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Quantifying microstructures in isotropic grain growth from phase field modeling: Topological properties

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Abstract

In a previous work [Acta Materialia 2012;60:4787], we developed a new method that utilizes discrete, voxel-based data for microstructure quantification. We successfully calculated some relatively simple microstructural quantities and relations. In this paper, we apply and extend this method to compute more complex microstructural quantities and, in particular, map out the connection between grain growth rate and various topological properties. We present detailed results for several local and average topological and geometric properties of the microstructures during grain coarsening, including the curvature of grain boundaries and triple junction lines, grain cell shape, and their relations with growth dynamics. We also examine several well-known topological relations, i.e. Euler relations, the Lewis rule and the Aboav–Weaire law. These quantities and relations are the centerpiece of the grain growth models and theories developed so far. We also compare our results with some existing results in three dimensions. The quantitative description of the dynamic behaviors of the microstructural attributes adds a valuable data set to grain growth that can be used for benchmarking for phase field modeling and comparison with other approaches.

Keywords: Microstructure; Grain growth; Quantitative characterization; Polycrystal; Phase field modeling

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1. Introduction

Grain growth in polycrystalline metals and cell growth in other types of cellular patterns, such as soap bubbles, are considered to be driven by the reduction of the excess free energies associated with the interfaces. The rate of grain growth is therefore related to the interface curvature, which is directly connected to either the pressure difference across the interface in the case of bubble growth [1] or the excess free energy in metals from Gibbs–Thompson effect [2]. On the other hand, it is recognized that certain microstructural quantities of a topological nature are also behind the cell growth [3,4]. For example, in the von Neumann model of two-dimensional grain growth, the growth rate is related to the number of edges or the number of neighboring grains [5,6]. The two are equivalent in two dimensions. Although empirical observation by Glazier from a Potts model indicated that the growth rate in three dimensions is proportional to the number of faces of a cell [3], an equivalent von Neumann theory has been proposed only recently, by MacPherson and Srolovitz [7], that also directly invokes topological quantities such as triple junction lines and their length, as well as the number of faces of a grain. While these models and theories can give general trends, detailed information about the relations between the topological quantities and their time evolution is difficult to observe during grain growth except in a few simple cases, such as in two dimensions.

The challenging issue is to reveal the local topological information down to each grain cell during growth. So far, such local quantitative information has not been obtained easily from either experiments or theoretical models, where usually average quantities are used. As

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stated succinctly by Glicksman [4], however, “it is the local geometrical attributes of the internal interfaces … that primarily determine how bounded volumes of matter fill space and respond to fields imposed within their network”.

In this work, which is a sequel to Ref. [8], we investigate the topological attributes and their relations to grain growth during isotropic grain growth from a phase field model simulation. Our focus here is not to validate existing theories and models for grain growth; in fact, as such theories and models are always based on certain specific conditions that may differ from those in the phase field model, difference in the results are unavoidable. One example is the exterior dihedral angle, which, according to the von Neumann [5,6] and MacPherson and Srolovitz theory [7], should remain strictly a constant at $2\pi/6$ during growth. As we have already seen from our previous work (see Figs. 11 and 12 in Ref. [8]), this assumption may not necessarily hold in the phase field model. Therefore, validating or comparing the physics of these theories and models fall outside of this work. Our primary purpose is to test and validate the numerical methods developed to handle the discrete microstructural data, particularly in a dynamic setting, such as grain growth, for the phase field model.

Nevertheless, a certain amount of comparison is needed to shed light on the influence of the technical approaches used in the models and theories. For this purpose, we compare our results to Lazar et al.’s recent work [9], in which the three-dimensional (3-D) von Neumann relation is supposedly followed exactly during their grain growth simulation. In addition, our results allow us to take a close look at topological properties in the grain growth process that have not been widely available before. The quantitative information about the microstructures from the phase field model adds a valuable set to the body of grain growth data that can be used for benchmarking (for phase field modeling) and comparison with theories and other models.

The paper is organized as follows. In Section 2, we present topological quantities, such as the number of faces, edges, vertices and their statistical distributions, for all 3000 grains in the sample. We also obtain their dynamic behavior during growth, in particular, the Euler relations from these quantities. We examine the relations between the number of grain faces and the growth rate, i.e. how grains with different numbers of face grow, shrink or vanish, and whether the growth rate scales with the mean number of faces, edges and vertices of a grain. This provides a different scenario from that of the von Neumann type of models in three dimensions [3,7,9]. In Section 3, we examine two well-known topological relations, the Lewis rule and the Aboav–Weaire law, during growth. In Section 4, we present a method and use it to calculate the mean curvature of grain boundaries (GB) and triple junction (TJ) lines. Various relations between the mean curvatures and other topological quantities, such as the number of faces per grain or the area of the grain boundary, are also revealed. We discuss the results and methods used in this paper in Section 5. Finally, in Section 6 we present conclusions drawn from this work.

2. Topological properties and relations

Using the grain index method shown in Ref. [8], we can identify the neighbors of a grain, which enables us to obtain the information of the number of faces, edges and vertices for each grain. Fig. 1 shows the average number of faces per grain during the grain growth. The distribution functions of the number of faces of each grain (Fig. 1a) are normalized, so comparison can be made with the results from other models and theories [9]. The data roughly follow a Gaussian distribution. The average number of faces per grain (Fig. 1b) ranges from 12.85 at the beginning of the growth to 13.60 when the growth reaches a steady state. The steady-state value is less than Meijering’s analytical result and other geometric models, such as Voronoi tessellation ($\langle F \rangle = 15.5335$ [10]) and the 3-D Potts model ($\langle F \rangle = 14.08$ [3]), but close to the prediction by DeHoff (13.60 [11]) and the result of Lazar et al. (13.769 ± 0.016) [9]. It is interesting to notice that the average number of faces per grain in our phase field simulation approaches the steady-state value differently when compared to Lazar et al.’s result. We will discuss this in Section 6.

In the von Neumann model, the grain growth rate is proportional to the number of grain edges. Since, in two dimensions, the number of edges equals the number of faces due to the dimension reduction, the equivalent von Neumann model in three dimensions should be related to the number of faces per grain. As argued by Glazier [3], if the grain growth rate follows the scaling relation of the ideal growth (Eq. (1) in Ref. [8]), the growth should exhibit a linear scaling relation with the number of faces in three

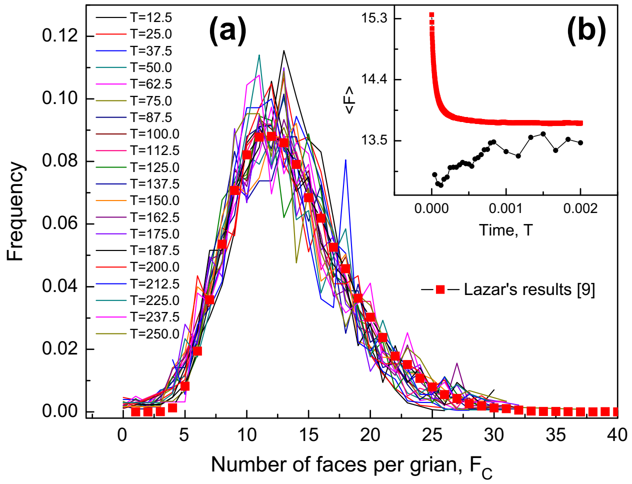

Fig. 1. (a) The time evolution of the distribution of number of faces per grain calculated from $t = 12.5$ to $t = 600$ at time intervals of 50. (b) The time evolution of the average number of faces. Lazar et al.’s result is plotted for comparison [9].