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COMPARISON OF DOMAIN GROWTH KINETICS IN TWO AND THREE DIMENSIONS

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I. INTRODUCTION

During the past five years, we¹⁻⁴ have been investigating the kinetics of systems with a high ground state degeneracy which have been quenched from a high temperature disordered state, $T \gg T_c$, to a final temperature below the transition temperature T_c . After the quench the system spontaneously develops local domains which are highly ordered. The average domain size then grows in order to reduce the excess free energy associated with the domain walls. For the non-conserved Ising model⁵ which has a ground state degeneracy of two, it has been known since the work of Lifshitz⁶ and Allen and Cahn⁷ that the correlation length R grows algebraically as $t^{1/2}$ for all dimensions above one. This result has been well documented by both analytical⁵⁻¹¹ and computer^{9,12-14} studies as well as experimental studies on ordering alloys⁷ (e.g., FeAl and CuAu). However five years ago little was known about the growth kinetics for more complex models which have a higher ground state degeneracy. Lifshitz⁵ was the first to predict slow kinetics in systems with several degenerate equilibrium states. Safran¹⁵ extended these arguments to show that domains may become pinned if the number of degenerate ground state $Q \geq d+1$, where d is the dimension of space. They suggested that the system could become trapped in locally stable metastable states which would then greatly slow down the kinetics. When Safran, our colleague at Exxon, showed us his results, we decided that computer simulations would be a very good method to test his suggestions. In collaboration with P. Sahni, we began at that time a study of the kinetics for the Potts model, for a wide range of Q 's from the $Q=2$ Ising model to $Q=64$. While we^{1,2} found that the growth remained algebraic, independent of the value of Q , we also found that the higher ground state degeneracy had a large effect on the growth kinetics, the microstructure and the topology. In this paper, we will review the recent progress in our understanding of the kinetics of domain growth for the Potts model and its connection to experiment.

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Examples of systems with highly degenerate ground states ($Q > 2$) include the superlattice structures observed for adsorbed atoms on surfaces, such as O/W(110), O/Ni(111) and H/W(001) which are chemisorbed and physisorbed systems such as rare-gas atoms adsorbed on graphite. In addition to surface studies, similar structures have also been observed in intercalation compounds such as SbCl_5 intercalated into graphite, for which $Q=7$. In addition, we observed that large Q was very important for describing grain growth in polycrystalline metals (e.g., pure Fe, Al and MgO), if it is assumed that all grain boundaries are energetically equivalent. Since there is an abundance of data on the growth kinetics, grain size distribution and topological distributions of grain edges from the metallurgical literature, it is possible to make comparisons between our model simulations and experimental data. It turns out that the Potts model captures all the essential features of grain growth in real materials. We also found that many of the properties of the domain growth kinetics, in particular the microstructures and topological distributions, were essentially the same, independent of dimensionality. When we compared the distribution of grain areas from our two dimensional simulations with the cross sections of our three dimensional systems, we found very good agreement. While the shape of the distribution function changes with Q , it is relatively insensitive to d .

One of the essential features of domain growth involves the competition between individual ordered regions or domains, of different orientations Q which share a common boundary. Since most analytical theories implicitly assume that domains can be described as spherical, and that growth occurs in an average environment, it is easy to understand why they are relatively poor in describing more than the simple qualitative aspects of experimentally observed kinetics and topology. In general, most analytic theories have been concerned with the time dependence of the average grain radius

$$\bar{R} \propto B t^n \quad (1)$$

where B is a temperature dependent constant. Many analytic descriptions give $n=1/2$, as observed experimentally for the $Q=2$ Ising model. However, experimental data for grain growth in polycrystalline materials consistently give $n < 1/2$, although the data has substantial scatter. This value for n is in agreement with experimental results for low Q . Homer and Clarke found $n \approx 0.5$ for $Q=7$ using x-ray scattering. There have also been two experimental studies using low-energy electron diffraction for O on W(110) ($Q=4$) and O on W(112) ($Q=2$) which also found $n \approx 0.5$. Some theories have tried to predict the domain size distribution function but have largely been unsuccessful. There are no predictions at all for many topological quantities, like the distribution of the

number of grain edges. These failures and inabilities may be traced to their treating the growth in terms of a grain in a mean environment. This type of mean field theory averages out much of the important, topological effects associated with connectedness of the actual microstructure. For this reason, they obtain results which best describe the Ising model ($Q=2$), for which $Q < d+1$ and the topology of the network is irrelevant. Generalizations of this type of theory to include many interacting spherical grains are also not sufficient as they still do not include the simple space-filling requirements which result in a topologically connected structure.

Because the outlook for finding a solution of an analytic model for domain growth, which describes not only the average growth of the grain radius R but also the domain size and topological distributions, does not seem hopeful, we have concentrated on obtaining this information from large scale computer simulations. In our early studies, we observed that the exponent n for growth in two dimensional (2-d) Potts model was dependent on Q . As Q increased from 2, n decreased slowly from 0.5 to approximately 0.41 ± 0.02 for Q greater than 30. As Q increased the domain size distribution function narrowed as the domains become more compact. For Q larger than approximately 30, we found both n and the domain size distribution function become independent of Q . This result for large Q was confirmed independently by Wearie et al. and Mouritsen. However, as pointed by a number of authors including Kaski et al, Dasgupta and Pandit, Valls and Mazenko and Huse, it is difficult to determine whether the exponents one obtains from fitting the simulation results are really asymptotic or not. This is true even when the available data give an excellent fit to Eq. (1). It is always difficult to rule out slow transients. Our original simulations were carried out on lattices of size 200×200 , already much larger than used to study equilibrium critical phenomena. Such large lattices were necessary since we were interested in following the kinetics for long times. However, even for this size system, we had to stop the simulation when the average grain size was on the order of 200 sites, in order ensure that there were enough domains in the system to give representative results. Because the average area grows as $R^2 \propto t^{2n}$, very large systems are needed to extend the time regime significantly. Here we will present results previously unpublished for $Q=48$ on a 1000×1000 lattice that show in fact when the simulations are extended to much larger systems and longer times the value of n for large Q appears to increase to $n=0.49 \pm 0.02$, consistent with that for the Ising model. However, all of our other results for the domain and topological distributions remain unchanged.

We have recently extended our simulations to three dimensions (3-d), where we have studied systems as large as 100^3 . Here we observe values of n which are significantly

less than $1/2$ for large Q . We find that for Q larger than approximately 12, n no longer depends on Q and $n = .38 \pm 0.02$. While we have seen no difference between the value of n for systems of size 60^3 and 100^3 , we cannot say for certain that this value of n is asymptotic. What we have been able to show is that both the observed value for n and the grain size distribution functions for the high- Q Potts model agrees very well with grain growth in real polycrystalline materials.

While the growth kinetics is an interesting problem to study theoretically, to make progress experimentally one often has to be concerned with the presence of quenched impurities. These impurities can occur in many different forms; for example, second-phase particles in grain growth in polycrystalline materials and/or surface defects in the ordering of atoms physisorbed on solid surfaces or intercalated into graphite. As a routine matter, second-phase particles are added to metals and ceramics to control grain size. In these cases the final grain size is affected by both the particle concentration and size. We found that in 2-d the domain growth becomes pinned for quenches to $T=0$ and that the average domain area A_f varies inversely with the concentration of impurities. For quenches to $T>0$, the asymptotic growth for long times is expected to be slower than a power law. Huse and Henley predicted that in 2-d the long-time growth would be $(\ln t)^4$. This is consistent with simulations by Grest and Srolovitz for the Ising model who were unable to distinguish a $\ln t$ from a power of $\ln t$, but did find that the growth was not a power law. A more recent work by Chowdhury et al have studied the cross-over from the early time power law regime to the late stage logarithmic regime. While simulations for quenches to $T>0$ have not been carried out for the Potts model, we expect similar slow growth for long times.

In this paper, we will review our simulation results for domain growth, with particular emphasis on comparing growth in two and three dimensions. In Sec. II, we will describe the model and Monte Carlo procedure. We will then review our findings for the growth kinetics and describe the changes which occur in the microstructure morphology as Q increases in Sec. III. We will also present results for the domain size distribution and compare our large Q results with experimental data for polycrystalline materials. Finally, in Sec. IV, we will give some conclusions and discuss future directions of this work. In this paper, we will consider only models with a ground state degeneracy Q greater than two. The reader is referred to excellent reviews for the domain growth kinetics for both the conserved and non-conserved Ising model by Gunton et al and Binder. In addition, we will not discuss lattice gas models for adatoms ordering on surfaces, for example $O/W(110)$, for which $Q>2$ but cannot be described by the simple Potts model considered here. The reader is referred to the papers by Sadiq and

Binder and Vinals and Gunton for Monte Carlo simulations of this interesting problem.

II. MODEL AND METHOD

We studied the Q-component ferromagnetic Potts model with a nonconserved order parameter,

$$H = -J \sum \delta_{S_i S_j} \quad (2)$$

where S_i is the Q state of the spin on site i ($1 \leq S_i \leq Q$) and δ_{ab} is the Kronecker δ function. The sum is over all spin pairs with a specified distance and $J > 0$. For all of the simulations, we started the system in a random state and rapidly quenched to $T=0$. The kinetics of the boundary motion were simulated via a Monte Carlo method in which a site is selected at random and re-orientated to a randomly chosen orientation. If the change in energy associated with the re-orientation, ΔE , is less than equal to zero the re-orientation is accepted. However, if $\Delta E > 0$, the re-orientation is accepted with probability $\exp(-\Delta E/k_B T)$. A generalization of Bortz et al's "n-fold" or continuous time technique to the Potts model was used to make the simulations more efficient. Without this method, the number of runs and size of the systems which we would have been able to study would have been greatly reduced. This is particularly true for large Q and late times, when most of the spins are not on the boundary. N re-orientations attempts are referred to as 1 Monte Carlo step (MCS), where N is the number of lattice sites. In all of our simulations we used periodic boundary conditions

In 2-d, we have carried out simulations on both the triangle and square lattice of size 200^2 , 380^2 and 1000^2 . For the triangle lattice, we include only nearest neighbors (nn) in Eq. (2). We found that on the square lattice if only nn are included, the domains become pinned for quenches to $T=0$ and the growth exponent n is zero for $Q \geq 3$, in accord with the predictions of Lifshitz and Safran. When the range of interaction is extended beyond nn to include next nearest neighbors (nnn) with coupling J equal for nn and nnn pairs, the growth is not pinned and $\bar{R}$ increases algebraically with the same value of n as on the triangular lattice. Vinals and Gunton found that if J is not equal for the nn and nnn interactions, the domains become pinned for quenches to $T=0$. When the final quench temperature $T > 0$, the growth on the square lattice with nn interactions becomes unpinned and we observed an effective growth exponent n which was T dependent rising toward the values observed on the triangular lattice as T approaches T_C . In 3-d, we observed similar effects for the simple cubic (sc) lattice. When the sum is only taken over nn in Eq. (2), growth becomes pinned as there is no local driving force on the vertices where four domains meet. However, the introduction of further neighbors in the sum,

Eq. (2), unpins the system and growth occurs even for $T \neq 0$. We have studied systems of size 60^3 and 100^3 on the sc lattice, including 6, 18, 26 and 124 neighbors in the sum in Eq. (2). This corresponds to the inclusion of nn sites, nn plus nnn sites, all sites within a cube out to (111) and all sites within a cube out to (222), respectively. We refer to these as cases $k=1, 2, 3$ and 4. We have only investigated the case in which the coupling J is equal for all pairs within the range of interaction. When the final quench temperature $T > 0$, the growth on the sc lattice with only nn interactions becomes unpinned, but the effective exponent n increases only slightly before T_c is reached. Since our main aim has been to search for universal features which describe the growth kinetics, we have concentrated on systems which do not become pinned due to local lattice effects when quenched to $T \neq 0$.

In this paper, we will mainly present simulation results for the square lattice with nn and nnn interaction. In 2-d, all of the results presented are averaged over 5 runs on a 380^2 lattice. We will also present results for the $Q=48$ model on a 1000^2 triangle lattice averaged over 2 runs. In 3-d, we will present results on a 100^3 sc lattice for $k=2$ and 3. For low Q , our results are averaged over 2-3 runs, while for high- Q , we typically made only one run. This is for two reasons. The first is computer time. One run for a $Q=48$ 100^3 simulation takes approximately 12-15 hours of CPU time on an IBM 390/150 computer. Since the continuous time method we use in the simulations is very scalar in its design, the amount of CPU time decreases only slightly on a Cray supercomputer. The second is that we see little fluctuation in our results from sample to sample. For high- Q , there is a sufficient number of grains to obtain good statistics for both the grain size and topological distributions from one run. Two runs for the case $k=3$, $Q=48$ on the 100^3 lattice gave nearly identical results for all properties studied. However, for low- Q the small linear dimension of our 3-d simulations does begin to play a role, limiting the time we can follow the growth and increasing the size of the fluctuations. For the Potts model, unlike the Ising model, the growth kinetics can easily be monitored by measuring the average grain area or volume directly by using a cluster-enumeration routine. This is computationally efficient and gives an accurate measure of the growth without having to average over many samples as is usually necessary for the Ising model. What would be useful is to be able to use larger lattices in 3-d to follow the growth for very long times, but this does not appear to be possible at the present time.

III. RESULTS

Fig. 1, we display the microstructures for $Q=3, 6, 12$, and 48 on the square lattice with nnn interactions. The boundary is drawn as the perpendicular bisector between

misoriented sites. One can clearly see the gross morphological changes that occur as Q increases from small Q near the Ising value ($Q=2$) toward the limit of high Q . The low Q configurations consist of very irregular and asymmetric domains. This irregularity decreases as Q increases. For high Q , the domains are significantly more compact and equiaxed. This dependence of the domain boundaries on Q is very similar in 3-d, as shown in Fig. 2 where we show a (100) planar section on the sc lattice for $k=3$ (26 neighbors) for the same values of Q . The cause of these large differences can be clarified by considering the temporal evolution of the domains in the low and high Q limit. In Fig. 3 we present results for growth on the square lattice with nnn interactions for $Q=6$ and 30. In Figs. 4 and 5 results for the same values of Q for a (100) planar section on the sc lattice with interaction range $k=3$ and 2, respectively. Steps are clearly visible in the micrographs in Figs. 2, 4 and 5 due to the small size of the simulated volume (100^3 lattice sites). This is less visible in Figs. 1 and 3, where we show a 200^2 section of a 380^2 simulation. Comparison of these figures indicates that in the low- Q limit, large discontinuous changes in the area of individual grains can occur when one domain meets and coalesces with another domain with the same orientation. The probability of such chance meetings decreases as Q increases, though one can see occurrences of this in the micrographs for $Q=30$. Since such coalescence events are strictly forbidden in the limit $Q \rightarrow \infty$, the rarity of such events for $Q \geq 36$, indicate that the infinitely degenerate system can be modeled with a large finite Q . An example of a highly degenerate system is the grain structure in polycrystalline materials, where the Q orientations can be associated with the local orientations of the crystalline lattice. It is interesting to note that the grain morphologies for the two 3-d model are not identical. The boundaries for the $k=2$ case are more flatter, reminiscent of the 2-d square lattice with nn interaction, which become pinned by "T" shaped vertices where three domains meet. The longer range interaction in the $k=3$ case seems to eliminate these, producing grain boundaries which on a coarser scale meet at 120° even though the sc lattice grain boundaries which meet at triple lines are constrained to have included angles of either 90° or 180° due to the symmetry of the lattice.

From Figs. 3-5, it appears that the domain size distribution is nearly identical between 2-d and 3-d. This correspondence is made more quantitative in Fig. 6, where the grain area distribution function for the 2-d square lattice is compared with that obtained from the (100) planar crosssections of both the $k=2$ and 3 models on the sc lattice for $Q=6$, 12 and 48. Results for the triangular lattice with nn interactions are identical to those for the square lattice with nnn interactions. For $Q \leq 4$, the 100^3 lattices are too small to obtain good statistics for the volume or cross-

sectional area distributions. The 2-d results are nearly identical with the k=2 sc results and both differ slightly from the k=3 sc case. In cross-section there appear to be more small grains for the k=3 sc case than for the other two cases. These distributions were found to be time invariant when normalized by their respective means. This property, which Mullins refers to as statistical self-similarity, was always observed. The only data available to test how well our model compares with experimental data is for the polycrystalline materials. In Fig. 7, we present the cross-sectional area grain size distribution from our simulations for the k=3 model with $Q=48$ and data for pure Fe. Note that the grain size distribution function for the simulations and experiment agree remarkably well.

Also shown in Fig. 6 as the continuous curve is the log-normal function $f(\log_{10}x)$, where $x=A/\bar{A}$, plotted using the values for the mean μ and standard deviation σ measured for each distribution. Note that the log-normal function is symmetric with tails extending to $\pm\infty$ while the data is actually skewed. The log-normal form is a better representation of our data for small Q . The development of the log-normal distribution in domain growth has been rationalized in terms of a probabilistic mechanism in which individual domains are assumed to change area or volume in a random and uncorrelated manner. This argument is not appropriate for high- Q , where the density of vertices is high. The presence of vertices couples each domain to its neighbors, so that changes in area or volume are correlated. In this limit, we find a better fit to the data is Louat's function $f(x)=\exp(-x)$, where $x=A/\bar{A}$. However, the volume distribution $f(\log_{10}(V/\bar{V}))$ is best fit by a log-normal function. In the low- Q limit, the density of vertices decreases and the correlation between domains becomes smaller so that the log-normal function is expected to give a better fit.

The kinetics of growth were evaluated by monitoring the time evolution of the mean chord length $\bar{L}$, mean cross-sectional area $\bar{A}$ and mean domain volume $\bar{V}$ (in 3-d). Data for the time dependence of the area $\bar{A}$ are shown in Fig. 8 for four values of Q on the 2-d square lattice with nn and nnn interactions. The lattice is size 380^2 and the data is presented as both a log-log and linear-linear plot. Data for the k=2 and k=3 model in 3-d on a 100^3 lattice are shown in Fig. 9. The data can be fit to the kinetic equation:

$$X(t)^m - X(0)^m = Bt \quad (3)$$

where X is equal to either $\bar{L}$, $\bar{A}$, or $\bar{V}$. For $X(t) \gg X(0)$, Eq. (3) reduces to $\bar{R} = Bt^n$, Eq. (1), where $\bar{R} = X^{1/d}$ and $n=1/(md)$, where $d=1$ for $\bar{L}$, 2 for $\bar{A}$ and 3 for $\bar{V}$. The average growth exponent, n , determined from fitting $\bar{L}$ or $\bar{A}$ in 2-d or $\bar{L}$, $\bar{A}$, and $\bar{V}$ give the same result within statistical error. Results for growth in 2-d indicate that $n=0.49 \pm 0.02$ for all Q . As can

be seen from Fig. 8b, the results seem to be quite linear on the plot of $\bar{A}$ versus t . Our new results for $Q=48$ on a 1000^2 triangle lattice out to 60,000 MCS, give n in agreement with this result for the square lattice. Both of these results give a value of n which is greater than our previous estimates of $.41 \pm 0.02$ for $Q \geq 30$. As seen from Fig. 8a, there is significant curvature in the early time regime for high- Q and this is apparently the reason we obtained a lower estimate of n for high- Q from fitting Eq.(3) to our data. If we fit our new data for $t \leq 6000$ MCS, we obtain estimates for n which are consistent with our previous results, indicating the rather slow crossover to the asymptotic time regime.

In 3-d, we find $n=0.38 \pm 0.02$ for $Q \geq 12$ for the $k=3$ case and $n=0.30 \pm 0.02$ for $k=2$. It is not possible to determine if this small difference between the $k=2$ and 3 cases is significant or if the exponent n is time independent. However, a plot of $\bar{A}$ versus t , Fig. 10, shows significantly more curvature in 3-d than in 2-d, suggesting that either the crossover to larger values of n occurs for times much larger than we have been able to study or that n is actually less than 0.5. The lower value of n for $k=2$ with only 18 neighbors within the range of interaction maybe a result of a weak pinning at the vertices which is not strong enough to pin the growth completely as for $k=1$, but is strong enough to effect the kinetics. For $Q \leq 12$, we again find results intermediate between these values and that for the Ising model, $n=0.5$. From our data, it appears that the kinetic exponent n saturates for $Q \geq 12$, while the grain size distributions do not become independent of Q until $Q \geq 30$.

We have studied the effect of quenched random impurities on the growth kinetics for a range of concentration from 0.5% to 20%. The model was initialized by placing N_c impurities with $S_i=0$ on the lattice. The remaining sites were assigned a random value from 1 to Q . The impurities were immovable and were noninteracting. These simulations were carried out on the triangle lattice of size 200^2 for $Q \geq 4$ and 400^2 for $Q=3$ and 4. Simulations for high- Q in 3-d are presently in progress. In all cases studied the domain growth becomes pinned after an initial power law regime. This crossover from a power law regime to pinning occurs at later times with increasing Q and/or decreasing impurity concentration. The averaged pinned domain area A_f varies inversely with the concentration of impurities as shown in Fig. 10. Note that the product cA_f clearly depends on the degeneracy of the model, Q . For high- Q , the domain growth stops when the domain size is comparable with the interimpurity spacing. Since domain growth occurs when small domains are annihilated and domain annihilation occurs by the meeting of three domain vertices, domain growth stops when domain vertices can no longer meet. Motion of vertices is prevented when the three domain boundaries meeting at the vertex are pinned. Therefore, in 2-d, where the mean number of edges (or

vertices) per domain is six (Euler relation), the average number of impurities needed per domain is three: six edges per domain divided by two to account for the fact that each edge is shared by two domains. This is in agreement the value $cA_f=3$ obtained from Fig. 11 for $Q=48$. As Q decreases, the domains become increasingly less compact and the value of cA_f increases as the number of impurities to pin the growth increases.

IV. DISCUSSION

One interesting problem which has often arisen is why the growth exponent n appeared to be less than $1/2$ for high- Q in our 2-d simulations and still does appear to be for both the simulations and experiment for 3-d. In 2-d, Mullins has shown that only by assuming statistical self-similarity (which our simulations demonstrate) and local equilibrium that n must equal $1/2$. He uses the result, first proven by von Neumann and Mullins, that for both bubble growth and idealized grain growth in 2-d, the rate of change of the area A_i of an individual grain (or bubble) depends only on the number of sides,

$$\frac{dA_i}{dt} = \frac{\pi k}{3}(N_e - 6) \quad (4)$$

where k is a constant. This equation should be valid for an arbitrarily shaped 2-d grain of N_e -sides under the assumption that $u=k/R$ and the angle between the intersecting grain boundary is 120° . Here u is the local velocity and R is the signed local radius of curvature lying in the plane, counted positive when it lies along n . Thus $A_i > 0$ for $N_e > 6$ and is < 0 for $N_e < 6$. Writing the statistical self-similarity hypothesis in the form

$$f_{N_e}(A, t) = \phi(A/\bar{A})/\bar{A} \quad (5)$$

where $f_{N_e}(A, t)$ is the probability that a grain has N_e edges and area A between A and $A+dA$, Mullins then proves that if local equilibrium is satisfied, i.e. Eq. (4) is valid for all grains at all times, then $n=1/2$.

Since we have already shown that Eq. (5) is valid, it is of interest to examine Eq. (4) more closely in order to understand the apparent slow cross-over to asymptotic behavior. This is particularly interesting in light of the simulations by Wearie et al for 2-d soap bubbles, who using a procedure similar to ours introduced the additional constraint that Eq. (4) be satisfied at all times. They found that the growth kinetics followed Eq. (1) with $n=1/2$ even for very early times. Without this constraint they obtained our previous result, $n=0.41$. To test the local equilibrium

property of the growth, we carried out a simulation for the $Q=48$ Potts model in which we followed each grain, monitoring its number of edges as a function of time. We first performed a normal domain growth simulation in 2-d for $Q=48$ on a 200^2 triangle lattice for 1,000 MCS until there were 960 grains remaining. In Fig. 12, we present results for the temporal evolution of the area of several individual grains with the same number of edges. Those grains monitored in Fig. 12 were highly unusual in that their number of edges did not change during the majority of the 10,000 MCS run. For convenience we have reset the clock to 0 after we started monitoring the number of edges and we have plotted a symbol only when the number of edges equal the number N_e specified in the figure. From Fig. 12, we see that the slope of A_i is approximately zero for $N_e=6$ and that for $N_e=4$ is approximately of equal magnitude and opposite sign from that for $N_e=8$. An average slope for $N_e=5$ and 7 is harder to determine. We must point out that most of the grains change N_e too often to be plotted in this way. Shown in Fig. 13 is the temporal evolution of the area A_i for five more typical grains observed during the 10,000 MCS run. A different symbol is used to label the number of edges at a given time. Note how often N_e changes. The data in Fig. 13 are the norm, while those in Fig. 12, are the exceptions.

Thus it appears that for those grains which keep the same number of sides for a long time, Eq. (4) is satisfied. However, there are large fluctuations around the mean slope and for most grains N_e changes too often for Eq. (4) to be applicable. From these results, we may be able to understand why the asymptotic growth regime was hard to obtain in our earlier simulations. Since local equilibrium was never established, the apparent grain growth was slower than expected and n appeared to be less than $1/2$. Even though the grains were several hundred sites in size, they were continuously changing their number of edges N_e too rapidly for the system to reach local equilibrium. Every time N_e changes, the microstructure rearranges to accommodate the new growth rate, as per Eq. (4). This accommodation process is not instantaneous but requires a finite amount of time τ . If this time had scaled with the grain size, we would have expected that n would remain less than $1/2$. Apparently, τ grows more slowly, leading to the observed cross-over to $n \approx 0.50$ kinetics for long times. In the future, we hope to analyze how local equilibrium is attained for longer times in our 1000^2 simulations.

In addition to our studies of domain growth for the Potts model with and without impurities, we have also studied growth when the boundary energy is anisotropic. In 2-d for $Q=48$, we studied a generalized Hamiltonian, Eq. (2), in which the interaction energy between different orientations depended on their relative mismatch. For weak anisotropy, n was observed to remain at $n=0.41 \pm 0.02$ and decrease quickly to

0.25±0.02 when the anisotropy became large and remain there, suggesting two universality classes for the domain growth exponent n . We also observed that the domain size distribution broadened as the anisotropy increased. While the exponent $n=0.41$ most likely should be interpreted as $n=0.5$ in light of the results discussed above, the value $n=0.25$ we observed for large anisotropy has been found by Mouritsen for a number of other models, including one with $Q=2$. These models are characterized by their ability to support soft domain walls, in which there exist a spatially smooth gradient of the order parameter across the domain boundary. This is in contrast to systems with hard walls, in which the domain boundary is sharply confined in space. Hard walls result from using discrete Potts-type or lattice gas variables as in Eq. (2). At least for systems of a non-conserved order parameter, there are several numerical results which suggest that there exist two universality classes for domain growth kinetics, depending on whether the type of domain walls, soft or hard. As suggested by Mouritsen, the domain wall softness appears to be more important than the degeneracy of the order parameter for classifying the growth classes, at least in 2-d. In 3-d, the only studies of which we are aware are on discrete models which have hard walls, so that the interesting question of classifying the growth kinetics into universality classes has not been addressed.

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Figure Captions

Figure 1 Domain-boundary configurations for $Q=3, 6, 12$ and 48 Potts model on a square lattice that were quenched from $T \gg T_c$ to $T=0$. Solid curves represent the boundaries between the regions of different orientations. The times were chosen to yield comparable domain sizes. A 200^2 section of the 380^2 sample is shown.

Figure 2 Planar cross-section of the 3-d microstructure for a 100^3 sc lattice with $Q=3, 6, 12$ and 48 for case $k=3$. The times were chosen to yield comparable domain sizes.

Figure 3 Temporal evolution of the domain-boundary for (a) $Q=6$ and (b) $Q=30$ Potts model quenched from $T \gg T_c$ to $T=0$ on the square lattice. A 200^2 section of the 380^2 sample is shown.

Figure 4 Temporal evolution of a (100) planar cross-section from the 3-d microstructure for (a) $Q=6$ and (b) $Q=30$ on a 100^3 sc lattice for case $k=2$.

Figure 5 Temporal evolution of a (100) planar cross-section from the 3-d microstructure for (a) $Q=6$ and (b) $Q=30$ on a 100^3 sc lattice for case $k=3$.

Figure 6 Time averaged domain size distribution function $f(\log_{10}x)$, where $x=A/\bar{A}$ for $Q=6, 12$ and 48 for the square lattice (curve a) and sc lattice with $k=2$ (curve b) and $k=3$ (curve c). Curves b and c have been displaced vertically by 0.03 and 0.06 , respectively, for clarity. The solid line corresponds to the log-normal function with appropriate values for the mean and standard deviation as determined from the histograms.

Figure 7 Cross-section of a high purity polycrystalline iron sample which was etched to highlight the grain boundary.

Figure 8 Plot of average area $\bar{A}$ versus $t(\text{MCS})$ for the $Q=6, 12, 24$ and 48 Potts model following a quench from $T \gg T_c$ to $T=0$. Data is averaged over 5 runs on a 380^2 square lattice with nn and nnn interactions of equal strength. In (a) we show the data on a log-log and (b) on a linear-linear plot. The exponent n is obtained by least square fitting this data to Eq. (3).

Figure 9 Plot of $\log_{10}(\bar{A})$ versus $\log_{10}(t)$ for the Potts model on a 100^3 sc lattice for four values of Q for (a) $k=2$ and (b) $k=3$.

Figure 10 Average area $\bar{A}$ versus t on a linear scale for $Q=48$ Potts model on (a) 380^2 square lattice with nn and nnn interactions, (b) 1000^2 triangle lattice with nn inter-

actions, (c) 100^3 sc lattice with $k=2$ and (d) 100^3 sc lattice with $k=3$.

Figure 11 Averaged pinned area $\bar{A}_f$ versus inverse concentration c^{-1} for five value of Q on the triangle lattice.

Figure 12 Time dependence of the area, A_i , of individual grains from the 2-d simulation with a specific number of edges, N_e , on the triangle lattice. Symbols are shown every 20 MCS when the grain has the number of edges specified. The simulations were started from a random starting state and run for 1,000 MCS, after which the clock was reset to 0. The data plotted are for grains which had the specified number of edges over unusually large portions of the next 10,000 MCS.

Figure 13 Time dependence of the area A_i of five randomly chosen grains from the 2-d simulations. The symbols represent the number of edges, N_e . As in Fig. 12, the clock was reset to 0 after an initial run of 1,000 MCS.

Fig. 1

Fig. 2

Fig. 3a

Fig. 3b

4a

4b

5a

5b

Fig. 6

Fig. 7

Fig 10