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EVOLUTION OF 2D POTTS MODEL GRAIN MICROSTRUCTURES FROM AN INITIAL HILLERT SIZE DISTRIBUTION

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Abstract

Grain growth experiments and simulations exhibit self-similar grain size distributions quite different from that derived via a mean field approach by Hillert [1]. To test whether this discrepancy is due to insufficient anneal times, two different two-dimensional grain structures with realistic topologies and Hillert grain size distributions are generated and subjected to grain growth *via* the Monte Carlo Potts Model (MCPM). In both cases, the observed self-similar grain size distributions deviate from the initial Hillert form and conform instead to that observed in MCPM grain growth simulations that start from a random microstructure. This suggests that the Hillert grain size distribution is not an attractor.

Introduction

It has long been observed that the grain growth process in polycrystalline materials is self-similar. The grain size distribution, scaled by the average grain size, is constant over time so that a coarsened structure is statistically equivalent to a magnification of its antecedent structure. Smith wrote in 1952 that "there is probably a tendency toward a fixed distribution of shapes and relative cell sizes..." [2] The nature of this distribution has been a topic of debate since then.

Several mean field models for grain growth begin from an equation for the flux of grains as a function of the grain size and time,

$$j = - D\frac{\partial f}{\partial R} + f(R,t)\, v, \tag{1}$$

where D is a diffusion coefficient for grains in grain size-time space, v is the boundary velocity R/t, and $f(R,t)$ is the grain size distribution as a function of grain radius R and time t. The first term on the right hand side of Equ. 1 is the diffusion term; the second is the drift term.

Hillert [1] solved for the presumably self-similar $f(R,t)$ by ignoring the diffusion term, and setting v to a physically motivated but non-rigorous growth function containing a critical grain radius R_c; Lücke *et al.* later justified Hillert's v more rigorously [3]. According to Hillert's analysis,

$$f(R,t) = (2e)^d \frac{\tilde{R}\, d}{\left(2-\tilde{R}\right)^{2+d}} \exp\left(-\frac{2\, d}{2-\tilde{R}}\right), \tag{2}$$

where d is the dimensionality, $\tilde{R} = R/R_c$, and R_c is a fitting parameter [1]. Several corrections and modifications to Hillert's analysis have been proposed, but none entail dramatic changes to $f(R,t)$ for normal grain growth [3,4].

In general, the Hillert distribution is more sharply peaked and skewed to larger R than experimental data [5]. In addition, various computer simulations of normal grain growth have produced distributions which appear self-similar over time and which have the characteristics of the experimental distributions [5-8]. These discrepancies have been attributed by some to the notion that the experiments and simulations span anneal times that are too short to allow a transition to the Hillert distribution.

It is not computationally tractable to increase grain growth simulation times significantly beyond their current maxima. Therefore, it is difficult to determine whether such simulations might, given sufficient time, realize a microstructure with the Hillert size distribution. Instead, we propose an alternate approach to this problem. We create topologically realistic microstructures that obey the Hillert grain size distribution, and observe their evolution under normal grain growth conditions. Presumably, if the Hillert distribution is an attractor, these structures should evolve self-similarly from the start, maintaining the Hillert grain size distribution as they grow.

Computational Method

In order to determine if the Hillert distribution is indeed an attractor, two-dimensional zero-temperature Monte Carlo Potts Model (MCPM) simulations were performed starting from microstructures with the Hillert grain size distribution. The starting microstructures were generated using two different methods as described below. A brief review of the MCPM is provided at the end of this section.

Microstructure Generation Methods

The Hillert grain size distribution specifies the relative radii of the grains in a microstructure. However, it says nothing about the shapes of the grains, nor does it specify the coordination that the grains must assume. In his original analysis, Hillert assumed that the grains were spherical, but this is certainly not topologically realistic. Therefore, in order to generate realistic grain microstructures which adhere to the Hillert grain size distribution, we specify two criteria: 1) the shape of size distribution must match (within a reasonable tolerance) the Hillert distribution, and 2) the topology must be "realistic." To satisfy these criteria, we employ two methods for generating microstructures.

Method of Rectangular Tiling: In the first of these methods, grains are tiled on a square lattice. The distribution of grain sizes is chosen to exactly match the Hillert distribution. Since the grain lattice is uniform and the grains are of varying sizes, the grains are irregularly shaped and non-compact after tiling. Therefore, after the grains are tiled, the system is evolved for 1,000 Monte Carlo steps using the zero-temperature MCPM procedure. This serves to "round out" the anomalous grain shapes, and makes the microstructure more "realistic," but it also causes the distribution of grain sizes to deviate slightly from the Hillert distribution.

Method of Tesselation: In the second method, a Laguerre tessellation is performed by grain nucleation and growth. Grains are seeded at random and allowed to grow radially until they impinge. The number of seeds is chosen to give the desired average grain radius. The Hillert distribution is approximated by varying the rate of grain nucleation, and by varying the growth rate of each grain according to its size. After this tesselation is complete, the microstructure is "annealed" for 5,000 Monte Carlo steps using the zero-temperature MCPM procedure.

Monte Carlo Potts Model

In the MCPM [9-12], a continuum microstructure is bitmapped onto a two-dimensional lattice by assigning each lattice site an index, s_i, corresponding to the orientation of the grain in which that site is embedded. Sites with one or more unlike neighbors are boundary sites; those with only like neighbors are interior sites. The total energy of the system is specified by assigning a positive energy to boundary sites and zero energy to interior sites via the Hamiltonian,

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$$H = \frac{E_0}{2} \sum_{j=1}^{N} \sum_{i=1}^{z} \left[1 - \delta(s_i, s_j) \right], \tag{3}$$

where E_0 is a positive constant which scales the boundary energy, N is the total number of lattice sites, z is the number of nearest neighbors j of site i, and δ is the Kronecker delta function with $\delta(s_i, s_j) = 1$ if $s_i = s_j$ and 0 otherwise.

Grain growth kinetics are determined through a zero temperature Monte Carlo technique. A lattice site and an orientation are chosen at random. The orientation of the chosen site is then changed to the new orientation if and only if the system energy remains constant or decreases. Time is incremented after each attempted reorientation by ($1/N$) Monte Carlo steps (MCS). Note that a Monte Carlo temperature of zero does not correspond to a physical temperature of 0 K, but rather to a system without thermally activated fluctuations in boundary positions.

Each of the microstructures described above was evolved via a MCPM simulation. The systems contain 2000x2000 sites on a square lattice with first and second neighbor interactions and full periodic boundary conditions. Grain growth is allowed to progress until self-similarity is observed, approximately 80,000 MCS in both cases. Grain size is measured by a cluster enumeration technique which exactly measures each grain area, A. The grain radius, R, is simply the square root of A.

Results and Discussion

This section contains brief descriptions of the characteristics of the initial microstructures, the evolution of the grain size distributions during the MCPM simulations, and the implications of these results for the mean field formulation of grain growth.

Characteristics of Initial Microstructures

The starting microstructures (after "annealing," as described above) are shown in Figs. 1a and 1b. The microstructure in Fig. 1a was generated using the rectangular tiling method, and has an average grain radius of 10.7 sites. The microstructure in Fig. 1b was tessellated, and has an average grain radius of 13.9 sites. The grain size distributions for these microstructures are shown in Fig. 2, and the Hillert distribution is plotted for comparison. Both of the initial microstructures in Figs. 1a and 1b exhibit nearest-neighbor coordination that is typical of "realistic" microstructures, as shown in Fig. 3, even though topology was not used as a criterion when the microstructures were generated.

MCPM Evolution of Grain Sizes

The initial microstructures in Fig. 1 were evolved for 80,000 MC steps using the MCPM described above. In the early stages of grain evolution, the grain growth exponent is approximately 0.35 and 0.32 for the tiled and tesselated cases, respectively. Self similar growth begins at about 20,000 MC steps in both cases, and the grain growth exponent in this regime is 0.51 and 0.52 for the tiled and tessellated microstructures, respectively. The final microstructures are shown in Figs. 1c and 1d, and the final grain size distributions in Fig. 2. The average final grain radii are 28.6 and 29.5 sites for the tiled and tessellated microstructures, respectively. A scaling distribution for a 4,000x4,000 site MCPM simulation, started from a random spin configuration, is shown in Fig. 2 for comparison. The distributions of grain sizes in the final microstructures deviate significantly from the Hillert distribution, and are very close to the typical MCPM distribution. The final distributions of nearest neighbors, shown in Fig. 3, are not significantly different from that of the typical MCPM microstructure.

Shortcomings of the Mean Field Formulation

The Smith - von Neumann - Mullins law for the evolution of grain area,

$$\frac{dA}{dt} = -C(6-n), \tag{4}$$

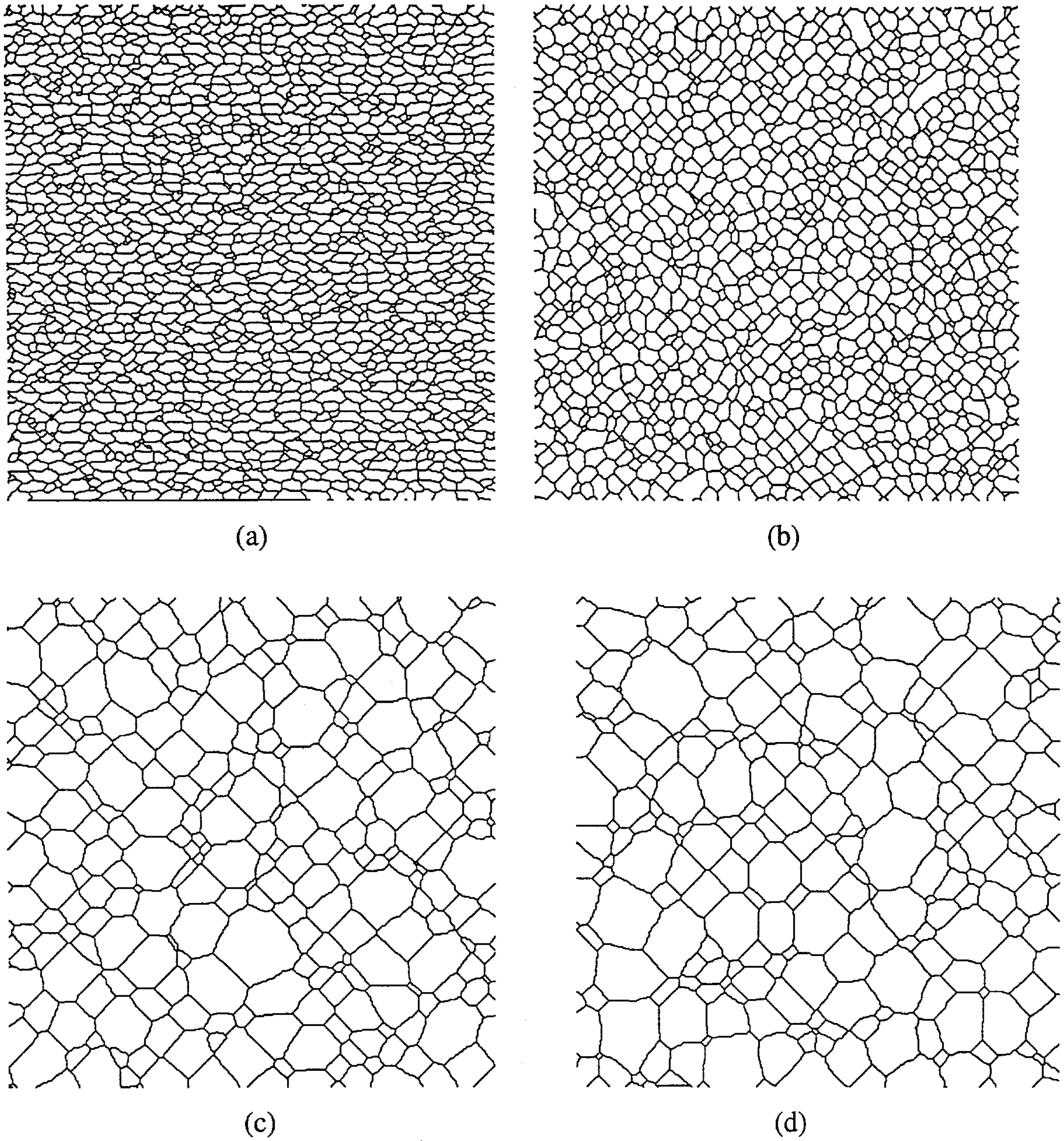

Figure 1. Images of the a) initial tiled, b) initial tessellated, c) final tiled, and d) final tessellated microstructures. The lattice size is 2,000x2,000 sites. Only 1/16 of each structure is shown.

is mathematically exact for two-dimensional, isotropic grain growth [13,14]. The rate of change in the area A of each grain is governed only by its number of corners n and is independent of the grain size and of any properties of the neighboring grains. Thus, grain growth is governed by local topology.

Since the Hillert structures generated for this study are topologically very close to a normal grain structure, their evolution should be nearly independent of their geometric details. Since they exhibit the correct topology and the Hillert grain size distribution, these structures conform to all the assumptions of the Hillert mean-field theory. The fact that they evolve away from the Hillert distribution during the MCPM simulations indicates that the Hillert distribution is not an attractor.

The dependence of grain growth on local topology also indicates a shortcoming of the radius-based mean field approach to grain growth. The rate of change in area of a given grain depends only on its topology and not on its size or the field of grains around it. However, the Hillert model postulates that a grain's trajectory in size space depends only on its size: small grains shrink and large ones grow. Although grain size and topology are empirically correlated,

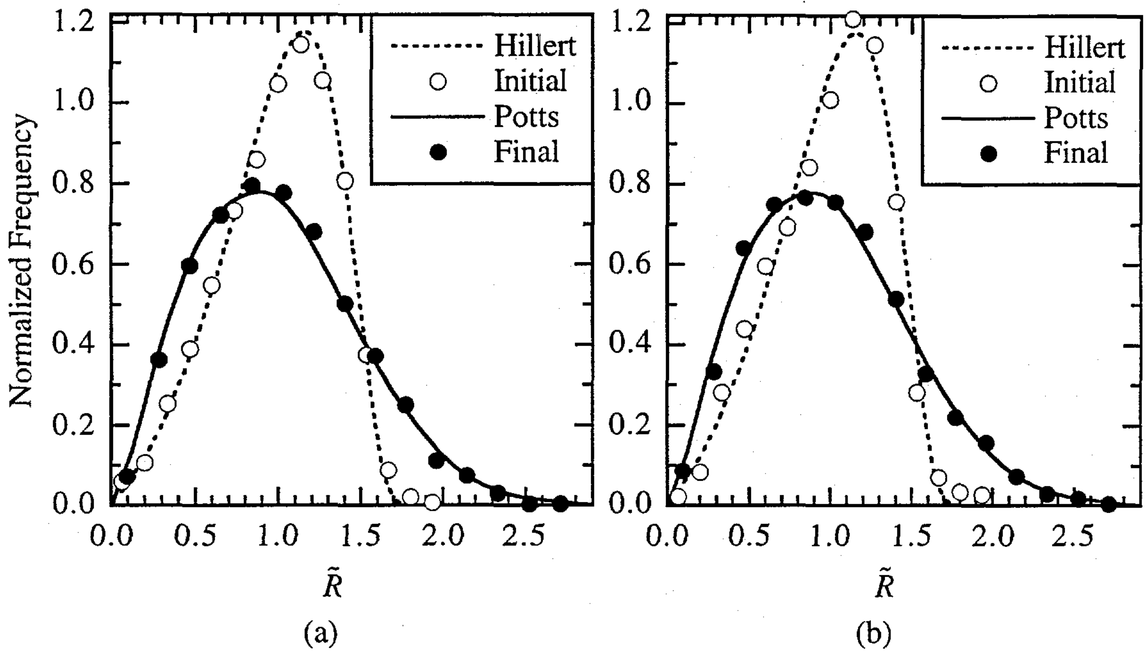

Figure 2. Grain size distributions for the a) tiled and b) tessellated microstructures. The dotted lines are the Hillert grain size distribution from Equ. 2, the solid lines are from a 4,000x4,000 site MCPM simulation started from a random grain structure, the open circles are the initial grain size distributions from this work, and the solid circles are the final distributions from this work.

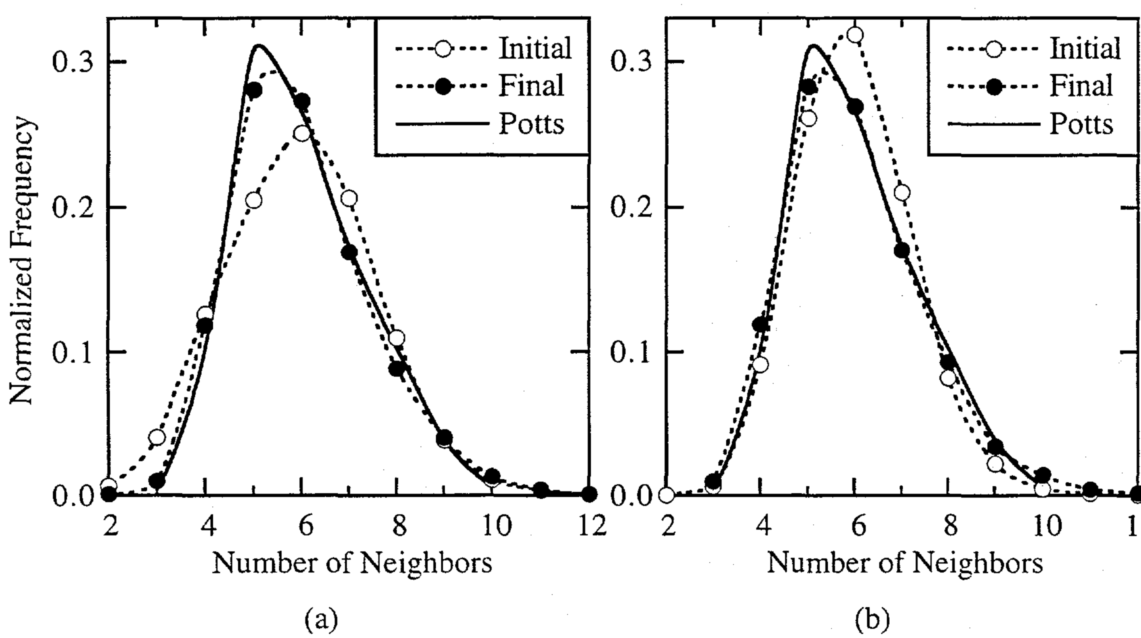

Figure 3. Grain coordination for the a) tiled and b) tesselated microstructures. The solid lines are the topology from a 4,000x4,000 site MCPM simulation, the open circles are the initial topologies from this work, and the solid circles are the final topologies from this work.

they are not necessarily linearly related. Mullins has recently shown that if the average number of neighbors is a linear function of grain size, then realistic mean field grain growth models give the Hillert grain size distribution [15]. However, even a small nonlinearity in grain neighbors vs. grain size can cause substantial deviations from the Hillert distribution. From the experimentally observed deviation from the Hillert distribution, Mullins concludes that this non-linearity is a feature of normal grain growth, attributed to size correlations between neighboring grains.

Conclusions

Two-dimensional zero-temperature Monte Carlo Potts Model (MCPM) simulations were performed starting from topologically realistic microstructures possessing the Hillert grain size distribution. During the course of the simulations, the microstructures evolved away from their initial Hillert structures, reaching self-similar grain size distributions very close to that observed in typical MCPM simulations and grain growth experiments. These results suggest that the Hillert grain size distribution is not an attractor, and that the grain size distribution observed in numerous grain growth simulations and experiments is the correct self-similar distribution.

Acknowledgments

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