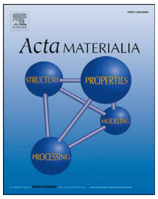
Acta Materialia 103 (2016) 681–687

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat



Full length article

Parsing abnormal grain growth

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ARTICLE INFO

Article history:
Received 10 July 2015
Received in revised form 19 September 2015
Accepted 22 October 2015
Available online 18 November 2015

Keywords:
Grain growth
Microstructure
Statistics
Processing

ABSTRACT

Abnormal grain growth, the enlargement of a minority of grains in a polycrystal at the expense of the surrounding grains, occurs in both metallic and ceramic materials and can have a profound impact on their mechanical and electrical properties. Somewhat surprisingly then, there is little consensus as to which specific microstructural features provide a signature of abnormal growth. Indeed, some workers describe this phenomenon in terms of a bimodal grain size distribution, often without justification, while others focus on very few, elongated grains. Using specialty alumina (i.e., high-purity aluminum oxide with tailored impurity composition) as our prototype, we describe here a set of practical maps and metrics that are useful in quantifying various microstructural features that are associated with abnormal grain growth. These maps provide a visual “fingerprint” of abnormal growth, while the metrics permit the design of processing routes to obtain desired microstructures. We then present an application of correlation analysis that illustrates the efficacy of data analytics in quantifying which input (i.e., processing) variables exert the strongest influence on abnormal grain growth. Finally, we outline the use of this methodology to examine correlations among processing variables and the thermomechanical and kinetic properties of materials (e.g., strength, hardness, thermal conductivity, etc.).

1. Introduction

When polycrystalline materials are held at sufficiently high temperatures, the grain structure coarsens in order to decrease the excess free energy associated with the grain boundaries [1]. Since this process determines important microstructural features over time, and therefore key mechanical and electrical properties of materials, it has been the subject of intense investigation over the years [2]. These investigations have focused on the driving forces for grain growth and the associated kinetics of microstructural evolution [3]. In describing the temporal evolution of a distribution of grains, it is useful to divide grain kinetics broadly into two categories, namely normal and abnormal grain growth. Normal grain growth (NGG), which occurs in a wide variety of metallic and ceramic systems, is characterized by a relatively narrow range in grain sizes and shapes and a grain-size distribution that obeys a simple scaling relation [1].

By contrast, abnormal grain growth (AGG) occurs in a polycrystalline material when a minority of grains having anisotropic boundary energies or mobilities becomes large and grows into the surrounding “normal” matrix [4]. AGG is ubiquitous in many systems, especially thin films, in which an anisotropy in grain-boundary properties leads to the fast growth of a subset of grains relative to others in the microstructure [5]. This fast growth may occur, in some cases, due to the presence of impurity excesses, such as Ca or Si in Al_2O_3 [6]. Recent studies have also linked the presence of AGG with grain-boundary complexion transitions in which boundary structure and chemistry change to produce a new interfacial state [7]. In many cases AGG is undesirable as the resulting heterogeneous microstructure leads, for example, to a degradation in mechanical properties (e.g., hardness) [8]. In some situations, however, AGG is, in fact, beneficial as elongated grains can facilitate crack-tip bridging and thereby improve fracture toughness [9,10]. Moreover, there is the well-known use of AGG to generate large grain sizes in electrical steels in order to optimize their magnetic properties [11].

Despite the important implications of this phenomenon for material properties in polycrystals, there is little to no consensus as to which specific microstructural features indicate that AGG has occurred. For example, while some workers may focus on the presence of a single relatively large grain, others may interpret AGG in terms of a subset of large, non-equiaxed grains. Indeed, different researchers have adopted varying in-house heuristic criteria, which often involve only limited grain-size information. In reality, the situation is much more complex, and it is clear that both the grain-size and grain-shape distributions are critical to characterize abnormality and to correlate features of AGG with materials parameters, such as composition, temperature, etc.

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http://dx.doi.org/10.1016/j.actamat.2015.10.034
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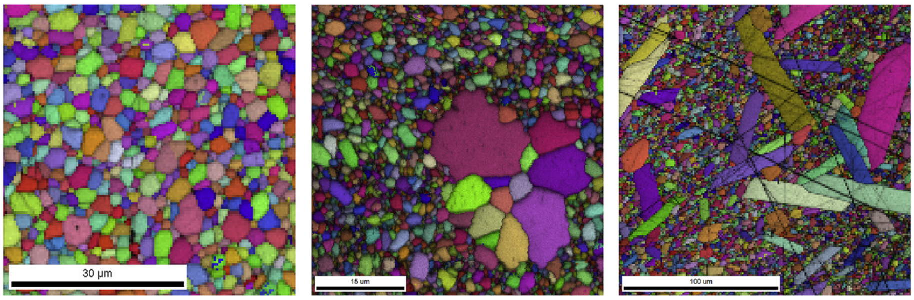

Fig. 1. Three illustrative microstructures for specialty alumina samples having different microstructures and processed under different conditions. a.) (Left) The system was annealed at 1750° C for 2 h. Each system contained the following dopants in different amounts: MgO, CaO, Na_2O and SiO_2. The main dopant was MgO. b.) (Middle) The system was spark-plasma sintered at 1300° C for 1 h. The main dopants were MgO and CaO. c.) (Right) The system was annealed at 1750° C for 2 h. The main dopants were SiO_2 and CaO.

In this paper we propose a set of microstructural maps and metrics that are useful in quantifying microstructural features that are associated with abnormal grain growth. We then present an application of correlation analysis that highlights relationships between the independent (i.e., processing) and dependent (i.e., microstructural metrics) variables. This methodology illustrates the utility of data analytics in quantifying which inputs exert the strongest influence on abnormal grain growth. In so doing it exemplifies the development of the techniques that are required for the implementation of the materials genome [12].

2. Methodology

2.1. Metrics

Given the large amount of microstructural data that must be processed in characterizing grain growth, it is useful to develop tools that will permit both a visual and a quantitative description of microstructural features associated with abnormality. For this purpose, it is convenient to construct first a map of the joint probability density function (pdf) of grain size, **G**, and aspect ratio, **a**, for a given microstructure. Consider three representative microstructures that are associated with specialty alumina having different chemistries and processing routes, as described below. Several pdf maps for these three microstructures, as shown in Fig. 1a–c, are presented in Fig. 2a–c. For the purpose of comparison, we employ the quantities, $\hat{G}$ and $\hat{a}$, which are the grain size and the aspect ratio, respectively, normalized by their microstructural averages. (In the latter case, this normalization of a dimensionless quantity is useful to relate it to its mean value, which typically differs from unity.) The dotted lines indicate the corresponding cutoffs for the grain size and the aspect ratio, G_c and a_c, used to identify "extreme" grains, as discussed below. While Fig. 1a is consistent with "normal" grain growth, Fig. 1b and c shows relatively large and non-equiaxed grains that are often taken as signatures of abnormality. Clearly, these pdf maps for disparate structures provide distinctive fingerprints that can be used to assess the degree of abnormality in terms of the number and distribution of outlying points.

To provide a quantitative description of AGG, it is essential to identify metrics that highlight specific features of the maps associated with abnormality. These metrics will necessarily focus on grains in the tail of the distribution. In our development, we borrow from the analysis of financial markets and risk analysis [13,14] to detect and quantify departures from grain size and shape distributions from that which is predicted by grain growth theory. In choosing quantities from the risk analysis and financial mathematics literature, we exploit an analogy between extreme events in a financial setting (e.g., unusually large monetary losses) and corresponding rare events in a microstructure (i.e., abnormal grains). In the former case, it is useful for planning purposes to have a measure of risk that reflects extraordinary occurrences, such as the mean value of the worse losses. Given that extreme events are of importance here, the corresponding quantities should be conditioned on being in the tail of the relevant distribution. As will be seen below, similar expressions based on conditional probabilities can be formulated for microstructural analysis. We note that, in this work, we focus on the moments of a distribution associated with finite sample sizes rather than on determining the limiting forms of statistics associated with very large sample sizes. This approach is appropriate in this context given the sample sizes considered and the fact that, in some cases, we are estimating multivariate probability densities with unknown limiting distributions.

In particular, we adapt to the current context the conditional probability $P(\mathbf{x}|\mathbf{x}>x_q)$ that a random variable **x** with associated pdf

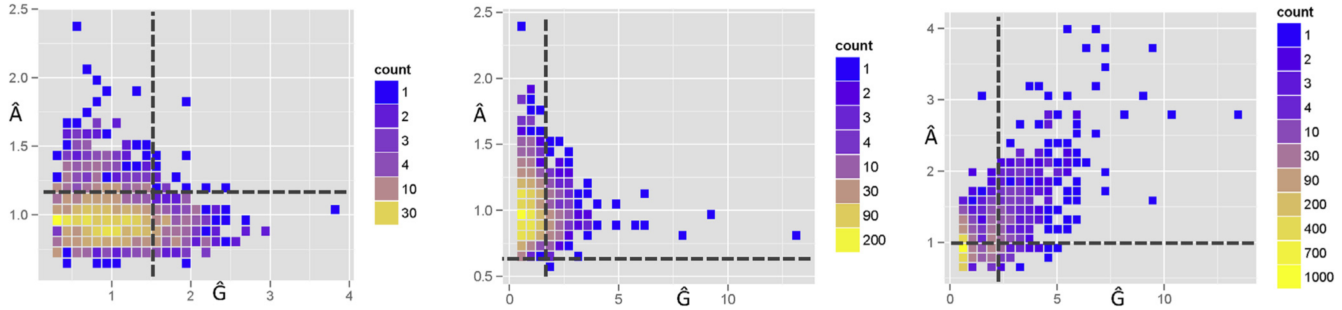

Fig. 2. The joint probabililty density function (pdf) maps corresponding to the microstructures shown in Fig. 1. These pdf maps summarize the density of normalized grain size, $\hat{G}$, and aspect ratio, $\hat{a}$, for the given microstructure, where each quantity is divided by its microstructural average. The dotted lines indicate the cutoffs G_c and a_c, used to identify "extreme" grains.