Simulation of growing grains under orientation relation - dependent quadruple point dragging

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Abstract. The growth behaviour of a specified grain embedded in matrix grains, for which the migration mobility of the quadruple points depended on the relation between the orientations of the growing and shrinking grains, was studied using a modified Potts MC-type three-dimensional simulation. Large embedded grains continued to grow without being overcome by coarsening matrix grains, whereas small embedded grains disappeared, under the influence of the relative mobilities of the quadruple points, the composition of the matrix grain texture and the width of the grain size distribution of the matrix grains. These results indicate that orientation relation-dependent quadruple point dragging can affect the recrystallization texture during the grain coarsening stage.

1. Introduction
It is known [1,2] that the quadruple junction mobility can affect the grain growth of polycrystalline materials. In the present report, the growth behaviour of a specified grain embedded in matrix grains, for which the mobility of the quadruple points depended on the relation between the orientations of the growing and shrinking grains, was observed using a simulation. The evolution of the texture component to which the specified grains belonged was estimated from the mean of the behaviour of individual embedded grains.

2. Simulation method
2.1 Construction of the specimen
The specimen contained 256×320×256 cubic cells, and the texture was composed of three components: S (specified grain component), M (matrix component) and B (background component). The starting structures that contained approximately 7100 grains were the same as those used formerly [3], and grains belonged to either the M or B components. Their grain size distributions were the same (figure 1). The number of faces of a grain is a number of grains sharing boundary planes with the grain concerned. The abbreviations ‘standard 21’ and ‘standard 12’ indicate standard starting structures with volume ratios M/B = 2/1 and 1/2, respectively, and ‘wide 21’ corresponds to a wide starting structure with M/B = 2/1.

Figure 1. Grain size distributions in the standard and wide starting structures.
2.2 Coarsening algorithm

As reported previously [3,4], the unit process for boundary migration was presented as the occupation of passive cell \( j \) by active cell \( i \) and was permitted with the probability \( p \). The value of \( \Delta E \) was calculated with respect to the Moore neighbourhood of cell \( j \):

\[
p^{\Delta E} = \exp\left(-\frac{\Delta E}{kT}\right) \quad \text{when} \quad \Delta E > 0 \quad \text{and} \quad p^{\Delta E} = 1 \quad \text{when} \quad \Delta E \leq 0 \tag{1}
\]

\[
p = \frac{p^{\Delta E}}{R} \tag{2}
\]

The permission ratio \( R \) was specified by the category of the occupation event, while the multiplicity of event \( m \) was defined as the number of grains to which the cells in the Von Neumann neighbourhood of passive cell \( j \) belonged. For \( m = 2 \) (boundary migration) and \( m = 3 \) (triple line migration), \( R \) was equal to unity. On the other hand, for \( m \geq 4 \), \( R \) was equal to unity only when the event yielded the growth of the embedded grain with shrinkage of the grains in component M, and was larger than or equal to unity otherwise. The coarsening process was performed by repetition of a systematic MC step, as formerly described [3,4].

3. Simulation results

3.1 Relation between the permission ratio and the migration rate of a quadruple point

The migration of quadruple points was observed in a configuration composed of columnar hexagonal grains with edge length \( a \) after Barrales-Mora et al. [1, 5]. Figure 2 (a), where ‘R1’ and ‘R10’ respectively indicate \( R = 1 \) and \( R = 10 \), shows examples of the changes in the distance between the corresponding two points observed for \( kT = 0.7, 0.87, 1.1, \) and 1.3 (\( kT0.7, kT0.87, kT1.1, \) and \( kT1.3, \) respectively), and \( a = 78/4 \) and 78 (\( a78/4 \) and \( a78 \), respectively). Runs for each set of the parameters were repeated 3 times. The straight parts of the curves represent the steady states. Figure 2 (b), where the gradients, being multiplied by \( a \), relative to the value obtained for \( a = 78 \) and \( R = 1 \) are shown, demonstrates the effect of the permission ratio on the mobility. \( kT \) equal to 0.87 was used in this report as formerly [3].

![Figure 2](image-url)

Figure 2. Migration behaviour of a quadruple point. \( kT = 0.87 \) was used in this report.

3.2 Coarsening behaviour of the embedded grains

A lenticular spheroid grain belonging to texture component S was embedded in a starting structure, as described previously [3]. Its size was controlled by the volume and the axial ratio. A reference structure was obtained using coarsening steps that decreased the number of the matrix grains by 10% (see figure 3 (a)). The volume of the embedded grain and the mean volume of the matrix grains in the reference structure are denoted by \( V_0 \) and \(<V>_0 \), respectively and those after coarsening are indicated by \( V \) and \(<V>_0 \), respectively. The following ratios are further defined:

\[
\text{referred coarsening ratio of the matrix grains} = \frac{<V>}{<V>_0}, \tag{3}
\]

\[
\text{referred coarsening ratio of the specified grain} = \frac{V}{V_0}, \tag{4}
\]

\[
\text{relative growth ratio of the specified grain} = \frac{(V/V_0)/(<V>)/<V>_0)}{<V>_0} \tag{5}
\]

Figure 3 shows 2D sections. The embedded grain is red; ‘matrix’ and ‘relative’ denote the referred coarsening ratio of the matrix grains and the relative growth ratio of the specified grain, respectively; \( N \) denotes the initial number of faces of the embedded grain. Figure 4 shows a collection of evolution curves for the individual embedded grains whose number of faces in the reference structure \( N \) happened to be 21 (a) and 23 (b). As can be
observed in the figure, for case 1, the relative growth ratio at a referred coarsening ratio of 32 was greater than 1, whereas for case 2, it was less than 1. The mean values for the relative growth ratios at referred coarsening ratios of 8 and 32 shown in figures 4 (a) and (b) were plotted in figures 5 (a) at numbers of faces = 21 and 23, respectively. The fractions of grains whose relative growth ratios were greater than 1 were similarly plotted in figures 5 (b). The population parameter for the statistics was approximately 15 grains (figure 4). Figure 5 contains the values obtained for $R = 2$ as well. Note that throughout in figures 5 ‘coarsening’ indicates the referred coarsening ratio of the matrix grain, and triangular and rhombic marks represent $R = 2$ and $R = 10$, respectively. When $R$ was small ($R = 2$), the relative growth ratio decreased as coarsening progressed or as the coarsening ratio of the matrix grains increased (see coarsening = 8 and 32 in figure 5 (a)); namely, even larger embedded grains disappeared with time. Furthermore, the fraction of embedded grains that continued to grow generally increased with an increase in the initial size of the embedded grain (figure 5 (b)). This fraction never reached unity, however, even for the largest embedded grain or when the number of faces was 40 (see figure 1). On the other hand, when $R$ was large ($R = 10$), the relative growth ratio increased as coarsening progressed, and the fraction reached unity.

4. Discussion

4.1 Migration rate of the quadruple point

The migration rate of the quadruple point decreased moderately with increasing $R$ (figure 2 (b)). The dependence of the migration rate on $a$ and $R$ coincided roughly with the theoretical calculation [1] in a manner similar to that discussed for triple line migration in a 2D model [4]. Additionally, while the effect of the simulation parameter $kT$ appeared more distinctly as the size of grain $a$ decreased, it did not seem to be critical.
4.2 Estimation of changes in the texture

The ordinate of figure 6 (a) was calculated using equation (6) as a function of the referred coarsening ratio of the matrix grains $j$.

$$\text{volume increasing ratio}(j) = \frac{\sum_i j r(j, i) f(i)}{\sum_i f(i)}$$

4.2.1 Estimation of changes in the texture

The numbers ‘8’ and ‘32’ in the legends of figure 6 (a) are the values for $j$. In equation (6), $f(i)$ represents the volume fraction of the specified grains in the reference structure whose number of faces is given by $i$, and the size distribution shown in figure 1 was used for it. The parameter $r(j, i)$ represents the mean of the relative growth ratios exemplified in figure 5 (a). The summation in equation (6) was made for values of $i$ ranging from 10 to 40, the value for $r(j, i)$ is practically zero when $i < 10$, whereas $f(i)$ is negligible when $i > 40$.

Equation (6) is a good approximation for the volume change of the texture component $S$ assuming that the initial grain size distributions are the same for all of the texture components, and the grains belonging to component $S$ do not collide with one another.

In figure 6 (b), the critical values for the number of faces of the embedded grain in the reference structure are shown. These values were obtained from the graphs exemplified in figure 5 (b). In the legends of figure 6 (b), ‘100%’ corresponds to the smallest number of faces for which the fraction shown in figure 5 (b) reached 1, whereas ‘50%’ corresponds to the smallest number for which the fraction reached 0.5. It can be clearly observed from this figure that when the width of the grain size distribution of the matrix grains was large, the effects were reduced (cf. wide 21 vs. standard 21).

5. Conclusions

Under the conditions where the migration mobility of quadruple points depends on the relation of the orientations of the growing and shrinking grains, the behaviour of a specified grain embedded in matrix grains has been observed using a modified Potts MC-type 3D simulation.

Critical sizes were found for the embedded grain. Notably, smaller embedded grains shrink absolutely, whereas larger grains continue to grow continually without being overcome by the coarsening matrix grains. Furthermore, the growth of the grains depends on the relative mobilities of the quadruple points, on the composition of the matrix grain texture and the width of the grain size distribution of the matrix grains.

It was also demonstrated that the volume fractions of texture components may vary during grain coarsening when the mobility of the quadruple points is affected by combinations of the orientations of the growing and shrinking grains in correlation with their texture components.

References

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