Particle-Assisted Abnormal Grain Growth

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Abstract. Abnormal grain growth is observed in systems that are nominally pinned by static particle dispersions. We used mesoscale simulations to examine grain growth in three-dimensional polycrystals containing stable, inert particles located at grain boundaries. In the absence of pinning particles, only normal grain growth occurs. When particles are present, some normal grain growth occurs, until a Zener-Smith pinned state is achieved. However, after a long incubation time, a few grains can thermally fluctuate away from their particle clouds and grow abnormally. The abnormal events are rare and stochastic. The abnormal grains are always among the largest initial grains, but most of the largest initial grains do not grow abnormally.

Introduction

Abnormal grain growth (AGG) occurs in a wide variety of metallurgical systems: textured and nontextured metals, thin films, strained systems, nanocrystalline materials, and systems with second phase precipitates. The proposed mechanisms for AGG are equally varied, including grain boundary energy anisotropy, inhomogeneous strain energy density, initial size advantage, favorable free surface energy, and grain boundary mobility variations. Clearly, AGG is one phenomenon with many causes.

Particularly baffling is the occurrence of AGG in polycrystals that are nominally stable due to the presence of inert, static pinning particles [1]. Dispersions of second phase particles are often used to inhibit normal grain growth in polycrystalline metals [2]. Since the particles exert a pinning force that balances the curvature driving force for grain growth (as first described by Zener and Smith in 1948 [3]), it stands to reason that they should prevent abnormal grain growth as well. However, AGG is observed in systems that are nominally pinned by static particle dispersions, such as nickel-based superalloys [4].

In this paper we describe a new mechanism by which static second phase particles not only fail to inhibit AGG, but actually cause it to happen. We term this phenomenon 'particle-assisted abnormal grain growth.'

System and Methods

We were inspired by a recent simulation result by Roberts [5], who observed a few instances of AGG in nominally pinned microstructures that contained particles preferentially located on grain boundaries. We wanted to devise a model system to better understand the cause and phenomenology of AGG in systems with static pinning particles.

We began with equiaxed, nontextured, 3D grain structures grown via a Monte Carlo Potts model (MCPM) grain growth simulation to various initial grain sizes [6]. We assigned uniform and isotropic grain boundary properties (energy and mobility), and then deposited pinning particles, which were 3x3x3 cubes of inert sites ($r = 3$), at random on the grain boundaries. The polycrystal

was then annealed using a standard MCPM simulation [7-10]. Under these conditions, the only driving force for microstructural evolution is the normal, isotropic curvature driving force for grain growth.

As with all particle pinning simulations, the system sizes are required to be rather large [11]. Each simulation used a system of at least 150^3 lattice sites evolved for at least one million Monte Carlo timesteps at a simulation temperature of 1.5. Because AGG in particle pinned systems is rare and stochastic, we ran many independent trials. Achieving this throughput required us to utilize an efficient, parallel kinetic Monte Carlo code that can run on both workstations and large cluster computers [12].

Results and Discussion

In the absence of pinning particles (particle volume fraction $f = 0$), the isotropic growth conditions ensure that grain growth proceeds normally and uniformly to a single crystal state.

For a grain diameter $R_0 = 10$ and particle fraction $f \leq 8\%$, the grain structure is not initially pinned. Upon annealing, some normal grain growth occurs until a pinned grain size is achieved. In the pinned state, not all the particles are located on grain boundaries. The final pinned grain size is approximately the Zener-Smith pinned size predicted by similar simulations for spatially random particle distributions [11]. This pinned state appears stable for at least 10^6 timesteps.
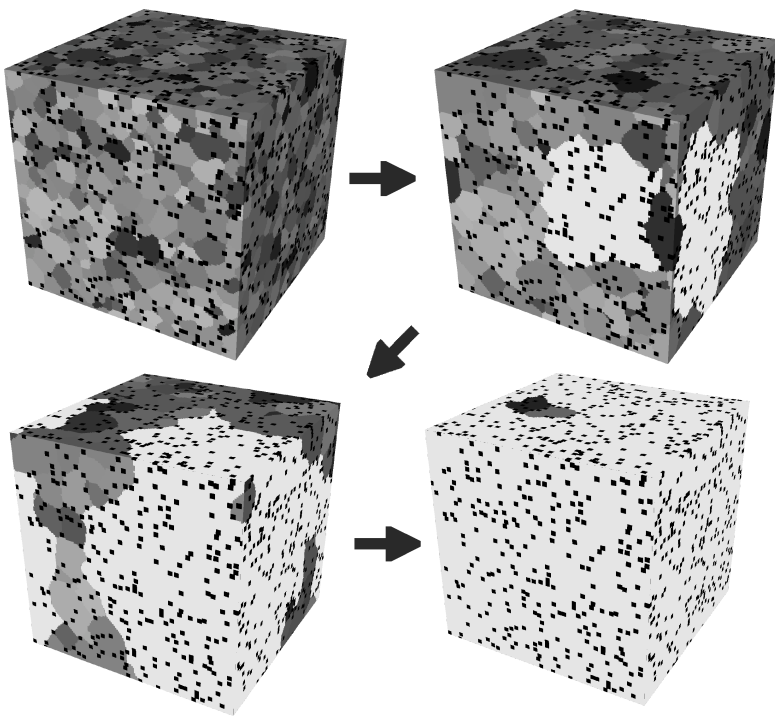

Figure 1. Abnormal grain growth in a particle-pinned system. The initial grain structure (upper left) is equiaxed, with particles decorating the grain boundaries. After some incubation time, an abnormal grain appears (light gray grain in upper right structure). The abnormal grain grows (lower left) and eventually consumes the other pinned grains (lower right). Particles are shown as black squares.

In a system with a particle volume fraction $f = 10\%$ and the same initial grain diameter, the microstructure also grows to a grain size approximately equal to the Zener-Smith pinned size. However, we found that after long anneals, a few grains grow abnormally, as shown in Fig. 1. The initiating event is a grain boundary that thermally fluctuates off of its pinning particles. If the free boundary belongs to a grain that is inclined to grow, it will grow without hindrance from its neighboring grains, since their boundaries remain immobile. Likewise, the particles do not inhibit the growth of the abnormal grain, since it has more neighbors, thus more driving force for growth, than the average, pinned grains. As the grain grows, its size advantage – thus its ability to grow at the expense of its neighbors – increases. In the right local environment, the result is persistent, abnormal growth of the free grain. Thus, we find the counterintuitive result that pinning particles cause AGG in systems not otherwise inclined to grow abnormally. This is particle-assisted abnormal grain growth.
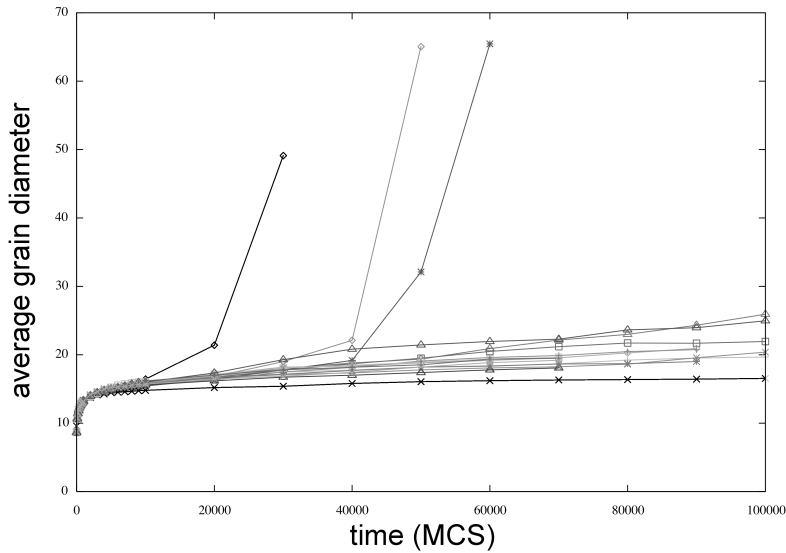
Figure 2. Grain growth kinetics for 15 independent simulations with particle volume fraction of 10%. All systems initially grow from initial grain diameter of 10 to the Zener-Smith pinned size of approximately 22. Most systems remain stagnant up to 10^5 timesteps, but in three cases, an abrupt increase in grain size indicates an abnormal grain growth event occurs.

Figure 2 shows grain growth kinetics for 15 independent simulations with $R_0 = 10$ and $f = 10\%$ over 10^5 timesteps. All the systems grow briefly, then stagnate at a grain size approximately equal to the Zener-Smith pinned grain size of 22 [11]. However, three simulations result in AGG events, indicated by a sudden increase in average grain size. It is interesting that AGG occurs at different times in different systems, indicating that it is a stochastic process. Once AGG takes place, the abnormal grain grows quickly to consume the system, so we typically can observe only one abnormal event per system. Although the other systems in Fig. 2 appear to stagnate, we found that in longer anneals (up to 10^6 MCS) every one eventually underwent an AGG event.
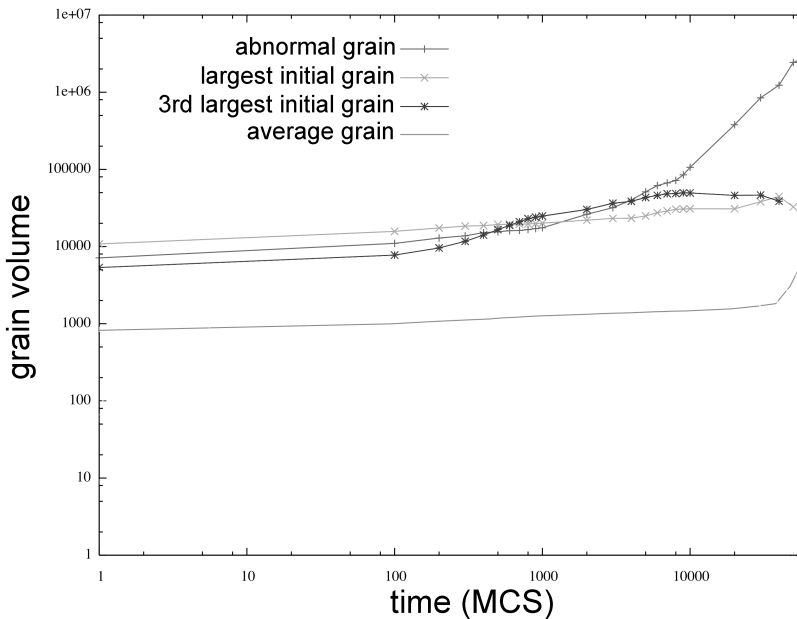

Figure 3. The kinetics of growth of the three largest grains and the average grain in a system that evolves via particle-assisted AGG. The eventual abnormal grain begins as the second largest grain. The largest grain shows no signs of abnormal growth.

In analyzing the abnormal grains, we find that they are always among the largest initial grains, but they are often not the largest, which is in agreement with experiments that suggest that size must be coupled with some additional advantage to cause AGG [13]. Figure 3 shows the kinetics of growth for the three largest grains in a microstructure that eventually undergoes AGG. These three large grains are about 14 times bigger by volume than the average grain, which is only a factor of about 2.4 in grain diameter; thus, the largest grains are well within the normal grain size distribution for an equiaxed microstructure.

The eventual abnormal grain begins as the second largest grain in the system and initially grows at about the same rate as the largest grain. Interestingly, the third largest grain initially grows faster

than both of the larger grains and surpasses them in size for a while. However, at around 1000 MCS, the abnormal grain begins growing much faster, presumably due to a critical boundary breakaway event. It quickly becomes the largest grain in the system and ultimately consumes the others. The average grain size evolves very little until the abnormal grain has become very large.

While the abnormal grain always begins as a large grain, most large grains never grow abnormally. We were unable to find a simple marker to determine which grain in an initial microstructure would become abnormal. For example, in a particular underlying grain structure, different random particle placement causes different grains to become abnormal. In addition, in a given grain/particle structure, different grains may become abnormal depending on simulation parameters (i.e. simulation temperature, choice of computer code, etc.). These observations reinforce the conclusion that particle-assisted AGG is a stochastic phenomenon.

Conclusions

Abnormal grain growth is a single phenomenon with many causes. The observation of AGG in polycrystals that are nominally stable due to the presence of inert, static pinning particles is particularly perplexing. Mesoscale grain growth simulations of 3D polycrystals containing static particle dispersions exhibit AGG in systems that do not evolve abnormally in the absence of particles. The AGG mechanism is the thermal fluctuation of a grain boundary away from its particle cloud. Because AGG does not occur in these systems without a particle dispersion, we term this AGG mechanism particle-assisted abnormal grain growth. Particle-assisted AGG adds a new explanation for the AGG phenomenon in a previously baffling class of materials.

Acknowledgements

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