Growth of Grains in the Third Orientation in an Inhomogeneous Matrix Consisting of Two Orientation Groups - A Modified Potts–Monte Carlo Simulation -

Kunio Ito

Department of Materials Engineering, The University of Tokyo, Bunkyo-Ku, Tokyo, 113-8656 Japan

E-mail: ito_e-prof@material.t.u-tokyo.ac.jp

Abstract. The growth of a C-grain embedded in the matrix of A- and B-grains has been simulated. A, B, and C denote orientation groups. Boundaries were defined as "specified" if they consisted of A and C grains, else they were defined as "unspecified". The edges of an embedded grain were named according to component grains as CAA, CAB, and CBB triple lines. The inhomogeneity of the matrix structure was presented as the ratio between their numbers. When the mobility of specified boundary is higher than that of unspecified boundary, the volume fraction of the C-grain increases with grain coarsening, which is affected by the ratio between triple lines. The results suggest that the development of the grain growth texture is affected by the orientation distribution in a specimen and that the influence must be bigger when the mobility of the triple line depends on the combination of relevant grains.

1. Introduction

Changes in crystallographic textures have been examined by simulating the grain coarsening process[1]–[3] using the grain embedding method[3],[4]. Boundary energy and boundary mobility were controlled as a function of orientation relations between adjusting grains. In the embedding method, the orientations of grains are classified into three groups, i.e., A, B, and C. An increase in the volume fraction of grains in the orientation group C through the grain coarsening process was studied. Thus far, similar to other studies[5], grains in the orientation group A and those in the orientation group B were homogeneously distributed in the matrix.

In this paper, the growth of grains in the orientation group C in the matrix of inhomogeneous distribution of grains in the two orientation groups is reported.

2. Modelling

2.1. Preparation of the matrix structure

First, structures similar to those in the previous report[3] were prepared, where the grains in the two matrix orientation groups A and B were identical in both volume fractions and grain size distributions. Then, the specimen was divided into 8 (=2 × 2 × 2) subdivisions of categories I and II so that they were three-dimensionally alternatingly located. In the subdivision of category I, the orientations of grains of group B were changed to the orientations of group A and vice versa in the subdivision of category II. The orientations of grains lying over the two categories were unaltered. The specimens
made from this type of the matrix structure are called the 222 specimen, and those made by a similar process through 512 (=8 × 8 × 8) subdivisions are called the 888 specimen. The 888 specimen corresponds to the specimen with a random orientation distribution[3](figure 1).

Figure 1. Sections of initial matrix structures prior to embedding a grain in orientation group C. (a) 222 and (b) 888 specimens. Grains in the orientation groups A and B are, respectively, colored as □ and □.

2.2. Algorithm for coarsening
A grain belonging to the orientation group C was embedded at the center of the matrix structure, and the coarsening process was simulated by the same algorithm as that reported in[3],[4]. Boundaries between the embedded grain and matrix grains in the orientation group A are defined as “specified,” and the other boundaries are defined as “unspecified”. The energy of cell i in orientation $O_i$ was given by equation (1). $f_{in}$ represents the dependence of boundary energy on orientation difference. The orientation change from $O_i^h$ to $O_i^a$ was accepted by probability $p$. $R_{O_i^a/O_i^h}$ represents the dependence of boundary mobility on orientation difference.

$$E_i(O_i) = \left(\sum_{n=1}^{26} f_{in} \delta_{in}\right) / 100$$  \hspace{1cm} (1)

$$\Delta E = E_i(O_i^a) - E_i(O_i^h)$$  \hspace{1cm} (2)

$$p = p(\Delta E) / R_{O_i^a/O_i^h}$$  \hspace{1cm} (3)

In the case of discrimination of boundary energy, if the combination of $O_i$ and $O_n$ corresponded to a specified boundary, then $f_{in}$ was set to 65, else to 100, and $R_{O_i^a/O_i^h}$ was fixed to 1. In the case of discrimination of boundary mobility, if the combination of $O_i^a$ and $O_i^h$ corresponded to the migration of specified boundary, then $R_{O_i^a/O_i^h}$ was set to 1 else to 3, and $f_{in}$ was fixed to 100. In the following figures, the former and the latter cases are, respectively, designated as F065R100 and F100R033.

3. Statistical results of the grain growth of embedded grain

3.1. Parameters concerning the grain growth

$\langle V \rangle (t)$; mean volume of matrix grains at time $t$, $\langle V \rangle (t_0) = 2900$ in the initial matrix structure $v_0(t)$; volume of an embedded grain at time $t$

$\langle V \rangle (t_1)$; mean volume of matrix grains when $\langle V \rangle (t_1)/\langle V \rangle (t_0) = 1.1$

$C_r = \langle V \rangle (t_r)/\langle V \rangle (t_1)$; matrix coarsening ratio at time $t_r$

$t_2$, $t_4$, $t_8$, $t_{16}$; time for $C_r = 2$, 4, 8, 16
\[ R_{\text{growth}(t_f, t_i)} = \frac{V_0(t_f)}{V_0(t_i)} / C_r \]; relative coarsening ratio of an embedded grain at time \( t_f \)

\[ R_{\text{growth}(t_f, t_i)} > 1 \] means an increase in the volume fraction of the embedded grain in a specimen[4].

\[ r_{eq}(t) \]; equivalent radius of an embedded grain, \( V_0(t) = 4\pi r_{eq}(t)^3 / 3 \)

\[ R_{eq}(t) = r_{eq}(t) / \text{half length of specimen} \]; relative equivalent radius of an embedded grain

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3.2. Parameters concerning boundaries and triple lines surrounding an embedded grain

\( n_A \); number of specified boundaries

\( n_B \); number of unspecified boundaries

\[ X = n_A / (n_A + n_B) \]; “fraction of specified boundaries”

\( n_{AA} \); number of triple lines that include two neighboring grains belonging to the orientation group A.

\( n_{AB} \); number of triple lines including one neighboring grain belonging to the orientation group A and another one belonging to the orientation group B

\( n_{BB} \); number of triple lines including two neighboring grains belonging to the orientation group B

\[ Y = (n_{AA} + n_{BB}) / n_{AB} \]; “ratio of mixed triple lines”

Coarsening processes are exemplified in figure 2. The ordinate axis “Relative size” represents \( R_{eq}(t) \). Plural specimens were made using randomly made matrix structures by changing sizes of embedded grains[2],[3]. One kinked line shows a process of one specimen, and round-shaped marks represent the means of 222 and 888 specimens.
3.3. Parameters concerning correlations between the growth of embedded grain and the degree of inhomogeneity of matrix grains

\[ R_{\text{growth}}(t_i/t_f) = R_{\text{growth}}(t_i/t_f)/R_{\text{growth}}(t_i/t_f) \]; relative coarsening ratio of an embedded grain during the time interval between \( t_b \) and \( t_e \). In the case of different boundary mobilities, \( t_b = t_2 \) and \( t_e = t_8 \).

For different boundary energies, \( t_b = t_4 \) and \( t_e = t_16 \). Thus, the two conditions were compared under similar matrix grain sizes.

\(< X > (t_b,t_e) \); the mean of \( X \) from \( t_b \) to \( t_e \) along a kinked line (e.g., figure 2 (b)).

\(< Y > (t_b,t_e) \); the mean of \( Y \) from \( t_b \) to \( t_e \) along a kinked line.

3.4. Method for calculating correlation coefficients

Let \( X_i \), \( Y_i \), and \( Z_i \) represent \( < X > (t_b,t_e) \), \( < Y > (t_b,t_e) \), and \( R_{\text{growth}}(t_i/t_f) \) of the \( i \)th specimen. The data pooled over 222 and 888 specimens are expressed as \{\( X_i \}, \{Y_i \}, \{Z_i \} \).

X–Y iteration loop; analysis between \{\( X_i \} and \{Z_i \} followed by the analysis of the residue

1) get correlation coefficient \( R_{x1} \) and approximate equation \( Z_{\text{apr}}^{x1} = a_{x1}X_i + b_{x1} \) from \{\( X_i \} and \{Z_i \}.

2) get correlation coefficient \( R_{y1} \) and approximate equation \( Z_{\text{apr}}^{y1} = a_{y1}Y_i + b_{y1} \) from \{\( Y_i \} and \{Z_i \}.

3) similarly, get \( R_{x2} \) and \( Z_{\text{apr}}^{x2} = a_{x2}X_i + b_{x2} \) from \{\( X_i \} and \{\Delta Z_{i2} = Z_i - Z_{\text{apr}}^{i2} \}.

4) get \( R_{y2} \) and \( Z_{\text{apr}}^{y2} = a_{y2}Y_i + b_{y2} \) from \{\( Y_i \} and \{\Delta Z_{i3} = Z_i - Z_{\text{apr}}^{i3} \} and return to 3)

get \( R_{xy}, a_{xy} \) and \( (R_{xy}, a_{xy}) \) by iterating 3) \( \rightarrow \) 4).

Y–X iteration loop; analysis between \{\( Y_i \} and \{Z_i \} followed by the analysis of the residue

get \( R_{xy}, a_{xy} \) and \( (R_{xy}, a_{xy}) \) by iteration that is similar to the X–Y iteration

Figure 4. Correlation between the fraction of specified boundaries and the relative coarsening ratio of an embedded grain

Figure 5. Correlation between the ratio of mixed triple lines and the relative coarsening ratio of an embedded grain
As shown in figure 3, where $G$ and $R$, respectively, represent $a_x$ or $a_y$ and $R_x$ or $R_y$, both loops give the same convergent values. Plotted points are normalized with respect to them.

\{Z_i\} are plotted against \{X_i\} (figure 4) and against \{Y_i\} (figure 5). The values of $R_x$ and $R_y$ after convergence are given in the figures, and the lines correspond to $G$.

4. Observation of shapes of embedded grain

Three-dimensional shapes of embedded grain are shown by its surfaces in figures 6 and 7.

![Figure 6](image1)

**Figure 6.** Embedded grain in the 222 specimen; energy discrimination case, matrix coarsening ratio = 16. (a) Whole grain; one cell in the figure represents 64 (= $4 \times 4 \times 4$) cells in the original structure. (b) Part of the grain; the cell size is the same as the original one. The colors of the cells show the orientation groups of neighboring grains.

![Figure 7](image2)

**Figure 7** Grain embedded in a 222 specimen; mobility discrimination case, matrix coarsening ratio = 8. Differences in (a) and (b) are the same as those in figure 6.

5. Discussion

5.1. Expression of the inhomogeneity of the matrix structure by the “ratio of mixed triple lines” parameter

This triple-lines-based parameter is expected to be equal to unity under the present condition that the numbers and sizes of grains in two orientation groups are identical, when grains in the two groups are randomly distributed, and expected to become bigger than unity when grains in the same group are clustering to make colonies. With the growth of embedded grain, the difference in this parameter
increases between 222 and 888 specimens (figure 2). The increase corresponds to the inhomogeneity of 222 specimens in their internal structures (figure 1(a)). By responding to the intentional design of matrix structures, the triple-lines-based parameter of 222 specimens was bigger than that of 888 specimens at the time when the growth rates of embedded grains were compared (see the axis of abscissa in figure 5).

Triple lines and quadruple points have been pointed out to affect the grain growth process [5]–[7]. The ratio of mixed triple lines represents the composition of orientations of grains surrounding an embedded grain. Hence, it is suggested that the degree of inhomogeneity in orientation distribution in a specimen will yield a stronger influence on textural development by grain coarsening, if the mobility of triple lines and quadruple points depend on the combination of related orientations.

5.2. Comparison of boundary energy discrimination with boundary mobility discrimination

Embedded grains in 222 specimens grow anisotropically corresponding to the inhomogeneity of the matrix structure (figures 6 and 7). This trend appears more distinctly under condition of mobility discrimination than under condition of energy discrimination (figure 7). When the mobility was different, grains in the orientation group B interfere with the potential rapid growth of the embedded grain into grains in the orientation group A. Under the condition of boundary energy discrimination, an embedded grain grows by wetting into the space between two grains in the orientation group A. Grains in the orientation group B do not essentially obstruct this growth.

The effect of ratio of mixed triple lines on the growth of embedded grain is bigger in the case of mobility discrimination than in the case of energy discrimination (compare (a) with (b) in figure 5).

The observed growth of embedded grain, which consumes grains in the orientation group A that are obstructed by grains in the orientation group B, is similar to the retardation of grain growth by second phase particles [5],[8]. The colonies of grains in the orientation group B correspond to particles, and the size of colonies of grains in the orientation group A corresponds to that of grains.

6. Summary

The simulation showed that when the mobility of boundary between grains in the third orientation group and matrix grains in one of their orientation groups is preferentially higher than those of other boundaries, the volume fraction of grains in the third orientation group increases more with grain coarsening in the case of matrix structure where grains make colonies of the same orientation group than in the case of matrix structure of homogeneous orientation distribution.

The observation of shapes of growing grains showed that this phenomenon corresponds to the retardation of growth of colonies surrounded by the higher number of higher mobility boundaries and the lower number of lower mobility boundaries by colonies surrounded by the higher number of lower mobility boundaries and the lower number of higher mobility boundaries.

The ratio of mixed triple lines, which is defined in this paper, represents the composition of orientations of grains surrounding an embedded grain. It is suggested that the degree of inhomogeneity in orientation distribution in a specimen will yield a stronger influence on the textural development by grain coarsening if the mobility of triple lines and quadruple points depends on the combination of related orientations. The ratio might be one of hidden factors that control this texture development.

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