is a trivial consequence of geometry. The lack of coupling at $k=0$ in (8) and (9) is due to particle and spin conservation.

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Kinetics of the Q-State Potts Model in Two Dimensions

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An efficient Monte Carlo procedure is applied to the study of the kinetics of low- and high-Q-state Potts models quenched from an initial high-temperature ($T \gg T_c$) state to very low temperatures ($T \simeq 0$). After an initial transient period, the mean domain size, R, increases algebraically with time as $R \sim Ct^n$. The exponent n decreases from $\frac{1}{2}$ for $Q=2$ (Ising model) to 0.38 for large Q. The change in n is attributed to a coalescence process which becomes increasingly effective with decreasing Q. For large Q, the prefactor C is proportional to $Q^{1/2}$.

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The kinetics of domain growth is a subject of considerable interest in the fields of surface science[1,2] and metallurgy.[3] Both phenomenological[4-8] and field-theoretic approaches[9] have been developed to explain the growth of domains in the ordering of alloys (e.g., Fe-Al, Cu-Au, etc.) with two equivalent sublattices quenched from high to low temperatures ($T < T_c$). The kinetics of domain growth has also been studied in binary alloys by Monte Carlo (MC) techniques with a simple Ising model.[10,11] All of the above investigations showed that the characteristic length R of a domain grows (or shrinks) algebraically with time [i.e., $R(t) \sim t^{1/2}$]. This growth law has been experimentally observed in various alloys.[9] In recent years, the kinetics of domain (or island) growth of adsorbed atoms on surfaces with more than two degenerate ground states has also been investigated. In a number of MC studies on chemisorption[1,12,13] and physisorption systems, domains of multiply degenerate ground states have been reported to grow very slowly. Analytical results on simple domain geometries have also suggested that the characteristic domain size grows slowly, as a logarithmic function of time.[6,14] A similar slow evolution has been observed by Lagally *et al.*[2] for ordering of oxygen atoms on a tungsten substrate [O/W(110)]. However, it is difficult to conclude from the experimental studies whether this slow growth is due to surface heterogeneities (steps, terraces, vacancies, etc.) or to more basic topological effects. A similar situation is encountered in the experimental study of grain growth in polycrystalline materials.[15]

In this Letter, we report the results of our computer simulations on the kinetics of a ferromagnetic Q-state Potts model which is rapidly quenched from $T \gg T_c$ to $T \simeq 0$. For low Q ($Q=2,3,4,6$), Potts models provide a good approximation to many chemisorption and physisorption systems, while for high Q, this model can be used to study the kinetics of continuous (infinitely degenerate) systems such as grain growth in a polycrystalline material.

We study the Q-component ferromagnetic Potts model,

$$H = -J \sum_{\mathrm{NN}} \delta_{S_i, S_j}, \tag{1}$$

where S_i is the Q state of the spin on site i ($1 \leq S_i \leq Q$) and δ_{S_i, S_j} is the Kronecker delta. The sum is taken over nearest-neighbor spins and $J > 0$. Using MC techniques, we study the domain growth of systems originally quenched from a high temperature to a very low one. To reduce the boundary effects, we employ very large systems (200×200 sites on a triangular lattice) with periodic boundary conditions. Standard MC procedures, in which a randomly chosen spin is allowed to flip into any of the $Q-1$ other orientations, was found to be very inefficient since, for large Q, the probability of acceptance of an arbitrary spin flip is very small. We have employed a variant[16] of the efficient MC procedure of Bortz

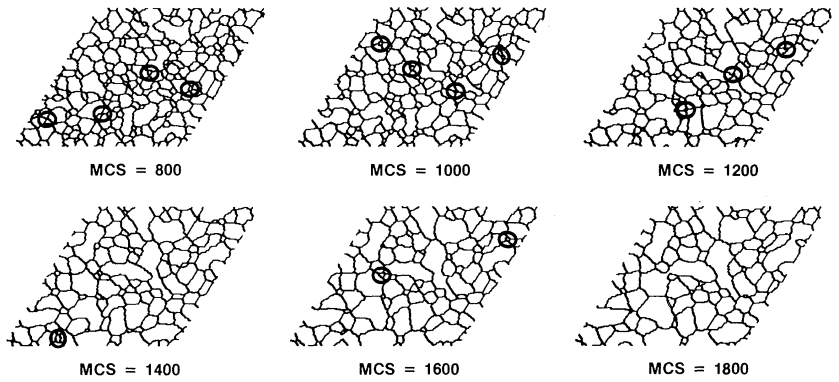

FIG. 1. The evolution of the quenched domains for $Q = 12$ at various times (in units of MC steps per spin) as indicated at the bottom of each snapshot. The circles indicate the location of a region in which coalescence is about to occur.

et al.,[17,18] where each time step is scaled by the probability that an attempt will produce a flip. Results obtained by this efficient procedure are found to be in excellent agreement with standard MC techniques.[16]

In analyzing the results of the present simulation, we monitored the mean area per grain $\langle A(t)\rangle$, which is simply related to $R(t)$, the characteristic domain size. While $R(t)$ is most frequently calculated via structure-factor analyses and $A(t)$ via cluster-enumeration techniques, we have adopted a new, much faster topological form of analysis. Using a generalized form of Euler's formula,[19] we calculate the total number of domains, $D(t)$, in terms of the number of edges, $E(t)$, and vertices, $V(t)$:

$$D(t) - E(t) + V(t) = \begin{cases} 0, & \text{infinite system} \\ 1, & \text{finite system} \end{cases} . \qquad (2)$$

Further, for an infinite system or one in which periodic boundary conditions are maintained, we know that every edge is two-ended and each vertex three-rayed, implying $2E(t) = 3V(t)$, and therefore $D(t) = V(t)/2$. Equivalently, the mean area is related to the total area A_T by

$$\langle A(t)\rangle = 2A_T/V(t). \qquad (3)$$

In Figs. 1 and 2, we display instantaneous snapshots of the evolution of spin configuration for $Q = 12$ and $Q = 64$, respectively. Results for $Q = 3$ and $Q = 6$ are presented elsewhere.[20] The morphology of the domains for high Q is significantly more regular and equiaxised than in the low-Q case. It is also evident that the domains in the $Q = 12$ case grow quite rapidly relative to the $Q = 64$ case. When two grains of like Q touch, they coalesce into one large grain. The point where the two grains of like Q meet is characterized by large local curvature, and, therefore grows extremely rapidly. The frequency with which coalescence events occur is observed to increase with decreasing Q, as is born out in Figs. 1 and 2.

The average domain radius is commonly fitted by either

$$R^m - R_0^m = Bt, \qquad (4)$$

where R_0 is the characteristic domain size at $t = 0$, or

$$R = Ct^n. \qquad (5)$$

For large times, when $R \gg R_0$, the two expressions are equivalent and $m = 1/n$. The exponent can be most easily extracted by using Eq. (5) in the long-time limit (inset, Fig. 3). The accuracy of the exponent can be verified by replotting the data over the entire time range in accordance with Eq. (5) (Fig. 3). The exponent n as a func-

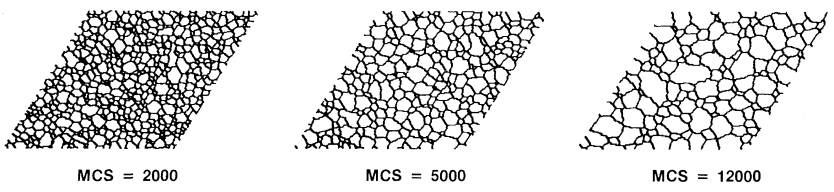

FIG. 2. Same as Fig. 1 for $Q = 64$.

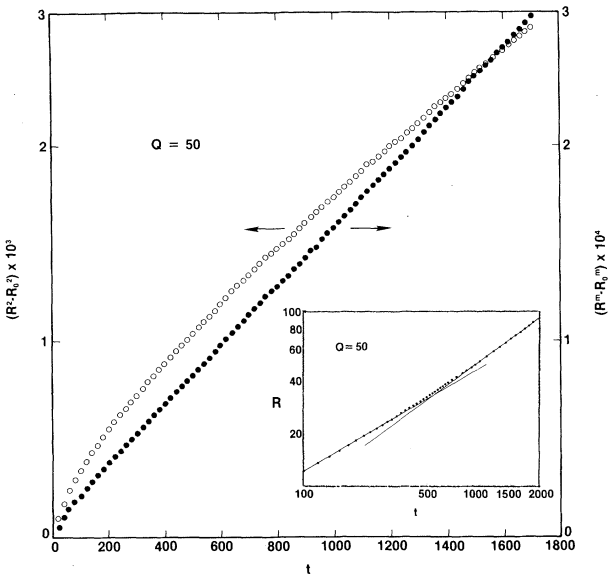

FIG. 3. $R^m - R_0^m$ vs time where m equals the classical value, 2 (open circles), and that derived from the slope of the inset, $\frac{8}{3}$ (filled circles). Inset: The characteristic domain radius R, as a function of time (in Monte Carlo steps), where the data have been averaged over five configurations.

tion of Q is shown in Fig. 4. The exponent n decreases linearly in the range $6 \leq Q \leq 20$. On extrapolating this linear behavior backwards, we find the usual result[3-7] of n equal to 0.5 for the Ising model ($Q=2$). For $Q \gtrsim 26$, we find n to be essentially constant, at a value of $0.38 \pm 0.01 \approx \frac{3}{8}$. For large Q the prefactor, C, is found to vary as $Q^{-1/2}$.

The change in the exponent, n, from $\frac{1}{2}$ for the Ising case to 0.38 for highly degenerate systems reflects a possible change in the fundamental growth mechanism. As is seen in Figs. 1 and 2, the effect of increasing Q is to decrease the number of coalescence events. In fact, for Q infinite no coalescence events can occur. For low Q, on the other hand, multigrain interactions are dominated by coalescence. The frequency of coalescence should be related to the probability of a domain having a second-nearest-neighbor domain of like Q. This probability may be estimated as

$$P(Q) = 1/Q[1 - (1 - 1/Q)^Z], \quad (6)$$

where Z is the mean number of second-nearest-neighbor domains. The asymptotic approach of $P(Q)$ to zero for increasing Q essentially eliminates the Q dependence of n (see Fig. 4). For the present simulation, $n(Q)$ is nearly constant for $Q \gtrsim 26$, suggesting that an infinitely degenerate system can be simulated with a (small) finite-Q Potts model.

The present results at $T=0$ on the triangular lattice are not in accord with the predictions of Lifshitz[6] and Safran[14] in that the growth exponent, n, is nonzero. On the other hand, our results on the high-Q Potts model on square lattice do show $n \simeq 0$ at $T=0$. We believe that these differences can be understood by considering the driving force for domain growth. In the continuum models, the driving force is provided by the decrease in boundary length accompanying reduction of boundary curvature. In lattice models, the curvature is discretized as kinks on the boundary. As illustrated in Fig. 5(a), boundary vertices are sinks for kinks on the square lattice. However, on the triangular lattice, kinks are transmitted through the boundary vertices [Fig. 5(b)]. Therefore, unlike on the triangular lattice, the driving force for domain growth can be quickly relieved

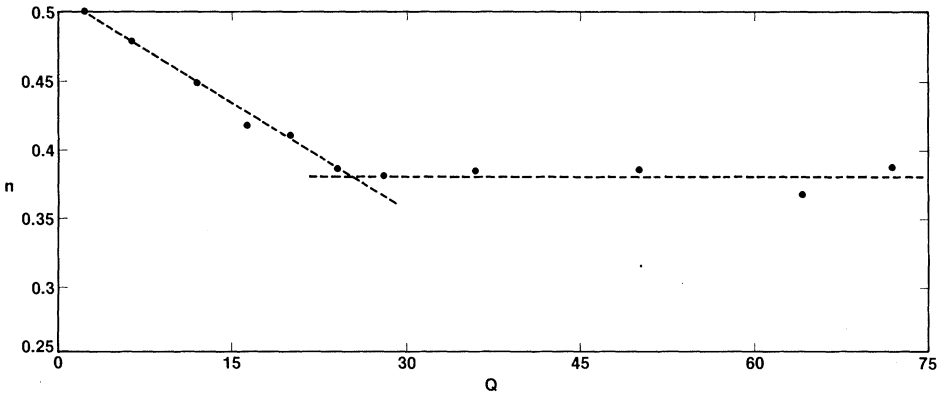

FIG. 4. The domain-growth exponent, n, as a function of Q, where the data for each Q value have been averaged over five configurations.

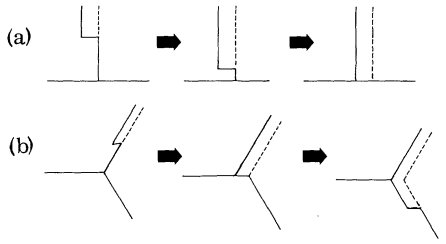

FIG. 5. (a) A kink moving down a boundary towards a vertex on the square lattice. The dotted line shows the prior boundary location. (b) Same as in (a), except for a triangular lattice. After the kink reaches the vertex, it proceeds along a different boundary.

on the dquare lattice. Normal, or curvature-driven, domain growth corresponds to the mutual annihilation of oppositely signed kinks. For increasing temperature, the effective kinetic exponent for the square lattice approaches the observed value for the triangular lattice, which is found to be temperature independent (below T_c). The unpinning at finite temperatures is attributable to the thermal generation of kinks.

Experience with Ising models[10,11] and previous domain growth theories[9] suggest that the exponent, n, is identical for $d=2$ and 3. Verification of this conjecture will be the subject of future inquiry.

In conclusion, we find that the characteristic length $R(t)$ for the high-Q Potts models scales as $t^{0.38}$, instead of the classic $t^{1/2}$ observed in Ising models and domain growth theories. Our results suggest that high-Q Potts models can be used to simulate continuous (infinitely degenerate) systems, such as grain growth in polycrystalline materials. In fact, experimental observations of grain growth in metals typically yield kinetic exponents less than $\frac{1}{2}$,[21] which is in accord with our findings.

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