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Long-range topological correlations of real polycrystalline grains in two dimensions

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ABSTRACT

The topological and geometric properties of real polycrystalline grains in two dimensions are investigated on the basis of a large dataset (14,810 grains). The distribution of grain edges, the grain topology–size relationship and the short- and long-range topological correlations between neighboring grains are characterized quantitatively. The results show a strong short-range topological correlation between a center grain and its first nearest neighbors, and a trivial long-range topological correlation beyond the first nearest neighbors (on average). Both the short- and long-range relations are well described by a generalized Aboav–Weaire law reported recently. Meanwhile, it is the perimeter law, rather than the Lewis law, that describes appropriately the relationship between the topology and geometry of metallurgical grains.

1. Introduction

Materials with a space-filling cellular structure, including metallurgical grain aggregates, foams and biological tissues, are ubiquitous in nature. A quantitative characterization of the topological and geometric properties of the grains/bubbles/cells is crucial for the understanding of the material [1–6], since the mechanical, electrical and chemical performances of materials strongly depend on the microstructural topology and geometry [7]. We take individual grains in a single phase, polycrystalline material as research objects in this paper. Historically, the topology of a grain has been commonly described by using only its number of edges in two dimensions or faces in three dimensions, i.e., the number of its first nearest neighbors [8–14]. Some good works have recently been done to provide a more detailed topological description of a grain [15,16] and analyze the affinities of a pair with different face classes in grain structures [17]. Some important topological relations concerning the first nearest neighbors have been summarized in the past, such as the Aboav–Weaire law [2,3] on nearest-neighbor topological correlations, the Lewis law [4] on the statistics of grain area, and the von Neumann–Mullins law [5,6] on the growth rate of individual grains.

Although such good advances have been made in the past, topology properties of grains are still far from a complete understanding. The Aboav–Weaire law describes the topological correlation between a grain and its first nearest neighbors (on average), i.e., short-range topological correlation. However, concentrating on the first nearest neighbors limits the available topological information about the microstructure, since everything about the microstructure beyond the first nearest neighbors is ignored. To investigate such long-range topological properties, some pioneer works have been done in literatures [18–21]. Very recently, the present author proposed a generalized Aboav–Weaire law [22,23] to describe both the short- and long-range topological correlations between a center grain and its neighbors (on average) on the basis of large-scale Monte Carlo simulation data. That is

$$m_j(f) = A_j + \frac{B_j}{q_j(f)} \tag{1}$$

where $m_j(f)$ is the average number of faces per grain in the jth nearest neighbor shell of f-faced grains, and $q_j(f)$ is the number of grains in the jth shell. A_j and B_j are two constants for each jth shell. For $j = 1$ (first nearest neighbor layer) and $q_1(f) = f$, Eq. (1) specializes to a form of Aboav–Weaire law [2,3]. The generalized Aboav–Weaire law is still awaiting experiment verifications both in two and three dimensions. It is very necessary to make a comprehensive research on both the short- and long-range topological correlations in a real material.

The aim of this paper is to investigate the statistical topology properties of 2D grains in a real polycrystal on the basis of a large dataset (14,810 grains). In Section 2, the materials and methods used in this paper are shown. Section 3 details the results including short- and long-range topological correlations, the distribution of grain edges,

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and the relationships between grain topology and geometry. Strong short-range and trivial long-range topological correlations are observed. The generalize Aboav–Weaire law, the Lewis law and the perimeter law are compared with the results and discussed in detail. These results might assist in a better understanding of the topological and geometric properties of cellular structures.

2. Materials and Methods

The chemical composition (wt.%) of the experimental steel was: C 0.18, Si 0.29, Mn 1.14, Cr 1.06, V 0.11, Ti 0.062, B 0.0027, Al 0.031, N 0.0044, P 0.024, and S 0.02. The alloy was melted in a vacuum induction furnace and cast into an ingot of 28.5 kg. The ingot was heated at 1250 °C for 1 h and forged into rods 13 mm in diameter. Then samples 10 mm in diameter and 12 mm in height from the rods were isothermally austenitized at 1050 °C for 30 s, water quenched and finally prepared into metallographic specimens by means of conventional standard procedures. Microscopic examination on three mutually perpendicular surfaces of the specimens showed that the microstructure is essentially isotropic and that the grains are nearly equiaxed. Conventional metallographic analysis revealed that the mean linear intercept size of the austenite grains is 32 μm. We investigated 14,810 grains within the dataset from more than 400 metallographic pictures. Fig. 1 shows the stratification into layers around a central grain colored in red, i.e., first, second, and third nearest neighboring grains are colored in green, yellow, and blue, respectively. A calculation program was developed by ourselves to measure the area, perimeter and the number of edges of each grain, respectively.

It is known that various material properties such as anisotropies of grain boundary energy and mobility, defects and impurities will affect the evolution of real polycrystalline microstructures to some extent. However, we did not consider these factors because they had no obvious influence on the observed structure (see Fig. 1) in this work. It is a typical single-phased polycrystalline structure like other space-filling cellular structures such as pure iron, bubbles, and biology tissues, which ensures that the topological and geometric properties observed in the following have its universality in cellular structures.

3. Results and Discussions

3.1. Distribution of Edges

The simplest way to classify the topology of a grain involves counting its number of edges [16,24]. This is the topological characterization most commonly quoted in the literature. Fig. 2 shows the distribution of edges per grain. The distribution functions of the number of edges of each grain are normalized, so comparison can be made with the result from other models. The result of the Potts model–Monte Carlo simulation [25] in a scale of 2000 × 2000 is also plotted in Fig. 2 for comparison (9725 grains in a steady-state grain-growth structure). Both the experiment and Monte Carlo simulation data accurately follow an asymmetric log-normal distribution with a fit correlation coefficient of 0.99. However, despite the same shape of distribution, there appears a little difference between experiment and simulation data in terms of the peak and the width of the distribution. The experiment data has a peak at nearly $n = 5$ and the observed largest edge number is 15, while the peak appears at nearly $n = 6$ and the largest edge number is 12 in the simulation. The little deviation between the experiment and simulation data is possibly due to the finite size/boundary effect in the experiment.

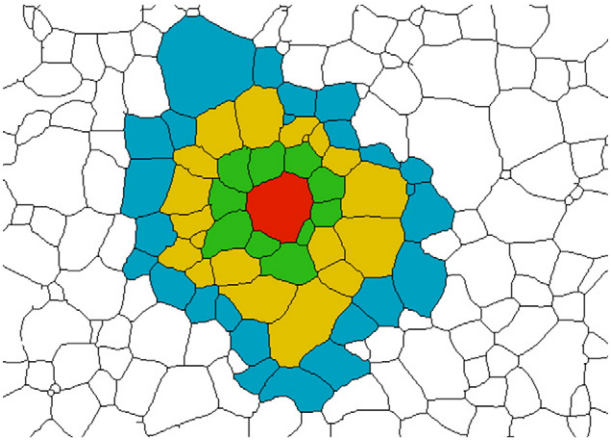

Fig. 1. Stratification into layers around a central grain colored in red in the experiment.

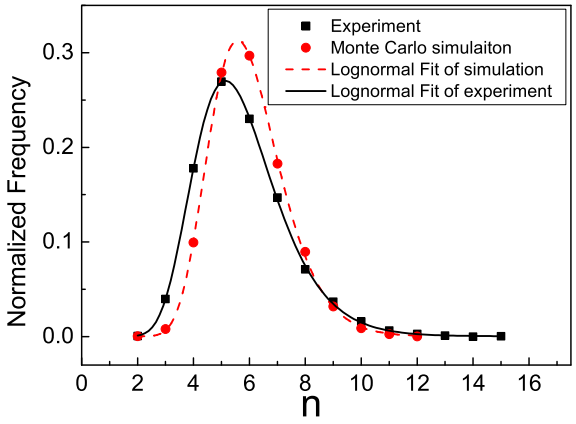

Fig. 2. Distribution of the number of edges per grain n.

3.2. Short- and Long-range Topological Correlations

For topological correlation studies, a definition of the jth nearest neighbors for a center grain is needed. A grain structure divides space into N individual grains. The local environment around a center grain can be treated as a concentric layer (coordination shell) structure [18–21]. The jth layer of a center grain is the set of its jth nearest neighbors. First nearest neighbors ($j = 1$) of a center grain are defined to be grains which are adjacent to it. For $j > 1$, the jth nearest neighbors are those adjacent to $(j - 1)$th layer, but do not belong to $(j - 2)$th layer (0 layer means the center grain itself). We consider that there are q_j grains in the jth shell of an n-edged center grain and the average number of edges per grain in this shell is v_j. For all grains in each n class, the topologically averaged values of v_j and q_j are $m_j(n)$ and $q_j(n)$, respectively; the total number of grain edges in the jth shell is $Q_j(n) = m_j(n)\, q_j(n)$.

Fig. 3(a) plots the average number of edges of each grain's jth nearest neighbors, v_j, vs. the number of edges per grain n. A distribution of v_j is observed for a given topological class. For grains in each topological class, we notice similar trends that v_1 covers the largest range of values and v_j becomes more and more centralized to a lower value with the increase of the topological distance j. The distribution of the value of v_j for all grains is shown in Fig. 3(b). With the increase of j, the peak of the distribution moves towards left, which means the centralization of v_j to a lower value. It is reasonable to predict that for $j = \infty$, v_∞ will be centralized to one certain value C for all grains (see the straight dash lines in Fig. 3(a)–(b)), meaning that v_j for the farthest neighbors is insensitive to n. This result is consistent with the fact that the farthest neighbors have little correlations with a central individual grain due to the longest topological distance j. It should be noted that the number of sampling grains decreased with the increasing j, resulting