Materials Microstructural Evolution in 3D Surface Front-Tracking Computer Simulations

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A fully three-dimensional surface front-tracking method for calculating the evolutionary grain growth behavior in materials has been implemented in the computer code Grain3D. Grain3D is now capable of finite element calculations for the evolution of the grain boundary surfaces on large systems, presently on the order of 1000 or more grains (over one million computational cells). In the present study, the grain growth ordering behavior is determined by examining the kinetics of a large cube of grains as a function of time.

Figure 1 shows the computation cube surfaces at the initial time of the simulation. The starting configuration for the grains is obtained by a pseudo-random generation of a specific number of nucleation sites followed by a space-filling algorithm that assigns a volume to each grain and identifies interfaces with adjacent grains. The algorithm has been constructed to approximate a Gaussian distribution of grain sizes as shown in Figure 2 for a typical starting condition of a 500-grain simulation. The present study is for the case of grain boundary motion proceeding with a velocity proportional to the local mean curvature at each point on the surface. As the calculation progresses, some grains become smaller and eventually disappear while others continue to grow. The distribution function for the system when there is a total of 328 grains is shown in Figure 3. The final state reached by all simulations is that of a single grain occupying the entire cube.

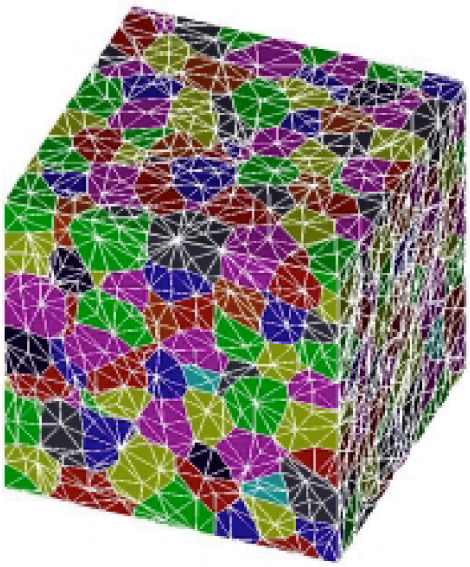

Figure 1: The computational cube at the initial configuration containing a total of 500 grains.

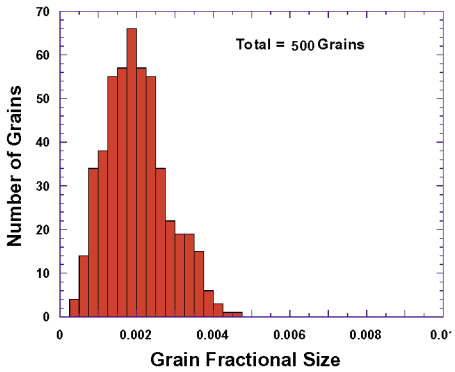

Figure 2: Histogram plot of the averge grain size distribution <size>, for the initial configuration.

As the simulation evolves in time, there are two specific grain growth rates that have been observed. First, there is an initial growth rate that is well characterized by an exponential in time. Second, there is a transition in the rate behavior to that of a power-law dependence. These growth behaviors are illustrated in Figures 4 and 5 and are in qualitative agreement of the predictions of the theory of phase ordering kinetics, i.e., initial exponential growth changing to a power-law dependence. (See the review article by A. J. Bray, Advances in *Physics*, 2000.) Further simulations are ongoing to obtain sufficient statistics to obtain accurate time dependent distribution functions of grain sizes by changing the initial conditions for the simulations.

One of the issues of the present study is the effect of the exterior surface of the computational cube on the growth rate behavior. The grains that are adjacent to this surface evolve differently in that their exterior surfaces are flat (as required by the boundary conditions) while their interior surfaces evolve according to the local curvature. By comparing results for increasingly larger size systems, and hence smaller surface to volume ratios, we hope to separate

the growth rate laws for interior bulk-like grains and surface grains. Understanding the different kinetic behavior in the two cases is important in providing a predictive capability for microstructural evolution in the presence of interfaces and where the geometry of interest is dominated by interfaces.

An important point to be made is that although the calculations described here are dependent on the evolution of the surface grid, Grain3D contains an internal volumetric grid that is necessary for the calculation of diffusion and stress properties.

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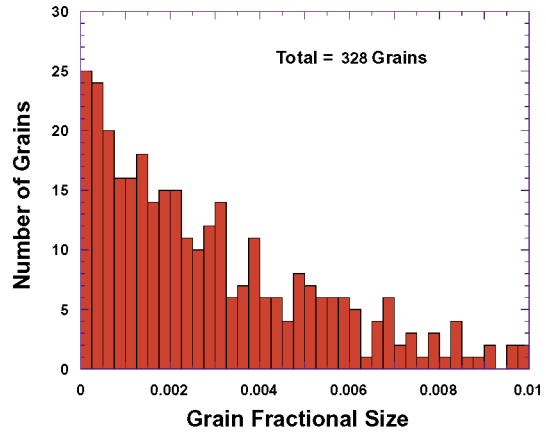

Figure 3: Histogram plot of the average grain size distribution, <Size>, after the system has evolved via the mean curvature algorithm until only 328 grains remain. The total volume is held constant.

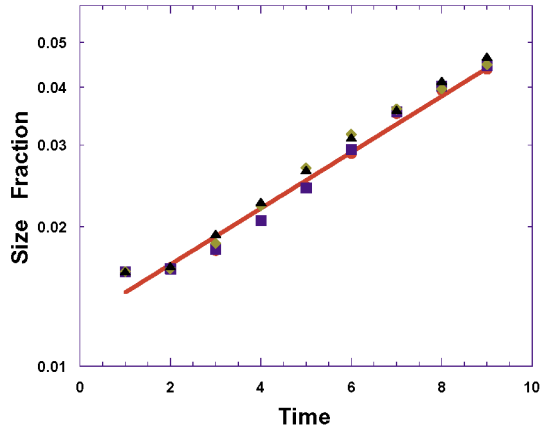

Figure 4: Log-linear plot of the early time growth rate behavior.

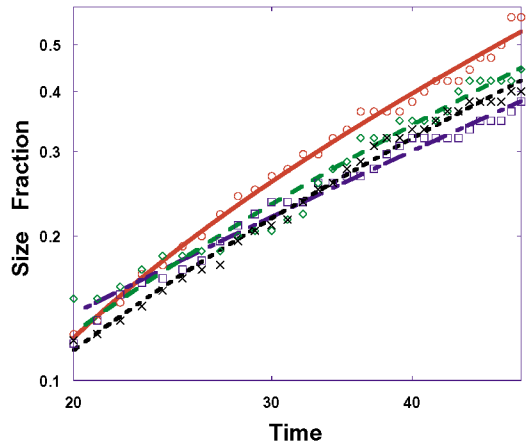

Figure 5: Log-log plot of the late time growth rate behavior. The lines are power law fits to four different simulations.