains in the dilute Ising model when the impurity-induced roughening of the interface dominates over the thermal roughening. The higher the concentration of the impurities, the smaller is the crossover time. This feature of the growth is valid both in two and three dimensions.

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REFERENCES

1. G. S. Grest and D. J. Srolovitz, *Phys. Rev. B* **32**:3014 (1985).
2. D. Chowdhury, M. Grant, and J. D. Gunton, *Phys. Rev. B* **35**:6792 (1987).
3. D. A. Huse and C. L. Henley, *Phys. Rev. Lett.* **54**:2708 (1985).
4. M. Kardar, *Phys. Rev. Lett.* **55**:2923 (1985).
5. D. A. Huse, C. L. Henley, and D. S. Fisher, *Phys. Rev. Lett.* **55**:2924 (1985).
6. M. Kardar, MIT Preprint (1987).
7. T. Natterman, KFA Julich Preprint (1987).
8. A. Sadiq and K. Binder, *Phys. Rev. Lett.* **51**:674 (1983).
9. J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, Vol. 8, C. Domb and J. L. Lebowitz, eds. (Academic Press, 1983).

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