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ScienceDirect

Acta Materialia 78 (2014) 125–134

Acta MATERIALIA

www.elsevier.com/locate/actamat

Grain growth in four dimensions: A comparison between simulation and experiment

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Received 6 January 2014; received in revised form 6 June 2014; accepted 7 June 2014
Available online 16 July 2014

Abstract

A 3-D isotropic phase field simulation was used to predict the morphology of individual grains during grain growth. The simulation employed a polycrystalline array of titanium alloy Ti-β-21S experimentally characterized by X-ray tomography as an initial condition. The non-destructive nature of X-ray tomography allowed for a second characterization of the same sample following coarsening induced by a heat treatment. Thus, direct comparisons of individual grains between simulation and experiment could be made. Although the experimental system appeared isotropic from a statistical standpoint, direct examination of individual grains revealed very distinct anisotropy in the grain boundaries on the local scale. The comparison between experiment and phase-field simulations revealed regions with excellent agreement, despite the complex topological changes grains may undergo during grain growth. Thus, the sequence of topological transitions that occurred experimentally is correctly captured by the phase-field model. We therefore conclude that this phase-field model for isotropic systems has been verified experimentally.

Keywords: Phase-field method; Grain growth; X-ray tomography; Simulation

1. Introduction

The dynamics of grain boundaries in polycrystalline structures has been a topic of great interest for many years. There has been a great deal of study on grain growth in two dimensions both theoretically [1–3] and experimentally [3,4]. Recently, there has been a resurgence of interest in the dynamics of 3-D grain growth, with the generalization of the 2-D von Neumann–Mullins relation to three dimensions [5], examination of the topology of ideal grain systems [6] and large-scale computer simulations of grain growth [7,8]. Although the growth rate of a grain in an isotropic system is known as a function of its interface morphology, predicting the evolution of even an isotropic polycrystalline material remains challenging due to the topological changes associated with face creation and elimination that occur during grain growth [9–11]. Experimental investigations of 3-D grain growth have typically focused on static structures, since the methods used to interrogate the samples were destructive. As a result, comparisons between theory, simulation and experiment were made using statistically averaged properties. To avoid the effects of initial conditions, studies of the grain structure are usually carried out in the self-similar coarsening regime. Because comparisons with the predictions of theory and simulation are, by necessity, statistical in nature, typical quantities measured tend to be limited to metrics such as number of faces per grain, grain size distribution and other averaged topological quantities. Thus, it is necessary to

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http://dx.doi.org/10.1016/j.actamat.2014.06.028
1359-6454/

collect large experimental data sets that contain many thousands of grains. These experimental studies have clearly illustrated the importance of grain boundary energy anisotropy in the evolution of grain structures [12–14] and grain topology [15] during grain growth.

By contrast, X-ray-based techniques are non-destructive in nature, and as such provide opportunities for direct studies of microstructure evolution during, for example, phase transformation, recrystallization or grain growth. For example, Offerman et al. examined the nucleation and growth of individual ferrite grains during the austenite-to-ferrite phase transformation in a carbon steel. The X-ray technique employed allowed the dynamics of individual grains to be measured, thereby enabling a direct comparison to theory without recourse to statistical measures [16]. Using 3-D X-ray diffraction microscopy it was possible to examine the growth of individual grains during recrystallization [17,18]. This has more recently been extended by Hefferan et al. to a full 3-D characterization of recovery and recrystallization in high-purity aluminum using high-energy X-ray diffraction microscopy [19]. 3-D X-ray diffraction microscopy has also been applied to studies of grain growth comparing the evolution of the same 3-D structure at two different annealing times in an aluminum alloy [20]. Syha et al. extended such non-destructive 3-D characterization to studies of grain growth in ceramics using diffraction contrast tomography [21,22]. These works clearly show the potential of grain-resolved X-ray diffraction techniques for studies of microstructural evolution in polycrystalline materials. However, although the spatial resolution of such diffraction-based techniques continues to improve, the currently attainable spatial resolution is lower than what can be achieved with direct X-ray imaging methods such as, for example, absorption-contrast tomography or phase-contrast tomography. Thus, in order to acquire the high-fidelity grain shape information necessary for modeling polycrystalline morphologies, the current study makes use of edge-enhanced tomography combined with special heat-treatment procedures to allow for detailed, yet non-destructive characterization of 3-D grain structures [23].

In addition to experimental investigations, insight into grain growth has also been sought through theory and simulation with a variety of different approaches. One such approach to modeling grain growth that allows the morphology of individual grains to be determined involves explicitly tracking the grain boundaries that separate each grain. Assuming a system with an isotropic grain boundary energy and mobility, the velocity at a point on the boundary is proportional to the local mean curvature of the grain boundary:

$$V = -MH \tag{1}$$

where V is the interfacial velocity in the interface normal direction, M is the orientation-independent reduced mobility (the product of the grain boundary energy and mobility), and H is the local mean curvature. This approach requires that the location and morphology of the boundaries be tracked explicitly. To reduce the complexity of meshing each boundary in the system, some approaches only follow the location of the grain boundary vertices, e.g. triple junctions in two dimensions or allow for some curvature in the boundary by introducing a point on the grain boundary in the center of a face [24–26]. Relatively few simulations have discretized the entire grain boundary surface due to the need to repair the mesh when a grain loses or gains a face. This rendered most of these methods computationally inefficient and was limited to systems with at most some hundreds of grains [27]. Recently, however, these limitations have been overcome allowing fully resolved 3-D calculations with hundreds of thousands of grains [8,11,28].

Phase-field methods also permit the curvatures and shapes of individual grains to be determined. In this case, an interface is described implicitly using an order parameter that varies smoothly across the boundary between grains. Thus there is no need to track the location of a sharp interface. Instead partial differential equations are solved at all positions in the system to determine the time evolution of the order parameters. There are three broad categories of phase-field methods used to model grain growth. The first was inspired by models of order–disorder processes in materials [29]. In this case, a non-conserved order parameter, η_i is assigned to grain i, where $i = 1, 2, \ldots N$ for a system with N distinct grain orientations. The free energy of the system, F, is then written as:

$$F = \int_V \left(f(\eta_1, \eta_2, \ldots, \eta_N) + \sum_{i=1}^{N} \kappa_i |\nabla \eta_i|^2 \right) dV \tag{2}$$

where V is the volume of the system, f is the bulk free energy, and κ_i is the gradient energy coefficient of grain i. The bulk free energy f is chosen to have minima of equal depth for each grain orientation, i.e. for $\eta_i = 1$, and $\eta_{j \neq i} = 0$. These order parameters are then evolved in time by the Allen–Cahn equation [30]:

$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta F}{\delta \eta_i} \tag{3}$$

where L is the mobility of the order parameter. There are no constraints on the value of the sum of the order parameters at grain boundaries or trijunctions, although the parameters can be chosen such that the sum of the order parameters is 1 across grain boundaries [31]. This method has been extended to systems with orientation-dependent and mobility-dependent grain boundary properties [31–34]. A second class of methods involves order parameters that are interpreted as the volume fraction of phases [35]. The sum of the order parameters must thus be one at all points by definition. An advantage of this approach is that they can easily be extended to the complexities of multi-phase multicomponent alloys. This model also recovers the classical motion by mean curvature result. Consistent with the constraint on the sum of order parameters, the