A Discrete Approach to Grain Growth Based on Pair Interactions: Effect of Local Grain-Boundary Curvature

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The concept of local grain-boundary curvature has been introduced in a discrete model for grain growth based on pair interactions. A Rayleigh-shaped quasi-stationary grain-size distribution (GSD) in a free system and log-normal-like distributions in the presence of inhibition have been obtained. In all cases, the commonly accepted theoretical results for the coarsening kinetics were preserved. In the present contribution, the dependence of the inhibition effects on time and on the geometrical model adopted for the polycrystal is discussed. Some advantages of the discrete model with respect to the introduction of physical quantities associated with the relative size of each pair of neighboring grains, such as, for example, inhibition, are suggested.

I. INTRODUCTION

In a previous article,\(^1\) it was shown that a discrete approach based on pair interactions can be formally used to describe grain growth in single-phase polycrystalline materials, with results similar to those from the mean-field model by Hillert\(^2\) and with realistic predictions of the topological features of three-dimensional (3-D) polycrystals. Conversely, in similarity to the mean-field models, it still predicts a left-hand-skewed quasi-stationary grain size distribution (GSD), which is in contrast to the experimental evidence.

All the analytical grain-growth models are based on the implicit assumption that the grain-boundary curvature appearing in the growth-rate equations is well approximated by the average curvature proportional to the reciprocal of the grain radius.

In the present work, using the theoretical framework of the discrete model of grain growth based on pair interactions,\(^1\) a generalized formulation of the local grain-boundary curvature is proposed, which enables the model to reproduce a right-hand-tailed quasi-stationary GSD, with a shape closely approaching the Rayleigh distribution proposed by Louat\(^3\) and Pande\(^4\) in the stochastic models for grain growth.

An alternative calculation of the pinning force due to second-phase particles, extending the result by Gladman,\(^5\) is also presented and discussed.

The Local Curvature and the Grain-Boundary Velocity

According to the discrete grain-growth model based on pair interactions\(^1\) and accounting for the grain-boundary curvature (\(\kappa\)), the equation for the relative rate of volume change of a grain belonging to the \(i\)th-size class sharing a common face with a grain in the \(j\)th class, with \(R_i > R_j\), can be written in a generalized form as

\[
\frac{dv_{ij}}{dt} = M \gamma A_{ij} (\kappa_i - \kappa_j - Z) \quad \text{for} \quad |Z| \leq \kappa_i - \kappa_j
\]

\[1a\]

where \(M\) is the grain-boundary mobility, \(\gamma\) is the interfacial energy, \(A_{ij}\) is the effective exchange area between grains \(i\) and \(j\), and \(Z\) is the inhibition due to second-phase particles, which is always opposed to the boundary motion.

The quantity \(\kappa_{ij}\) is the effective local curvature of an \(i\)th-versus \(j\)th-class grain in contact with a \(j\)th-class grain. The difference appearing in the growth-rate equations is well approximated by the average curvature proportional to the reciprocal of the grain radius.

Consequently, by differentiating Eqs. [6] and [3] with respect to \(R_i\), one obtains

\[\kappa_{ij} = \kappa_i = \frac{2 \pi}{R_i} \quad [7]\]
In Table II, the parameters of the GSDs and Kinetic Exponents after 1000 Seconds of Simulated Grain Growth as a Function of the Inhibition Level; the Estimated Stagnation Grain Size ($D_{\text{lim}}$) is Also Indicated When Clearly Present.

<table>
<thead>
<tr>
<th>$Z$ (mm$^{-1}$)</th>
<th>Variation Coefficient $k_{\text{GSD}}$</th>
<th>Average Number of Faces ($m$)</th>
<th>Growth Exponent</th>
<th>$D_{\text{lim}}$ ($\mu$m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.506</td>
<td>11.14</td>
<td>0.484</td>
<td>—</td>
</tr>
<tr>
<td>25</td>
<td>0.459</td>
<td>11.29</td>
<td>0.252</td>
<td>*</td>
</tr>
<tr>
<td>50</td>
<td>0.462</td>
<td>11.30</td>
<td>0.169</td>
<td>250**</td>
</tr>
<tr>
<td>100</td>
<td>0.434</td>
<td>11.37</td>
<td>0.084</td>
<td>129</td>
</tr>
<tr>
<td>200</td>
<td>0.418</td>
<td>11.41</td>
<td>0.026</td>
<td>69</td>
</tr>
<tr>
<td>300</td>
<td>0.425</td>
<td>11.40</td>
<td>0.011</td>
<td>49</td>
</tr>
</tbody>
</table>

*Not determined.
**Estimated by extrapolation beyond 1000 s.

Fig. 1—Grain-coarsening kinetics at different levels of constant inhibition.

**Table I. Parameters of the GSDs and Kinetic Exponents after 200 Seconds of Simulated Grain Growth as a Function of the Inhibition Level**

<table>
<thead>
<tr>
<th>$Z$ (mm$^{-1}$)</th>
<th>Variation Coefficient $k_{\text{GSD}}$</th>
<th>Average Number of Faces ($m$)</th>
<th>Growth Exponent</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.517</td>
<td>11.12</td>
<td>0.473</td>
</tr>
<tr>
<td>25</td>
<td>0.454</td>
<td>11.29</td>
<td>0.326</td>
</tr>
<tr>
<td>50</td>
<td>0.467</td>
<td>11.27</td>
<td>0.256</td>
</tr>
<tr>
<td>100</td>
<td>0.477</td>
<td>11.27</td>
<td>0.200</td>
</tr>
<tr>
<td>200</td>
<td>0.456</td>
<td>11.31</td>
<td>0.120</td>
</tr>
<tr>
<td>300</td>
<td>0.449</td>
<td>11.34</td>
<td>0.078</td>
</tr>
</tbody>
</table>

which is the general expression of the average spherical curvature, assumed to be independent of its neighbor’s size.

On the other hand, the concept of curvature can be further generalized by taking into account the local contact properties between two grains. By rewriting Eq. [4] as a specific function of the effective contact area between grains $i$ and $j$, it results that

$$S_{ij} = A_{ij} \cdot m_i$$

[8]

The effective local curvature derived from the ratio between the derivatives of Eqs. [8] and [3] can be written as

$$\kappa_{ij} = \frac{1}{4 \pi R_i^2} \left( A_{ij} \frac{dm_{ij}}{dR_i} |_{R_i} + m_i \frac{dA_{ij}}{dR_i} |_{R_i, R_j} \right)$$

[9]

where the subscripts indicate that the derivatives are evaluated with respect to $R_i$ at the $(R_i, R_j)$ point.

It is worth mentioning that the effective exchange area $A_{ij}$ in Eq. [8] is a local quantity, whereas $m_i$ is an average property derived from the topological model adopted. [1]

**II. RESULTS**

A. Model Behavior with Constant Inhibition

To facilitate the immediate comparison with the previous approach with the average grain-boundary curvature, the simulations have been carried out on the same ideal system as in Reference 1. A grain-boundary mobility of $9.03 \cdot 10^{-11}$ m$^2$ J$^{-1}$ s$^{-1}$ and an average grain-boundary energy of 0.5 J m$^{-2}$ have been used, with constant inhibition values of 0, 25, 50, 100, 200, and 300 mm$^{-1}$, respectively. In all cases, the initial GSD had a Gaussian shape, with a 5 mm average size and 2.5 mm standard deviation, and the discrete class width was $\Delta R = 2$ mm. The simulations were stopped after a coarsening time of 1000 seconds.

Figure 1 shows the plot of the average grain size vs time in double logarithmic scale. In Table I, the most significant parameters obtained from the simulations after 200 seconds are reported, namely, the variation coefficient $k_{\text{GSD}}$ (the ratio between the GSD standard deviation and the average size), the average number of faces per grain, and the growth exponent (the slope of the first linear part of the curves reported in Figure 1). This table can be easily compared with the results previously obtained in Reference 1.

In Table II, the same data are reported for comparison after 1000 seconds. Unfortunately, the quasi-stationary condition could not be achieved, as is shown in Figure 2. In particular, even if the log-log plot follows a linear trend (Figure 1), the self-preserving shape of the GSD has not yet been reached (Figure 2).

It is worth noting that, as expected, a clear linear correlation exists between the limiting grain size in the stagnation