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Affinities for topological arrangements in grain structures

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Abstract

Boundaries between neighboring grains with different numbers of faces exhibit a wide range of tendencies to occur in a structure, from high preference to high avoidance. These tendencies are described here in terms their contact affinity, which describes the extent to which an *i–j* faced grain pair actually occurs in the structure relative to that expected from statistically random contact. An affinity of unity indicates random occurrence and values above or below unity indicate the corresponding factor above or below random with which a particular pairing occurs. Grain contact affinities determined for both 3-D Monte Carlo grain growth simulations and experimental serial sectioned grains show similar trends of high affinity for contact between few- and many-faced grains, avoidance of contact between grains in similar face classes, and random contact between grains of intermediate face classes and all other classes. Contact affinities have been modeled in terms of the relative face curvatures, with high curvatures of opposite sign exhibiting the highest contact affinities, like signs the lowest, and relatively flat-faced grains showing near-random contact with all other classes. The measure of affinity is thus interpreted as the degree of stability or instability of boundaries against rapid face loss from topological events. The affinity approach overcomes a significant bias of the Aboav–Weaire analysis, which describes the average neighbors of face classes but is insensitive to the actual preference or avoidance for boundaries with other classes. The contact affinity term quantifies these tendencies.

Keywords: 3-D characterization; Grain growth; Monte Carlo simulation; Titanium alloys; Topology

1. Introduction

The geometry and arrangement of cells in a polycrystal has been a topic of study for many years [1–10]. This interest comes from the standpoint of understanding how grain shapes and structures occur, and, more importantly how they affect the grain growth process. Of particular interest is the evolution of the grain face and size distributions towards asymptotic states and whether there is a single [11,12] or multiple [13,14] such states.

Evolution of the overall structure is the combined result of numerous pair- and group-wise interactions among grains, termed topological events [13,15–18]. These unit processes that create and remove faces from grains are important since this face evolution maintains the supply of new tetrahedra for grain disappearance, which is the fundamental event of grain growth [13,15,16]. Changing the face class of a grain also sets its new boundary curvature and growth rate [19–28]. The overall grain structure and the occurrence of these topological events are strongly affected by the pairing of different face classes.

The topological events occurring in grain growth typically occur as a competition among grain pairs or clusters in which some grains grow or gain faces while their

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neighbors lose faces or are consumed. The size and topological path followed by a grain is determined by its face class and that of its neighbors, which together set their boundary stability and determine the resulting event. Understanding the arrangements of grain structures and their means of asymptotic evolution is a major step toward understanding the topological nature of grain growth.

This paper presents a means for quantitatively describing the frequency of occurrence, termed affinity, of grain-pair arrangements relative to that expected from random probability. This affinity term gives the factor greater or less than random at which the arrangement occurs. The affinity of different face class combinations at grain boundaries in titanium alloy Ti-21S [29] and in 3-D Monte Carlo (3DMC) grain growth simulations [30] are presented here and explained in terms of boundary curvatures and the resulting junction stability. The methodology employed will be shown to provide a significant improvement beyond the Aboav–Weaire approach, which describes each grain face class only in terms of its average neighbor.

2. Background: the Aboav–Weaire approach

The traditional means for describing grain arrangements is by the average numbers of faces, M_n, on the first neighbors *of* n-faced grains, termed the Aboav–Weaire relationship [1–4]. This long-followed approach is illustrated in Fig. 1 for a 3DMC grain growth simulation. The face class of the average neighbor is seen to range from 22 for 4-faced grains to 14 for 60-faced grains, indicating that few-faced grains have higher-faced neighbors and vice versa. It is significant to note that most average neighbors are in intermediate face classes. The average neighbor approach is thus relatively insensitive, and M_n decreases by only three face-classes, from 17 to 14, for neighboring face classes 10–60. Although the trend of generally high or low face class preferences between neighbors is qualitatively correct

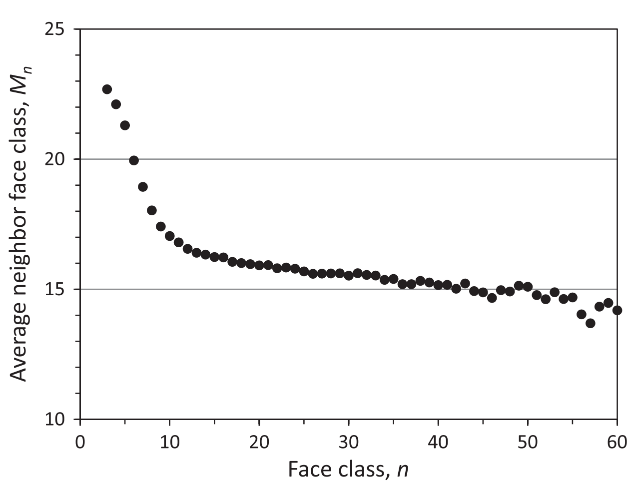

Fig. 1. Aboav–Weaire plot of M_n, the average neighbor face class of n-faced grains in 3DMC grain growth simulation. Average neighbor varies only from 17 to 14 between face class 10 and 60.

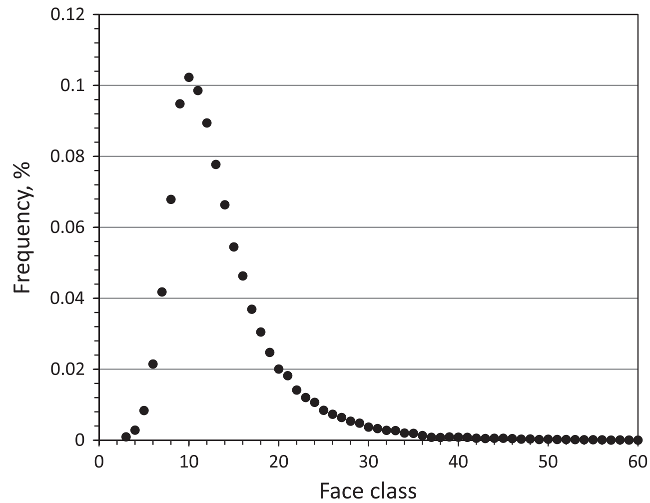

Fig. 2. Grain face-class distribution from 3DMC grain growth simulation, mean face class 13.7.

it does not address the marked tendencies for high or low contact that actually exist between classes.

As an example, in Fig. 1 the M_n statistic suggests that face class 60 prefers contact with class 14, of which there is a high fraction in the system. It will be shown below that independent of the effect of the high frequency of grains in face class 14, there is actually a lower than statistically expected presence of 14–60 pairs, 0.85 times the amount expected from random contact. In fact, intermediate face classes such as 14 have essentially random contact with all other classes due to having relatively flat faces, with neither excessively high nor low tendency for contact. M_n thus implies an attraction between grains that is actually not present.

The origin of the bias in the average neighbor description is the large fraction of grains that occupy the intermediate face range (Fig. 2); thus, the computed average neighbor is heavily weighted towards the center of the face distribution. Most n-grains contact these intermediate M-grains, not by attraction but by the fact that the intermediate grains are the most prevalent and cannot be spatially avoided. The resulting description greatly overestimates the M–n grain interaction and misrepresents this incidental contact as attraction. The goal of this paper is to describe the true tendency for high or low contact between grains of specific 3-D face classes, unbiased by the confounding effect of face class frequency.

3. Frequency-biased contact

The following example further illustrates the frequency-bias origin of the average-neighbor problem. Fig. 3 shows the fraction of contacts between grains of several particular n-face classes and their neighbors in the above 3DMC simulation. The four n-classes used as examples here, 5, 8, 14 and 35, illustrate behavior of relatively low, intermediate and high face classes, respectively. All of these classes have

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