Kinetics of Domain Growth: Universality of Kinetic Exponents

Gary S. Grest, David J. Srolovitz, and Michael P. Anderson
Corporate Research Science Laboratory, Exxon Research and Engineering Company, Annandale, New Jersey 08801
(Received 30 January 1984)

We have studied the growth kinetics of several systems with highly degenerate ground states which were quenched from a high ($T >> T_c$) to a low temperature ($T \cong 0$). The mean domain size R increases algebraically with time as $R \cong t^n$, where surprisingly the value of n is observed to fall into one of two universality classes for all the models studied. We observe a distinct crossover from one universality class to the other as the spin interaction is varied.

PACS numbers: 68.55.+b, 05.50.+q, 61.50.Cj

Recently, there has been considerable interest in studying the kinetics of domain growth.[1] Early work[2] in this field attempted to explain the growth of domains in simple ordering alloys which had been quenched from above T_c to below the critical point in systems like Fe-Al or Cu-Au. These systems may be simulated with use of an Ising model.[3] Theoretical studies,[3] computer simulations,[2] and experiments all show that in this type of model the characteristic length R of a domain increases algebraically with time, $R(t) \cong t^n$, where $n = \frac{1}{2}$.

When one goes from the simple two-component Ising model to more highly degenerate systems, Monte Carlo simulations have shown[4-6] that the value of n is typically less than $\frac{1}{2}$. For such highly degenerate systems, the topology of the domain boundary network plays an important role in modifying the kinetics. Our studies[4] of the kinetics of ordering for the two-dimensional Potts model have shown that the exponent, n, decreases continuously from a value of $\frac{1}{2}$ for $Q = 2$ to a value of 0.41 for $Q > 30$. Mouritsen[5] studied the ordering of N_2 molecules into a herringbone structure governed by an anisotropic planar rotor model on the triangular lattice and found $n = 0.25$. Since our large-Q results could be interpreted in terms of a discretized model of a continuous spin, our results may be compared with Mouritsen's.[5]

The fact that two different values of n have been observed in topologically connected systems of domain boundaries suggests that a variety of types of kinetic behavior are possible. One explanation of this type of variety is that the exponent n depends on the details of the model. If this is correct, additional simulations employing different model assumptions should produce different values of n. However, it is also possible that there are universality classes for kinetic exponents, and the two models studied to date are in different classes. This is a very intriguing possibility since if it were true, this would suggest that kinetic phenomena at $T << T_c$ have features in common with critical phenomena. We already know from earlier studies,[1] on systems which are far from equilibrium, that the growth is temporally self-similar and the structure function or cluster distribution satisfies scaling.

In this Letter, we report the results of our computer simulations which provide evidence for the existence of universality classes for kinetic growth phenomena. In these simulations, we have monitored the kinetics of domain growth for a generalized Q-state Potts model, where we have chosen Q large ($= 48$). The Hamiltonian employed is

$$H = -\sum_{nn}[1 - V(S_i,S_j)], \quad (1)$$

where S_i is one of the Q states of the ith spin and $V(S_i,S_j)$ is the spin interaction, specified below. The sum is taken over nearest neighbor (nn) spins on a triangle lattice. Using standard Monte Carlo procedures, we study the domain growth of a system orginally quenched from a high T to a very low one. To reduce boundary effects, we employ very large systems (200×200 sites), with periodic boun-

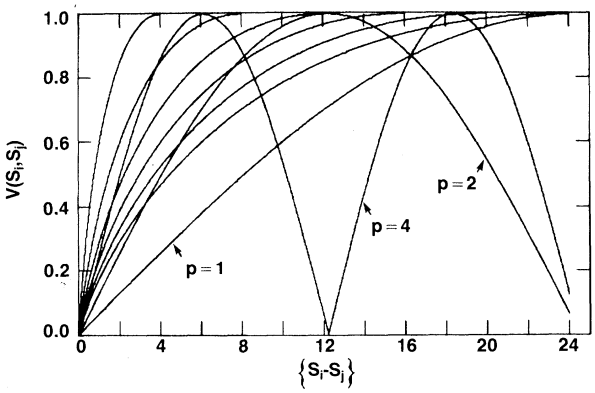

FIG. 1. Interaction potential $V(S_i - S_j)$ vs $\{S_i - S_j\} = \min(|S_i - S_j|, |S_i - S_j \pm Q|)$ for $p = 1$, 2, and 4 for V_1 [Eq. (2a)] and $Q^* = 4$, 8, 12, 16, 20, and 24 for V_2 [Eq. (2b)].

dary conditions. In all cases, after the system was quenched to $T \cong 0$, we ran our simulations for at least 3000 Monte Carlo steps per spin and averaged our results over 2–5 runs.

In the present simulation study, we considered a number of different potentials. For $V(S_i,S_j) = 1-\delta(S_i,S_j)$, where $\delta(S_i,S_j)$ is the Kronecker delta, the model reduces to the standard Potts model. This delta-function potential of the Potts model may be generalized to include nonequivalent interactions between sites of unlike orientation (S_i,S_j). In terms of the language of the Q-state Potts model, the continuous spin θ_i is discretized as $\theta_i = 2\pi S_i/Q$. This leads naturally to our first potential,

$$V_1(S_i,S_j) = \left|\sin\left(\frac{p\pi(S_i-S_j)}{Q+1}\right)\right|, \tag{2a}$$

where we have considered $p=1$, 2, and 4. Note that this potential is linear for small arguments S_i-S_j. The $Q+1$ term in the denominator was choosen to ensure that the ground state is a simple ferromagnet with a Q-fold ground-state degeneracy.

The second class of potentials considered is the Read-Schockley potential,[7] which describes the orientation dependence of low-angle grain boundaries in metals and ceramics,

$$V_2(S_i,S_j) = \begin{cases} \dfrac{-\{S_i-S_j\}}{Q^*}\ln\left(\dfrac{\{S_i-S_j\}}{eQ^*}\right), & \{S_i-S_j\} \leq Q^*, \\ 1, & \{S_i-S_j\} \geq Q^*, \end{cases} \tag{2b}$$

where Q^* is a parameter and $\{S_i-S_j\} = \min(|S_i-S_j|, |S_i-S_j \pm Q|)$. For $Q=48$, $Q^*=7$ can be used to parametrize tin and $Q^*=12$ for lead.[8] In Fig. 1, we plot this potential for several values of Q^*, along with V_1 for three values of p.

In addition to these two potentials, we considered a linear-isotropic potential,

$$V_3(S_i,S_j) = \begin{cases} \{S_i-S_j\}/Q^*, & \{S_i-S_j\} \leq Q^*, \\ 1, & \{S_i-S_j\} \geq Q^*. \end{cases} \tag{2c}$$

While this third potential is very simple, it has one feature which is rather interesting. Because the potential is linear, it is possible to insert a domain between two other domains, without any change in energy, as long as $\{S_i-S_j\} \leq Q^*$. For example, if a domain of orientation 1 is next to a domain of orientation 9, it is possible to insert any domain of orientation 2–8 in between the original two domains with no change in energy, as long as $Q^* \geq 8$.

In choosing these potentials, we avoided potentials with nondiscrete boundaries, for example, the clock model:

$$V(S_i,S_j) = -\cos[2\pi(S_i-S_j)/Q] + 1.$$

A study[9] on the clock model for $Q=26$ found an exponent n which claimed to be "not inconsistent with $n=0.5$"[6] for the late stages of growth. We reexamined the growth kinetics for the clock model $(Q=26,48)$ employing much larger systems $(4\times10^4$ sites) and longer times (6000 Monte Carlo steps) than in the previous study. Our simulations conclusively show that the clock model exhibits non-power-law growth and that following an initial transient the system rapidly becomes pinned.

We have fitted the domain radius by the form $R^m(t) - R^m(t=0) = Bt$, where B is a constant. In Fig. 2, we show $\log_{10}R$ vs $\log_{10}t$ for V_1 with $p=1$

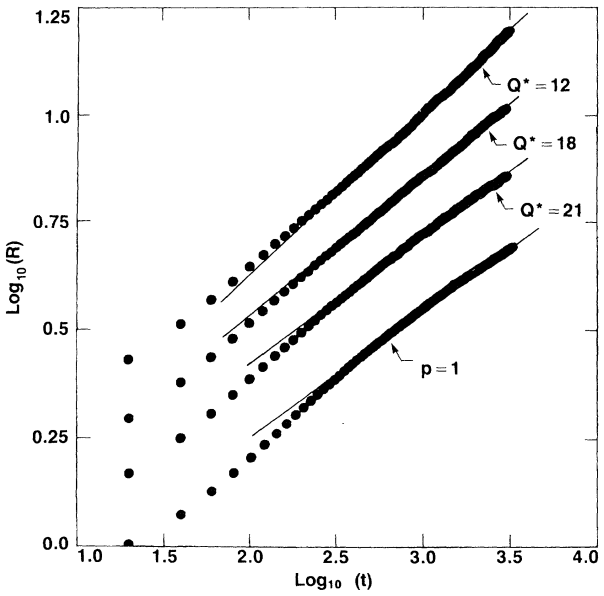

FIG. 2. Plot of $\log_{10}R$ vs $\log_{10}t$ for V_1, $p=1$, and V_2, $Q^*=21$, 18, and 12, after the system was quenched to $T \cong 0$. Dots represent data that have been averaged over four simulations and the curves have been displaced along the y axis for clarity. The slope for long times is extracted from a least-squares fit by $R^m(t) - R^m(t=0) = Bt$.

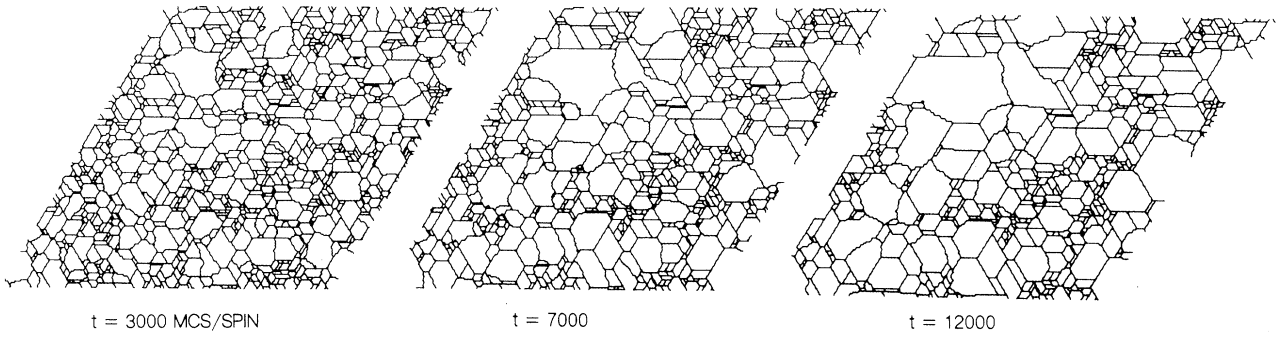

FIG. 3. The evolution of the quenched domains for V_1, Eq. (2a), for $p = 1$ at various times as indicated at the bottom of each snapshot.

and for V_2 with $Q^* = 21$, 18, and 12. The remarkable result is that for all three values of p for V_1, for $Q^* \geq 20$ for V_2, and for $Q^* \geq 8$ for V_3, $n = 1/m$ is found to be 0.25 ± 0.02 in agreement with the earlier results by Mouritsen.[5] However, for $Q^* \leq 12$ for V_2 and $Q^* \leq 4$ for V_3, we find $n = 0.42 \pm 0.02$, in agreement with our previous results for the Potts model, where we found $n = 0.41 \pm 0.02$. Only for $14Q \leq Q^* \leq 19$ for V_2 and $Q^* = 6$ for V_3 do we find values for n which do not fall within these two universality classes. For these values, we found that $n \cong 0.37$ for $Q^* = 14$, $n \cong 0.33$ for $Q^* = 16$, 18, and 19 for V_2, and 0.30 for $Q^* = 6$ for V_3. This is presumably a crossover effect, though we cannot rule out a third universality class with $n \cong 0.33$.

In Figs. 3 and 4, we display the domain boundary configuration at three instances of time during the evolution of the domains for V_1 with $p = 1$ and V_2 with $Q^* = 12$, respectively. The domain size distribution functions for potentials V_2 and V_3, in the parameter range where the growth exponent $n = 0.42$, are very similar to those observed for the Potts model. When Q^* is large enough to produce non-Potts-like kinetics, the domain size distribution functions are wider than for the Potts model. The widths of the distributions and the maximum domain size divided by the mean domain size were observed to increase with increasing Q^*.

The domain boundary configurations for potentials V_2 and V_3 in the range of Q^* where $n = 0.42$ closely resemble those seen for the Potts model.[4] At larger values of Q^*, the domain boundary configurations for all three potentials appear qualitatively similar. In this parameter range, the microstructure may be characterized as having a relatively uniform distribution of medium and large size domains with intervening regions composed of a large number of small domains. No doubt, the presence of regions of small domains is a consequence of the decomposition of domain boundaries into many boundaries when the difference in Q between adjacent domains, $\{S_i - S_j\}$, falls within the linear regions of the potentials. In this sense, the regions of small domains correspond to wide boundaries instead of many individual domains. Mouritsen[5] reached similar conclusions for his N_2 on graphite model. In the linear regions of the potentials, the disappearance of a low-angle boundary does not coincide with a decrease in energy and hence domains surrounded by low-angle boundaries

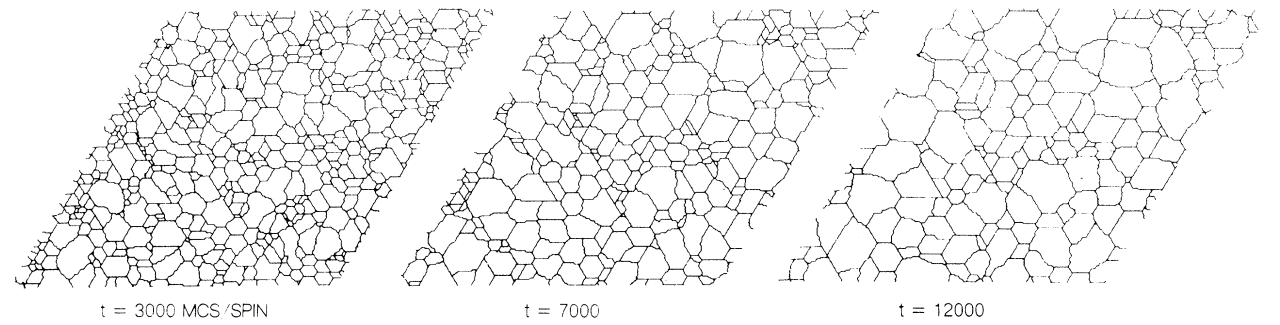

FIG. 4. Same as Fig. 3 for V_2, Eq. (2b), for $Q^* = 12$.

are very stable. In the limit that Q^* goes to its maximum value, 24, for the linear potential, V_3, nearly all of the observed domain boundaries are wide.

It appears that the domain of attraction of the two observed exponents is rather strong, since as seen in Fig. 1, there is very little difference between V_2 for $Q^*=12$ and 20 or for Q^* near 6 for V_3. Yet, the crossover from one universality class to the other occurs over a small region in the parameter space. These results suggest, for the first time, that there exist universality classes for kinetic exponents and that the exponent n is not dependent on the details of the model. The apparent difference between these two classes appears to be affected by the energy dependence of the low-angle boundaries. If the domain boundaries are stable against decomposition into low-angle boundaries, an exponent of 0.42 is observed. This is the limit of sharp domain boundaries, for which the Potts model is a good example. When boundaries readily breakup into a number of low-angle boundaries the kinetic exponent, n, is approximately 0.25. This is the wide boundary limit, for which V_3 with Q^* large is a good example.

In conclusion, we have performed Monte Carlo simulations to study the kinetics of domain growth for a wide variety of systems. We find that there exist two distinct kinetic domain growth universality classes when the number of components, Q, is large and nonconserved dynamics are employed. These classes are (1) $n \cong 0.42$, which corresponds to sharp domain boundaries, for example, a Potts model, and (2) $n \cong 0.25$, which corresponds to wide domain boundaries. These results should be contrasted with the domain growth exponent observed in nearest-neighbor Ising models, $n=\frac{1}{2}$. The difference between the Ising results and the high-Q results, presented here, can be attributed to the topology of the domain boundary network. The importance of the topology increases as Q increases and hence, the fixed points $n=0.42$ and $n=0.25$ should be expected to approach $\frac{1}{2}$ as Q decreases.[4] A study of the dependence of n on Q for the potentials examined here is currently being pursued.

[1]J. D. Gunton, M. San Miguel, and P. S. Sahni, *Phase Transitions and Critical Phenomena* (Academic, London, 1983), Vol. 8.

[2]S. M. Allen and J. W. Cahn, Acta. Metall. **27**, 1017, 1085 (1979).

[3]M. K. Phani, J.L. Lebowitz, M. H. Kalos, and O. Penrose, Phys. Rev. Lett. **45**, 366 (1980).

[4]P. S. Sahni, G. S. Grest, M. P. Anderson, and D. J. Srolovitz, Phys. Rev. Lett. **50**, 263 (1983); P. S. Sahni, D. J. Srolovitz, G. S. Grest, M. P. Anderson, and S. A. Safran, Phys. Rev. B **28**, 2705 (1983).

[5]O. G. Mouritsen, Phys. Rev. B **28**, 3150 (1983).

[6]A. Sadiq and K. Binder, Phys. Rev. Lett. **51**, 674 (1983).

[7]W. T. Read and W. Shockley, Phys. Rev. **78**, 275 (1950).

[8]J. G. Byrne, *Recovery, Recrystallization, and Grain Growth* (MacMillan, New York, 1965), p. 117.

[9]K. Kaski and J. D. Gunton, Phys. Rev. B **28**, 5371 (1983).