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SIMULATIONS OF THE RELATIVE IMPORTANCE OF INITIAL SIZE ADVANTAGE AND BOUNDARY ENERGY ANISOTROPY IN ABNORMAL GRAIN GROWTH (POSTPRINT)

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In textured materials, initial size advantage competes with boundary energy and mobility anisotropy as a driving force for grain coarsening. High local boundary anisotropy and large pre-existing size advantage encourage abnormal grain growth. In the present work, the importance of these driving forces relative to one another is explored for various initial grain size advantages and texture intensities using a Potts Monte Carlo approach with anisotropic grain boundary energy varying according to the Reed-Shockley model. A size greater than approximately twice the mean grain size was sufficient to virtually ensure a grain has a growth advantage regardless of texture intensity.

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Simulations of the relative importance of initial size advantage and boundary energy anisotropy in abnormal grain growth

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Abstract. In textured materials, initial size advantage competes with boundary energy and mobility anisotropy as a driving force for grain coarsening. High local boundary anisotropy and large pre-existing size advantage encourage abnormal grain growth. In the present work, the importance of these driving forces relative to one another is explored for various initial grain size advantages and texture intensities using a Potts Monte Carlo approach with anisotropic grain boundary energy varying according to the Reed-Shockley model. A size greater than approximately twice the mean grain size was sufficient to virtually ensure a grain has a growth advantage regardless of texture intensity.

1. Introduction

The control of grain size during processing is of practical significance because almost every important property of a structural metallic material is a function of grain size. Accordingly, a number of deterministic and statistical models have been developed to predict changes in grain size during annealing. These models are largely based on the original model of Burke [1] and Burke and Turnbull [2], who assumed that the pressure acting on the grain boundary is due solely to its curvature. The authors' analysis revealed that grain growth kinetics could be described by the equation D^n-$D_o^n = kt$ where D_o is the initial mean grain size, D is the mean grain size at time t, n is the grain growth exponent, and k is a constant. The original analysis yielded $n = 2$ for ideal grain growth, though this is rarely observed experimentally. Deviation from ideality may be due to specimen size, texture, or the presence of pinning defects like second phases and inclusions [3]. While numerous rules of thumb and models have been developed to describe specimen thickness and pinning particle effects, respectively, incorporating texture effects into analytical grain growth models has received considerably less attention. Notable exceptions include the work of Abbruzzese and Lucke [4] and Eichelkraut et al. [5]. These authors introduced orientation-dependent grain boundary energy and mobility into Hillert's statistical model [6] and showed that texture had a strong effect on grain growth kinetics and the development of the grain size distribution. The theory also introduced the concept that the critical grain radius, above which grains will grow and below which grains will shrink, is an orientation-dependent quantity. Thus, there is a competition in the early stages of grain growth that is set up by the spatially stochastic distribution of grains present upon the completion of recrystallization. Due to the complexity of recrystallization process (see [Doherty et al. [7] for a comprehensive review), one can expect that some grains have a slight size advantage compared to the neighbors while others have a slight mobility advantage due to having a larger misorientation angle with neighboring grains. Some small fraction of grains may have both a size and mobility advantage. In this work, we explore this competition using Monte Carlo simulations that account for the effect of grain boundary misorientation on grain boundary mobility.

2. Methodology

Potts Monte Carlo simulations with were run using the AppPottsRS code [8] in the Stochastic Parallel PARticle Kinetic Simulator (SPPARKS) framework [9]. Within AppPottsRS, the grain boundary properties (specifically, the trans-boundary diffusivity, or the product of grain boundary mobility and interfacial energy) are assumed to vary with grain boundary misorientation according to the Reed-Shockley equation. Unimodal orientation distribution functions (ODFs) were generated using MTEX [10], then random samples were taken from the ODFs and assigned to 3x3 px square blocks in a 1500x1500 px 2D grid, creating 2.5E4 simulated grains. A 180° halfwidth was used to approximate a uniform orientation density function (i.e., a polycrystal with randomly oriented grains). Upon this grid, another evenly-spaced grid of 400 grains was superimposed, with each of the 400 grains given sized uniformly as either 4x4 px, 5x5 px, 6x6 px, or 9x9 px. The superimposed grid thus presents a set of grains with a pre-existing size advantage. The 400 grains in the superimposed grid were all assigned an orientation of the modal value of the ODF. By assigning all grains without an initial size advantage to have identical sizes, the present work deliberately avoids the additional complicating role of grain size distribution (which is known to have an effect on final grain size and grain growth rates [11]). Potts Monte Carlo simulations were then run for 40 Monte Carlo steps (MCS), since after this time grains with the initial size advantage impinged upon each other under some simulation conditions.

3. Results and Discussion

Figure 1 shows pole figures (top row) corresponding to the ODFs from which the grain orientations in the corresponding inverse pole figure maps (bottom row) were sampled. The bottom row shows inverse pole figure (IPF) maps of the results after 20 MCS of the simulations that initially contained 6x6 px "seed grains" with pre-existing size advantage of the 6x6 px simulations after 20 MCS. In the pole figures, the texture intensity decreases from left to right, with 1°, 5°, 10°, 15° and 180° halfwidths. Note in the IPF maps that the grid of "seed grains" with the initial size advantage become more apparent from the left to the right, such that nearly all of these grains with the size advantage persist to 20 MCS while their neighbors are eliminated.

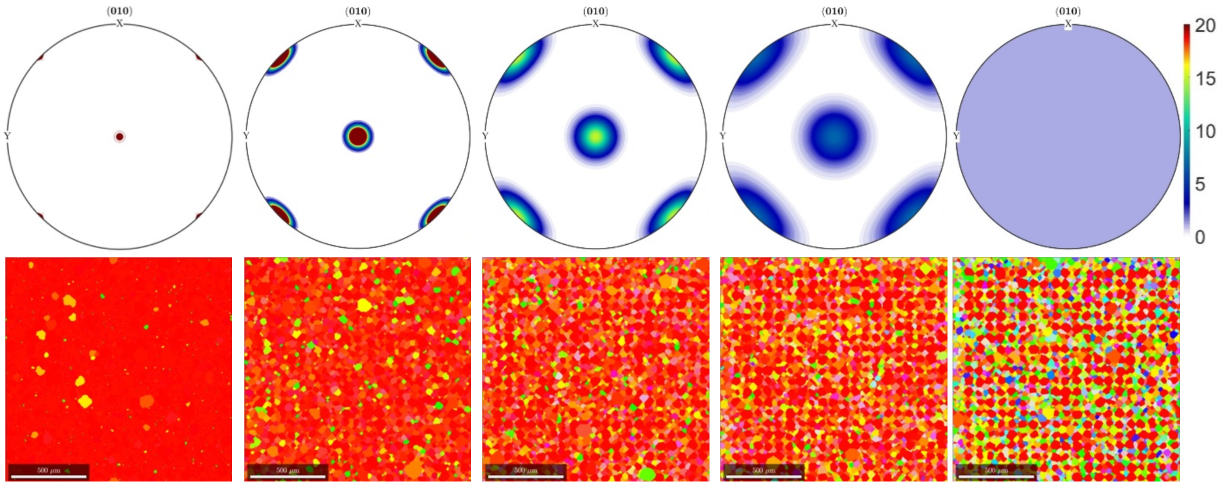

Figure 1: (001) pole figures for initial simulation conditions and corresponding normal-direction inverse pole figure maps after 20 MCS. Left to right: 1°, 5°, 10°, 15° and 180° halfwidths. The pole figure colorbar range is from zero to 20 in times random. Red in the inverse pole figure corresponds to the [001] crystal direction. Scale bar lengths correspond to 500 px.

The structure of the simulation is illustrated in figure 2, which displays snapshots of the results of simulated grain structure evolution for the case of the 180° halfwidth with 9x9 px square "seed" grains in a matrix of uniform 3x3 px square grains. The initial condition is shown on the left, while the center shows the results at 5 MCS and the right shows the simulated microstructure after 20 MCS. The whole microstructure is shown in the top row with each grain being plotted in a unique color, while the bottom row highlights the arrangement of the "seed" grains given an initial size advantage.

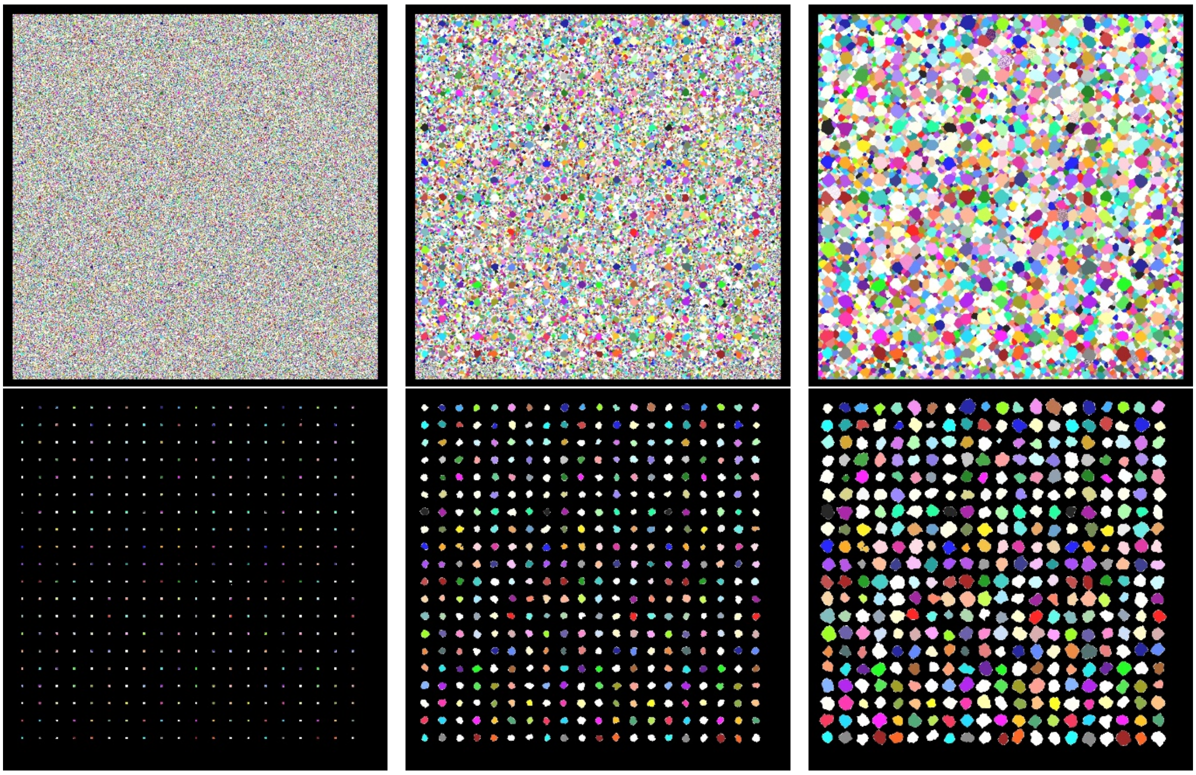

Figure 2: Simulated grain structure evolution for uniform boundary properties and 9x9 px "seed" grains in matrix grains uniform 3x3 px size. Colors indicate unique grain IDs. Left column: initial state; Middle column: 5 MCS; Right column: 20 MCS. Top row: overall structure; Bottom row: Only "seed" grains given a pre-existing size advantage shown.

Figure 3 shows the evolution of the mean circle equivalent grain size, <R>, in px with number of Monte Carlo steps (MCS) completed. The data has been split into four with each subplot displaying all texture intensity cases with the same initial seed grain size. The solid line (darkest color) corresponds to the case of a uniform ODF, the dashed line corresponds to the case of the 15° halfwidth, the dash-dot line to the 10° halfwidth, dotted line to 5°, and solid lightest color line to 1°. Since the grain growth rate varies significantly with the boundary energy on account of the texture, all subsequent analyses comparing the behavior in the different simulations are performed with respect to the mean grain size in the system as opposed to the Monte Carlo step, to facilitate comparisons between the different simulations.

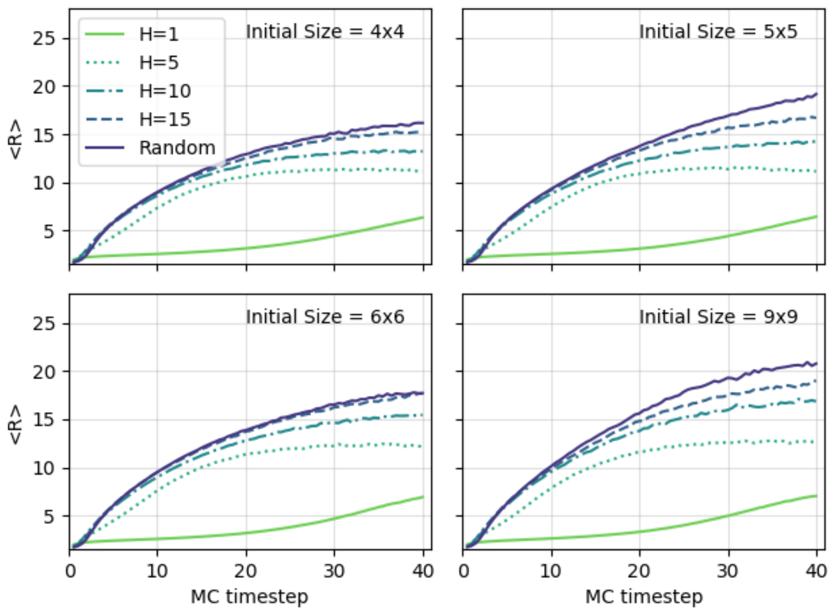

Figure 3: Evolution of mean grain size vs. number of Monte Carlo steps.

Figure 4 shows the number of retained "seed" grains vs mean grain size in the simulation. The linestyles are the same as those used for figure 3. Larger initial size results in a greater fraction of the "seed" grains persisting longer in the simulation. In the case of a size advantage of approximately two times the mean equivalent diameter, the probability of the neighborhood topology being such that the large grain is overcome by its neighbors becomes negligible for the 180° halfwidth ODF (approximating a random polycrystal, labeled "random" in figure legends). As texture intensity increases, the effect of pre-existing size advantage is reduced.

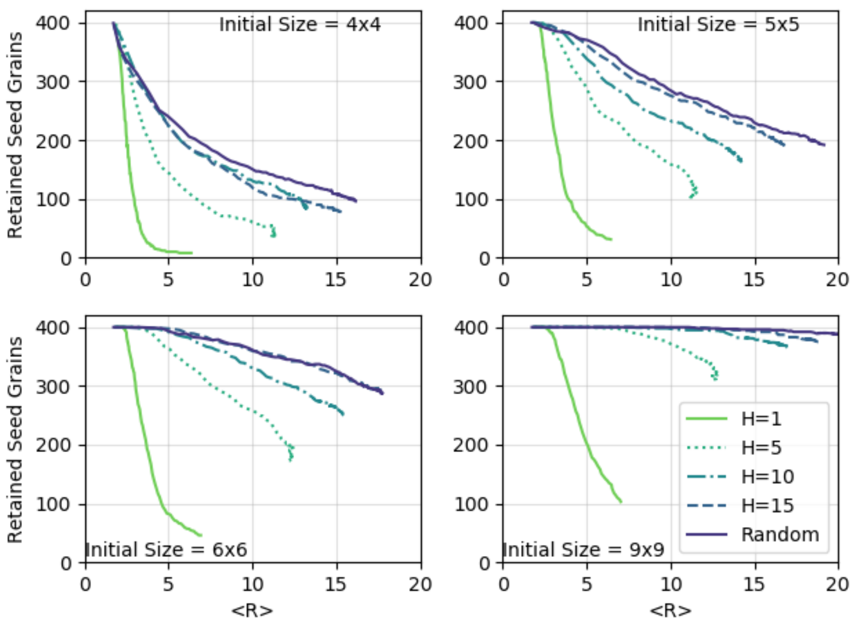

Figure 4: Number of retained seed grains vs. mean grain size during simulated grain coarsening. H=1 corresponds to a 1° halfwidth of the unimodal texture distribution, H=5 to 5° and so on. Line styles are the same as in previous figures.

The observation that pre-existing size advantage is mitigated by texture strength is reinforced in figure 5, which shows the evolution of the fraction of the grains in the system that were originally seed grains. If the seed grains exhibit no initial growth advantage, their line appears approximately horizontal, maintaining the initial ~0.02%. This only occurs for the highest texture strength, and is lost for the largest size advantage. For all other texture strengths investigated, even a small initial size advantage drastically increases the likelihood that a grain will be among the grains that remains at the end of 20 MCS.

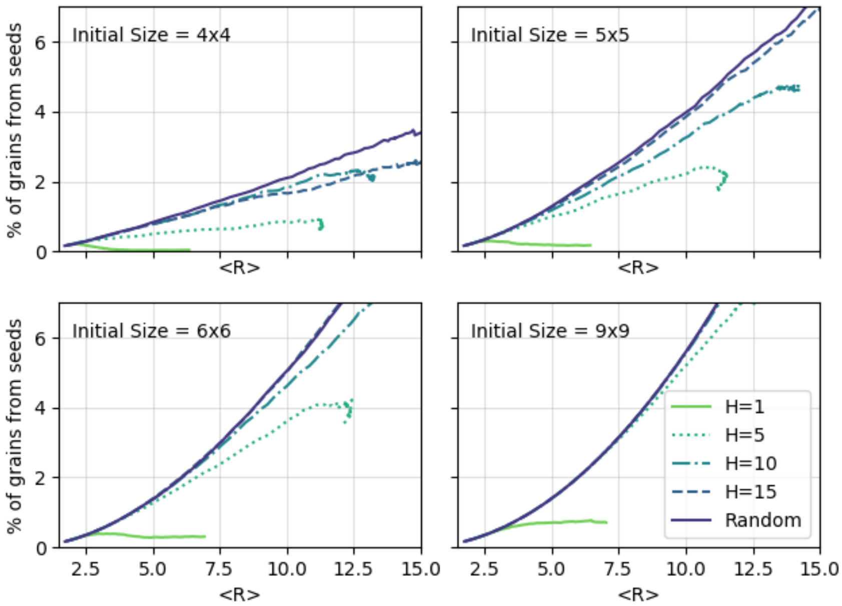

Figure 5: Evolution of the fraction of grains in the system that were “seed” grains given an initial size advantage. H=1 corresponds to a 1° halfwidth of the unimodal texture distribution, H=5 corresponds to 5°, and so on. Line styles are the same as in previous figures.

The misorientation angle distributions for the initial state and after 20 MCS are shown in figure 6. The shape of the 180° halfwidth distribution compares well with the expected Mackenzie distribution both initially and after 20 MCS. As evidenced by the increase in the peak of the 1° halfwidth distribution over the course of the 20 MCS (comparing left and right plots), the texture intensity increases during this simulation. This does not appear to be a strong effect in the other cases.

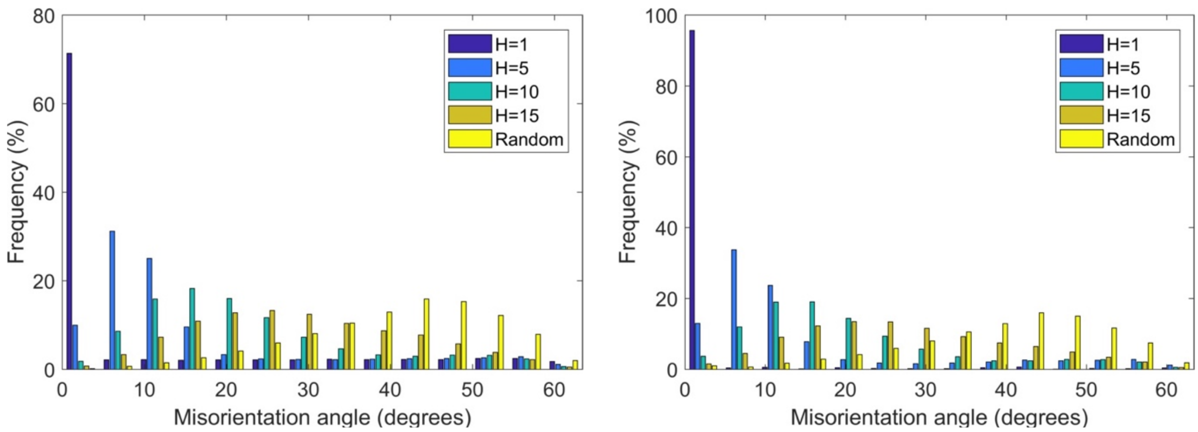

Figure 6: Misorientation distributions in the simulation. Left: Initial condition; Right: after 20 MCS.

The 10° halfwidth texture peaks around 15 times random. The present results suggest that, as a texture intensity reaches above 15 times random, the fraction of low angle boundaries increases to the point that grain neighborhood begins to matter to the extent that grains slightly larger than average do not have a significant advantage over other grains in the system which have randomly been assigned favorable neighborhoods. In light of this, a pressing question is how to characterize the frequency of neighborhoods that enable size advantages to develop in the first place, since obtaining a 2x the mean size advantage drastically increases the likelihood that a grain will persist for a long time during coarsening. Even in the absence of a size advantage, abnormal grain growth can occur when a single sharp texture component exists due to random fluctuations in local texture intensity. For mechanical processing routes that produce two or more texture components, an isolated grain that is highly misoriented with respect to its neighbors is likely to have higher volatility to its grain boundary mobility. These grains are either likely to rapidly disappear or become grains with an early size advantage, which may subsequently grow abnormally.

4. Conclusions

The present work analyzes a rather idealized case of grain coarsening in the presence of textures in order to gain insights into the relative importance of initial grain size on subsequent grain structure evolution in a textured polycrystal. Our results reveal the larger a grain is relative to the mean, the more likely it is to still exist at a snapshot of a later time during grain coarsening up to very strong texture intensities in excess of 15 times random. A size advantage of 2x the mean equivalent diameter appears to virtually guarantee that a grain has a sufficient size advantage over its neighbors to be among the grains that is not eliminated when less than 1% of the original grains remain.

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