Computational Materials Science 153 (2018) 382–391

Contents lists available at ScienceDirect

Computational Materials Science

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

On the topology and size advantage of potentially abnormal grains

Dana Zöllner[a,*], Paulo Rangel Rios[b]

[a] B CUBE - Center for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, Germany
[b] Escola de Engenharia Industrial Metalúrgica, Universidade Federal Fluminense, Av. dos Trabalhadores, 420, Volta Redonda, RJ 27255-125, Brazil

ARTICLE INFO

Keywords:
Coarsening
Polycrystalline materials
Abnormal grain growth
Topology
Computer simulation

ABSTRACT

Curvature driven grain growth progresses by the motion of grain boundaries to the center of their curvature. In polycrystals this leads over time to a decrease in the total interfacial area and therewith interfacial free energy. As a result, the grain microstructure evolves such that it has a unimodal size distribution. In contrast, abnormal grain growth proceeds in such a way that certain grains show an exaggerated growth, which results in a bimodal size distribution. In the present work, Monte Carlo computer simulations of grain growth are employed in two dimensions to determine how grains showing a very large size advantage behave within a matrix of finer grains that can grow without restrictions. We demonstrate in agreement with early analytical work that true abnormal grain growth does not develop from those large grains. In fact, the large grains tend to decrease their size advantage over time and may eventually be "captured" by the grain size distribution of the matrix. Particularly, we focus for the first time on the influence of abnormal grain growth on topological transitions and neighbor environments, where we find that even abnormally large grains follow the Aboav-Weaire-law, from which it can be concluded that its local environment is not essentially different from that of small grains. Still another phenomenon may happen: the persistence of the size advantage of these grains may lead to what can be called pseudo-abnormal grain growth.

1. Introduction

The investigation of abnormal grain growth (AGG) can be divided into the following key aspects: Firstly, there is the question on how abnormal grains form? Secondly, it is necessary to know whether a certain grain is indeed growing abnormally. Thirdly, it is important to determine how abnormal grin growth influences the local topology around itself. In addition, there is the question about the influence of the abnormal grains on structure-property-relationships.

These and other questions have been in the focus of researchers for many decades. In his classical work Hillert [1] presented a method for analytical treatment of normal and abnormal grain growth. In particular, he examined several mechanisms for a possible development of abnormal grain growth. He concluded that while ideal grain growth is characterized by a stable unimodal distribution, which has in two dimensions a maximum grain size of twice the average grain size, incorporating a very large grain with a size larger than twice the average of the total microstructure would grow abnormally on the expense of the smaller matrix grains. Although this idea seemed to be reasonable at that time, it has been shown among others by Thompson et al. [2] and Lücke et al. [3] that a mere size advantage of an abnormally large grain in an unrestricted matrix of finer grains does not lead to abnormal grain growth. This type of coarsening can rather be described as a special kind of transient grain growth [3]. In particular, Thompson et al. [2] predicted that if a large grain is inserted into a matrix that possesses a Hillert grain size distribution this large grain will not grow abnormally, but rather its scaled size will decreased and the large grain may eventually rejoin the grain size distribution.

Nevertheless, the investigation of the effect of the presence of a few large grains located within a finer polycrystalline grain ensemble has been and still is of utmost importance since it usually has a deleterious influence on the properties of the material. Such large grains may appear due to materials processing. They often result from grains growing into a matrix that contains grains, which have a somehow restricted growth compared to the few rapidly growing ones (compare, e.g., [2,4–14] and the literature within). The following three cases are given exemplarily for the wide variety of experimental investigations:

- Riontino et al. [6] investigated grain growth in unstrained and strained specimens of pure iron at different annealing temperatures. While the un-deformed samples showed characteristics of normal grain growth, for all the deformed specimen three characteristic stages of growth were observed: a first stage, where the grains increase their sizes overall only slightly, a second stage characterized

* Corresponding author.
E-mail address: dana.zoellner1@tu-dresden.de (D. Zöllner).

https://doi.org/10.1016/j.commatsci.2018.07.012
Received 8 May 2018; Received in revised form 2 July 2018; Accepted 6 July 2018

by an abrupt increase in average grain size corresponding to the onset of abnormal grain growth, and finally a third stage, where the growth is almost fully blocked.

- On the other hand, a situation that is typical for grain growth of austenite in micro-alloyed steels is that during heating large grains may develop from a unimodal but pinned matrix around 1000–1100 °C [9]. As heating continues the particles that pinned the matrix may dissolve and one is left with large grains within a matrix that is free to grow. When higher temperatures are reached, around 1200 °C, the resulting polycrystal may appear uniform again indicating that the size advantage of the large grain has probably decreased. In other words, the large grains may have been captured by the growing unpinned matrix grains at high enough temperatures.
- Another example is the investigation of 304L stainless steel, for which it has been shown for a broad range of annealing temperatures [13] that particularly for annealing temperatures between 65% and 70% of the melting temperature a transition in grain growth kinetics from normal to abnormal took place resulting in a bimodality of grain size distributions. In contrast, in Eurofer-97 steel deformed at different strains Oliveira et al. [14] found that grain boundaries with misorientations above 45° as well as local microstructural instabilities may explain AGG.

Hence, a size advantage—even a large one—may not necessarily lead to true abnormal grain growth. In order to say that a grain is undergoing abnormal grain growth two main criteria are possible: a metrical, e.g., [10] and a topological criterion [15]. The metrical criterion to determine, whether a grain is growing abnormally or not, can be written in a rather simple form:

$$\frac{\mathrm{d}(R_A/R_M)}{\mathrm{d}t} > 0, \tag{1a}$$

where R_A is the radius of the abnormal grain and R_M is the mean grain radius of the matrix. The grain radius, R, is defined as the radius of a sphere that has the same volume as the grain.

Therefore, a grain is growing abnormally if its linear grain size is "moving away" from the average grain size, that is, its scaled grain size R_A/R_M increases as coarsening progresses. In contrast, if

$$\frac{\mathrm{d}(R_A/R_M)}{\mathrm{d}t} < 0 \tag{1b}$$

holds, the large grain is decreasing its scaled grain size R_A/R_M and approaches the average grain radius. In this case it is not growing abnormally. Regarding the grain size distribution rather than the growth of an individual grain, Kang [16] pointed out that a more robust abnormal grain growth criterion would be the development of a bimodal grain size distribution. The latter assumes the existence of a size gap between the largest grains of the matrix and any abnormal grains.Rios and Glicksman [15] demonstrated that a topological criterion for abnormal growth is also possible and can be written as:

$$\frac{\mathrm{d}N_A}{\mathrm{d}t} > 0, \tag{2}$$

where N_A is the number of faces or neighbors of the abnormal grain. This topological criterion shows that an abnormal grain grows by gaining faces, whereas during normal grain growth, when the grain size distribution is self-similar, all grains, whether they are growing or shrinking, are always losing faces [17,18].

One method to investigate the behavior of large grains within a finer matrix that is free to undergo grain growth in detail in two and in three dimensions is the usage of computer simulations. In particular, mesoscopic computer simulations can access information that analytical models are—at this moment—unable to deal with. For instance, computer simulations allow a detailed investigation of the topological aspects of the evolving grains, particularly, topological transitions and the nature of the grains surrounding the large grains. Of course, computer simulations are not a substitute for analytical investigations, however, over the last decades they have been used more than once to provide a new approach to a deeper understanding of the phenomenon of grain growth and offer at the same time a unique possibility to close the gaps between analytical theories and experimental investigations. This is especially important since our understanding of grain growth is limited by the difficulty of accessing the details of three-dimensional polycrystalline grain microstructures experimentally as well as by anisotropies regarding grain boundary energy and mobility and by impurities in the samples. Computer simulations also enable us to investigate phenomena like topological transitions, which are problematic to access analytically.

The present work intends to fill this gap in the literature by reporting results from Monte Carlo Potts model simulations on the metrical and topological behavior of large grains within a fine grained matrix free from any growth restrictions. One particular phenomenon that has to our knowledge never been investigated in such detail is simulated here: namely, the persistence of the size advantage of large grains that may lead to what can be understood as pseudo-abnormal grain growth.

2. Simulation algorithm

In order to analyze the growth behavior of individual very large grains with many faces (clearly larger than the largest matrix grains) embedded in a matrix of smaller grains under ideal grain growth conditions the Monte Carlo Potts model is applied (compare, e.g., [19–23] and the literature within).

To that aim, the grain microstructure is mapped onto a quadratic lattice in two dimensions. The number of nearest neighbors for all lattice points is selected such that the first and second nearest neighbors, nn, are taken into account. Each lattice point (pixel in a graphical representation) is called a Monte Carlo Unit and abbreviated as MCU comprising a certain but unassertive area of one grain. Each grain and therewith all lattice points associated with this grain have assigned their specific crystallographic orientation making the Potts model a sharp-interface model.

Following the standard algorithm [22], the time unit of the simulation is one Monte Carlo Step (abbr. MCS) containing N reorientation attempts, where N is the total number of MCUs of the lattice fixing time and size scale of the simulation. Generally, only two materials parameters enter the calculation, namely, the specific grain boundary energy per unit length γ and the grain boundary mobility m, both of which are a function of the misorientation between neighboring grains. However, for a simulation of ideal grain growth, where it is assumed that all boundaries are of high angle characteristics, both parameters are identified by a unique maximum value of m_{max} and γ_{max}, respectively. And since we need within the algorithm only the relation between mobility and energy with respect to their maximum values (m: m_{max} and γ: γ_{max}), these relations are always set equal to one resulting in a rather simple procedure, where each reorientation attempt consists of the following four steps:

1. At first, one lattice point is chosen at random. It has a certain orientation Q_i characterizing the current state of the lattice.
2. In the second step a new state is generated. This new state differs from the old original state by the flip of just one (the selected) MCU giving it a new orientation Q_j.
3. Then the energy of the two states is calculated each given by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{nn} 1-\delta(Q_i, Q_j). \tag{3}$$