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A NEW PERSPECTIVE ON TEXTURE EVOLUTION

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Abstract. Modeling and analysis of texture evolution in polycrystalline materials is a major challenge in materials science. It requires understanding grain boundary or interface evolution at the network level, where topological reconfigurations (critical events) play an important role. In this paper, we investigate grain boundary evolution in a simplified one-dimensional system designed specifically to target microstructural critical event evolution. We suggest a stochastic framework that may be used to model this system and compare predictions of the model with simulations. We discuss limitations and possible extensions of this approach to higher-dimensional cases.

Key Words. Grain boundary character, Coarsening, Texture, Continuous time random walk, Boltzmann equation.

1. Introduction

Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites, grains separated by interfaces, grain boundaries. The energetics and connectivity of the network of boundaries are implicated in many properties across all scales of use, for example, functional properties, like conductivity in microprocessor wires, and lifetime properties, like fracture toughness in structures. Engineering a microstructure to achieve a desired set of performance characteristics is a major focus in materials science. In contemporary terms, this has led to new automated data acquisition techniques, and now we are confronted with the issue of providing accurate and predictive descriptions, theories, and models. Even though this is an important and interesting subject by itself, it is also an excellent prototype for the study of multiscale phenomena.

Of course, from a multiscale viewpoint, one may aspire to begin with a molecular description of a subset of a large granular system or cellular network, and then derive a theory for its local or mesoscale behavior, and finally pass to the macroscopic state. A special advantage in our situation is that there is a well developed local thermodynamic theory based on work of Mullins [5], Herring [2], and many others, that covers normal evolution, which is the mesoscale regime. To accomplish the passage to macroscopic level, what is frequently termed upscaling in porous media networks, we need to introduce some new quantities. Indeed, it is commonly accepted that material characteristics can be traced to statistical properties of the grain boundary network. A significant advantage of the simulation platform is our ability to alter various features to assess their role or importance in a manner more flexible than nature herself permits. Historical emphasis here has been on the geometry, or more exactly, on statistics of simple geometric features of experimental

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and simulated polycrystalline networks, like grain area. More recently, attention has been turned to texture, the mesoscopic description of arrangement and properties of the network described in terms of both crystallography and geometry. However, the mechanisms by which the robust distributions develop from an initial population are not yet understood. As a polycrystalline configuration coarsens, facets are interchanged, some grains grow larger, and other grains disappear. Further, when triple junctions collide, new boundaries are created. We refer to these topological rearrangements as critical events. They play an important role in the evolution of distribution functions, as we explain below. In this paper, we investigate a simplified a one-dimensional system designed specifically to target critical event evolution in microstructure and its effect on texture. We use ideas from the kinetic theory of gases to study the stochastic characteristics of a one-dimensional system of grain boundaries moving under a gradient flow. We think that this model possesses some of the main features of an interacting grain boundary network in a typical polycrystalline microstructure.

In recent years, we have witnessed the introduction of automated data acquisition technologies in the materials laboratory. This has permitted the collection of statistics on a vast scale and stands to enable an important bridge between experiments and mesoscopic simulations. There are situations, for example, where it is possible to quantify the amount of alignment or misalignment sufficient to produce a corrosion resistant microstructure [1]. To rise beyond this level of anecdotal observation, the thermodynamics of the material system must be related to texture and texture related properties. Said in a different way, are there any texture related distributions which are material properties? Some geometric features of the configuration, like relative area statistics have these properties in the sense that they are robust but they are not strongly related to energetics. Recent work has provided us with a new statistic, the grain boundary character distribution, which has enormous promise in this direction. Owing to our new ability to simulate the evolution of large scale systems, we have been able to show that this statistic is robust and, in elementary cases, easily correlated to the grain boundary energy [9]—[11].

As mentioned, the regular evolution of the network of grain boundaries in two dimensions is governed by the Mullins equations of curvature-driven growth, supplemented by the Herring condition of force balance at triple junctions—a system of parabolic equations with natural boundary conditions [12]–[7]. For the higher dimensional formulation of capillary driven growth, see [8]. When applied to a single evolving $n-$sided grain with constant grain boundary energy, this mechanism leads to the Mullins-von Neumann $n-6$ rule [3]—the rate of change of the area of the grain is proportional to $n-6$, i.e.,

$$\frac{dA_n}{dt} = \gamma(n-6) \text{ where } A_n \text{ is the area of an } n\text{-sided grain,} \tag{1}$$

and $\gamma > 0$ is some material constant. MacPherson and Srolovitz [13] have given, very recently, higher dimensional generalizations of the $n-6$ rule. In particular, from (1), grains with $3, 4$ or 5 sides decrease in area. When averaged over a population of grains, equation (1) results in

$$\frac{d\bar{A}_n}{dt} = \gamma(n-6) \text{ where } \bar{A}_n \text{ is the average area of } n\text{-sided grains.} \tag{2}$$

Inspection of Fig. 1 shows that, contrary to (2), the average area of five-sided grains in a columnar aluminum structure increases several fold over the course of