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On the Aboav–Weaire-law for junction limited grain growth in two dimensions

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ABSTRACT

In the present work the validity of the Aboav–Weaire-relation in polycrystalline grain microstructures obtained by junction limited grain growth as it may occur in nanocrystalline materials is tested. To that aim, two-dimensional Monte Carlo Potts model simulations have been performed, and it follows that while the kinetics as well as the grain size–topology–relationship shows significant differences for grain boundary controlled grain growth and triple junction controlled growth, the Aboav–Weaire-relation is fulfilled independent of the grain feature controlling the growth kinetics.

1. Introduction

In 1970 Aboav has undertaken the task to determine how the grains of a typical polycrystal are arranged in space [1]. As a result he concluded that grains in a polycrystalline solid are not simply disposed at random, but are rather arranged in a certain order. In particular, for the investigated case of sections through polycrystalline magnesium oxide he found that the relation between the number of faces s of a grain are related to the average number of faces of all neighboring grains m_s by the following simple approximation

$$m_s \cdot s = 5 \cdot s + 8. \tag{1}$$

Only four year later Weaire [2] pointed out that such a conclusion of "nonrandom" ordering in polycrystals cannot be drawn this simple. To that he cited Euler's Theorem as an elementary example. In particular, Euler's Theorem states that in an infinite two-dimensional polyhedral network, where only three fold vertices exist, the average number of faces of all polyhedral equal six. Hence it gives quite well a microstructural correlation in a cellular network, while the grains can still be distributed randomly.

However, Weaire also presented a relatively simple derivation of an equation similar to Eq. (1) based on Euler's Theorem as well as an extension taking the second moment of the neighbor distribution μ_2 into account such that

$$m_s \cdot s = 5 \cdot s + (6 + \mu_2). \tag{2}$$

It should be noted that Eq. (2) is not such a strict general rule as Eq. (1). Any possible two-dimensional cellular network that is associated with an own distribution of number of faces is characterized by an own distinct value for the constant term in Eq. (2).

Considering the distribution of cells in a planar section of soap foam led to a further modification by Aboav [3] yielding the today well-known Aboav–Weaire-law

$$m_s \cdot s = (6 - \alpha) \cdot s + (6\alpha + \mu_2), \tag{3a}$$

where α is a constant. Its value depends on the type of cellular pattern under investigation and is assumed to take for polycrystalline grain microstructures obtained by normal grain growth a value that is close to unity. Eq. (3a) can additionally be written in terms of the average number of faces as

$$m_s \cdot s = (\langle s \rangle - \alpha) \cdot s + (\langle s \rangle \cdot \alpha + \mu_2). \tag{3b}$$

Ever since then, Eqs. (3) have been used very successfully to describe different kinds of cellular pattern, as for example polycrystalline metals and ceramics, soap froth or biological tissues (compare, e.g., [4–10]).

In the following, two-dimensional Monte Carlo Potts model simulations have been performed. It follows that while the kinetics as well as the grain size–topology–relationship shows significant differences for grain boundary controlled grain growth and triple line controlled growth, the Aboav–Weaire-relation is fulfilled independent of the grain feature controlling the growth kinetics.

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2. Topology

For polycrystalline materials it is commonly known that for normal (grain boundary controlled) grain growth the average (linear) grain size increases according to

$$\langle R\rangle = (b\cdot t + \langle R\rangle_0^{1/n})^n, \tag{4a}$$

where R is the grain radius, which is defined in the present work as the radius of a grain area equivalent circle, b is the growth constant, and n is the growth exponent, which is supposed to have theoretically a value of 0.5.

Then again, recently it has been shown that in case of triple junction control a linear time law follows (compare, e.g., [11,12])

$$\langle R\rangle = b\cdot t + \langle R\rangle_0. \tag{4b}$$

Both kinetics have been observed using Monte Carlo Potts model simulations (details see [13–15]) and have been shown to be characterized by statistical self-similarity regarding the grain size distribution as well as regarding the topology–size–relation [16].

In the following analyses we consider at first the relation between number of faces s of a grain and its relative grain size x defined as $x = R/\langle R\rangle$ (compare [17,18]) as follows: A central grain of size R is surrounded by s grains of average size $\langle R\rangle$. The perimeter U of the central grain through the centers of the surrounding grains can be calculated in two different ways. Firstly, it holds $U = \pi\cdot(R+\langle R\rangle)$. Secondly, the average diameters of s grains add up to $U = s\cdot 2\langle R\rangle$. Assuming that those two perimeters are identical it follows

$$s = \pi\cdot x + \pi. \tag{5a}$$

Alternatively, a similar argument concerning the area, which can be calculated either as $A = \pi\cdot(R+\langle R\rangle)^2$ or as $A = \pi\cdot R^2 + s\cdot 0.5\pi\cdot\langle R\rangle^2$, yields

$$s = 4\cdot x + 2. \tag{5b}$$

Sadly, this very simple argument is not reflected by normal grain growth simulations. In particular, we find by use of the Potts model a quadratic relation between s and x as presented in Fig. 1a. The deviations from Eqs. (5) are quite obvious. Then again, the quadratic (non-polynomial) term has been found to be very important for the mean-field theory of grain growth by Streitenberger and Zöllner [19–21] yielding deviations from Hillert's classical solution.

However, for the case that the triple junctions control the growth kinetics we find that $s(x)$ can be represented very well by a linear function as shown in Fig. 1b. Moreover, Eq. (5a) is an adequate representation of the self-similar simulation data, although the slopes differ slightly. In comparison, the results of grain boundary controlled growth show deviations to higher grain boundary faces for small grains ($x < 0.5$) as well as large grains ($x > 1.75$).

Then again, for both kinetics the average number of faces is indeed quasi identical to the expected value of six. Also the maximum in the distribution of the number of faces $f(s)$ is close to six for both cases (compare Fig. 2a). However, the distributions themselves vary rather strongly. $f(s)$ for grain boundary controlled growth is narrower, while the distribution for triple junction controlled growth has a long right-hand tail and is not as peaked as the other one. Hence, the second moment for grain boundary controlled growth is with $\mu_2 = 2.1650$ visibly smaller than the value for triple junction controlled growth with $\mu_2 = 2.9019$.

A direct comparison of the number of faces versus relative grain size for all data each from one time step of the two growth kinetics is given in Fig. 2b. While the grains with approximately five up to eight faces spread across the same size range, those with nine faces or more show significant differences. In particular, for triple junction controlled growth considerable higher relative grain sizes are reached without showing any tendency to higher number of faces. This reduces the curvature of the least-squares fit for large grain sizes. At the same time, as also visible in Fig. 2a, there are distinctly more grains with three and four faces in case of triple junction control. This also reduces the curvature of the least-squares fit only this time for small grains.

3. Aboav–Weaire-law

The question arises whether the observed deviations in the self-similar topology–size–relations are coupled with deviations in local topological relations like the relationship between the number of faces of a grain and the average number of faces of all neighboring grains as described by the Aboav–Weaire-law. The latter in terms of Eq. (3b) as $m_s\cdot s = (\langle s\rangle - \alpha)\cdot s + (\langle s\rangle\cdot\alpha + \mu_2)$ can be calculated directly from the above given simulation results.

The microstructure of grain boundary controlled normal grain growth is characterized by an average value for the number of faces of 5.9979 (Fig. 1a) and the associated distribution by $\mu_2 = 2.1650$ (Fig. 2a). Assuming $\alpha = 1$ it follows

$$m_s\cdot s = 4.9979\cdot s + 8.1629. \tag{6a}$$

For triple junction controlled growth the microstructure is characterized by $\langle s\rangle = 5.9857$ and $\mu_2 = 2.9019$, from which it follows with $\alpha = 1$

$$m_s\cdot s = 4.9857\cdot s + 8.8876. \tag{6b}$$

On the other hand, for the simulations the measured Aboav–Weaire-relations are given in Fig. 3 for both growth kinetics. It can be seen that the simulated microstructures show indeed the

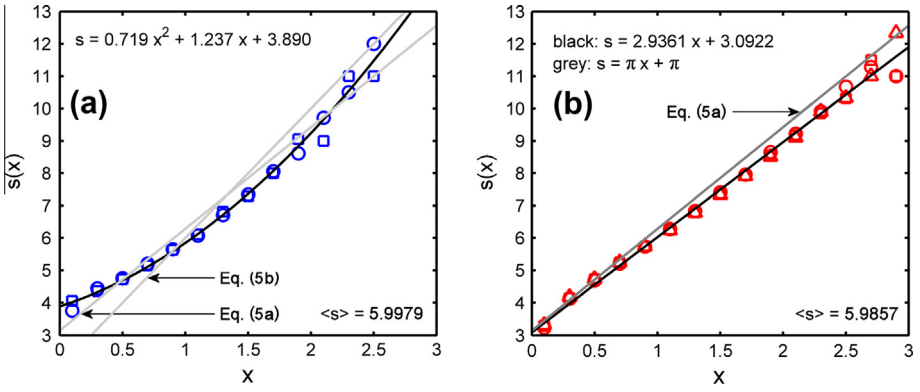

Fig. 1. Self-similar relation between number of faces and relative grain size for: (a) grain boundary controlled growth; (b) triple junction controlled growth.