1. Introduction

The properties of steel and other metallic materials depend much on their texture. Therefore, it is extremely important to predict and control their texture in the manufacturing process. Various models have been proposed for predicting changes in texture. Among such models, the statistical method is used, for example, to understand the mechanism of orientation selectivity in abnormal grain growth that is found in grain-oriented electrical steel sheets in the steelmaking process. However, this method cannot be used to study the orientations of individual grains. Thanks to the dramatic advances in electron backscatter diffraction (EBSD) technology in recent years, it has become easier to analyze the individual grain orientations and the individual orientation relationships with adjacent grains in the two dimensions. Under such a condition, the development of a grain growth simulation model that allows for the full use of EBSD observation data is desired.

Models that describe grain growth, such as the stochastic method (Monte Carlo method) and the phase field method, which has also been applied to grain growth models, requires grain boundaries to be set to finite widths. Therefore, in the early stage of grain growth in which a large number of fine grains exist, this method does not always achieve sufficient calculation accuracy. Moreover, introducing physical principles such as the tension balance at triple junction is not easy.

The phase field method, which has also been applied to grain growth models, requires grain boundaries to be set to finite widths. Therefore, in the early stage of grain growth in which a large number of fine grains exist, this method does not always achieve sufficient calculation accuracy. Moreover, introducing physical principles such as the tension balance at triple junction is not easy.

The front tracking model approximates the grain boundaries using curved lines, which migrate to the curvature centers. In the two-dimensional front tracking model, several virtual vertices (double junctions) are arranged along a grain boundary between two triple junctions, and the grain boundary is approximated in a curved line expressed by a polynomial equation, which allows for calculation of the local curvatures of a grain boundary. In this calculation, a local grain boundary or a double junction migrates at a velocity \( v_{gb,i} \).

\[
\frac{\rho_{i}}{M_{gb,i}} F_{gb,i} = \gamma_{i} \kappa_{gb,i} \tag{1}
\]

where \( M_{gb,i} \) is the mobility of the grain boundary to which the double junction \( p_{i} \) belongs; \( F_{gb,i} \) is the driving force per unit length acting on the grain boundary with a direction...
from the double junction \( p_i \) to the curvature center; \( \gamma \) is the grain boundary energy per unit length; \( \kappa_{gb,i} \) is the curvature vector with the magnitude of the grain boundary curvature at the double junction \( p_i \) and with the direction from the double junction \( p_i \) to the curvature center. However, the triple junction, which is a real junction, is not handled physically but rather mathematically. The position of the triple junction is mathematically adjusted so that the grain boundaries intersect one another at angles such that the grain boundary tensions due to the grain boundary energies achieve equilibrium.\(^5\) For example, when the energies of three grain boundaries are equal, the intersection angles are adjusted to 120 degrees.

In the initial vertex model, the grain boundaries are always approximated by straight lines,\(^7,8\) and the driving force for grain growth is the vector summation of the grain boundary tensions acting on the triple junction. In this model, as shown in Eqs. (3) and (4), grain growth is expressed by the migration of the grain boundary triple junction \( p_i \) at a velocity \( \vec{v}_{p,i} \),

\[
\vec{v}_{p,i} = M_{p,i} \vec{F}_{p,i} \quad \text{.............................. (3)}
\]

\[
\vec{F}_{p,i} = \sum_{j=1}^{3} \gamma_j \vec{q}_j  \quad \text{............................ (4)}
\]

where \( M_{p,i} \) is the mobility of the triple junction \( p_i \); \( \vec{F}_{p,i} \) is the driving force acting on the triple junction \( p_i \); \( \gamma_j \) is the grain boundary energy per unit length of the grain boundary to which the triple junction \( p_i \) and the adjacent triple junction \( p_j \) belong; and \( \vec{q}_j \) is the vector from the triple junction \( p_j \) to the adjacent triple junction \( p_j \).\(^7\) The unit of the energy per unit length is the same as that of the force. Therefore, the right side of Eq. (4) indicates the force acting on the triple junction, and the migration of the triple junction is accurately described from a physical viewpoint. However, the initial vertex model has a drawback in that it approximates grain boundaries by straight lines, regardless of the fact that the grain boundaries are normally curved lines.

Such the initial vertex model has been improved by placing virtual vertices along the grain boundaries, or converting it into a multi-vertex model.\(^9,10\) This improvement has allowed for grain boundaries to be approximated by polygonal lines. The motion of each virtual vertex is described by the variational principle based on the motion equation that contains a viscosity term or a friction term. As the improved vertex model is based on a physical principle, it is considered suitable for describing grain growth. However, when the number of virtual vertices along a grain boundary is small, significant error can occur as a result of approximating the grain boundaries not by curved lines but by polygonal lines. For example, in the contraction of an isolated n-sided polygon, the velocity of the virtual vertices described by the improved vertex model is about \( 1/\cos(\pi/n)^2 \) times faster than the velocity calculated by the curvature obtained from the front tracking model.\(^9\) Although they become equal at the limit of \( n \rightarrow \infty \), the error is as much as about 11% when \( n = 10 \).

The purpose of this paper is to propose a new two-dimensional topological network model, or a local curvature multi-vertex model, that can overcome the above-described problems of the improved vertex model and can express physical principles in a straightforward manner. More specifically, this paper particularly focuses on (1) the concept of this model, (2) the contrivance and the optimization of the conditions on handling distances, time intervals, and triple junctions when conducting a simulation, and (3) the verification of the model.

### 2. Proposal of a Model - Local Curvature Multi-vertex Model -

#### 2.1. Principle of Grain Boundary Migration

In order to elaborate a two-dimensional grain growth model that is more accurate and more straightforward than conventional models, we introduce two types of junctions using the same method adopted by Frost et al.\(^5\) and Fuchizaki et al.\(^9\) One of the junctions is a triple junction, which is a real junction. The other is a virtual junction, or a virtual vertex, discretely located along a grain boundary. Using this method, the migration of grain boundaries expressed by lines can be converted to the migration of junctions. Because a virtual vertex is connected to the two adjacent junctions for convenience sake, it can be referred to as a double junction. In addition, a real junction is connected to three adjacent junctions, so it can therefore be referred to as a triple junction. The migration of virtual vertices and real junctions follows Eqs. (1) and (2), and Eqs. (3) and (4), respectively. The local curvature vector \( \kappa_{gb,i} \) is calculated by the following equation,

\[
\kappa_{gb,i} = -\frac{1}{R_i} \frac{\vec{R}_i}{|\vec{R}_i|} \quad \text{.......................... (5)}
\]

where \( \vec{R}_i \) is a radius vector with the magnitude equal to the radius of circle \( C_i \) determined by the double junction \( p_i \) and the two junctions adjacent to the double junction on the grain boundary, and with the direction from the center \( O_i \) of the circle \( C_i \) to the double junction \( p_i \) (Fig. 1). The direction of the local curvature vector \( \kappa_{gb,i} \) is opposite that of \( \vec{R}_i \).

The driving forces in Eqs. (2) and (4) can be derived from the grain boundary energy gradient, or \( \vec{F} = -\nabla E \), where \( \vec{F} \) is the driving force and \( E \) is the grain boundary energy. Therefore, it is possible to say that Eqs. (1) to (5) are relational expressions based on physical principles. However,
it should be noted that the units of the driving force in Eqs. (2) and (4) are the force per unit length and the force (See the Appendix).

Many studies on grain boundary energy have been conducted. The energy of a Σ1 coincidence site lattice (CSL) boundary, which is a low-angle grain boundary, is smaller than the energy of a general high-angle grain boundary, and the Read-Shockley relationship is applied for the energies of Σ1 CSL boundaries.13) As is the case of Σ1 CSL boundaries, the energy of a CSL boundary, which is a high-angle grain boundary, with a high density of coincidence site lattice points as a Σ3 CSL boundary is smaller than the energy of general high-angle grain boundaries.12) However, without sufficient available quantitative data on the grain boundary energy, particularly those of the BCC metal, the Read-Shockley relationship is also applied for the energies of the Σ3 CSL boundaries. At the same time, the energies of the general grain boundaries are assumed to be constant, except for the energies of CSL boundaries that have a high density of coincidence site lattice points.

2.2. Appropriate Arrangement of the Virtual Vertices in the Local Curvature Multi-vertex Model

The distances between triple junctions and double junctions change with time evolution. In order to prevent the calculation accuracy from being reduced, it is necessary to prevent such junction distances from becoming extremely long or short. In the new model presented in this paper, it is proposed to generate or annihilate virtual vertices in order to maintain their distances at appropriate lengths. The appropriate lengths are described in the subsequent Sections 2.3 and 2.5.

When the distance between two adjacent vertices becomes the specified maximum length \( L_{\text{max}} \) or more, a new virtual vertex is generated between the two adjacent vertices. As shown in Fig. 2(a), the virtual vertex \( p_b \) is generated between the virtual vertex \( p_2 \) and the virtual vertex \( p_3 \). The virtual vertex \( p_a \) is arranged on the perpendicular bisector of the line segment \( p_2p_3 \), and the curvature \( \kappa_a \) of the virtual vertex \( p_a \) is the average of the curvature \( \kappa_2 \) of the virtual vertex \( p_2 \) and the curvature \( \kappa_3 \) of the virtual vertex \( p_3 \).

On the other hand, when the distance between two adjacent vertices becomes the specified minimum length \( L_{\text{min}} \) or less, one new virtual vertex is generated and two existing virtual vertices are annihilated. As a result, one virtual vertex is annihilated. As shown in Fig. 2(b), the virtual vertex \( p_b \) is generated near the virtual vertices \( p_2 \) and \( p_3 \), and the virtual vertices \( p_3 \) and \( p_4 \) are annihilated. The virtual vertex \( p_b \) is arranged on the perpendicular bisector of the line segment \( p_2p_3 \), and the curvature \( \kappa_b \) of the virtual vertex \( p_b \) is the average of the curvature \( \kappa_2 \) of the virtual vertex \( p_2 \) and the curvature \( \kappa_3 \) of the virtual vertex \( p_3 \).

Because of above-mentioned generations and annihilations of virtual vertices, the distance \( L \) between two adjacent vertices can be expressed as

\[
L_{\text{min}} < L < L_{\text{max}}
\]  

(6)

At this time, in order to generate or annihilate virtual vertices stably, it is necessary to set the maximum length \( L_{\text{max}} \) to more than twice as long as the minimum length \( L_{\text{min}} \):

\[
2L_{\text{min}} < L_{\text{max}}
\]  

(7)

As mentioned above, using the simple process of generating and annihilating virtual vertices and the conditions of Eqs. (6) and (7), the distances of the vertices can be prevented from becoming extremely long or short as time passes during grain growth. In this way, the vertex distances can be stabilized, and the calculation accuracy can be maintained.

2.3. Optimization of the Distances between the Virtual Vertices in the Local Curvature Multi-vertex Model

In this section, the impact of the virtual vertex distance on the calculation accuracy is examined. It is considered that the impact on the calculation accuracy can be established not by the absolute value of the virtual vertex distance but by a relative value based on the length of the grain boundary, which is the grain diameter. In this study, the average grain diameter was used as reference, and the initial grain radius was assumed to be 10 (arbitrary units) as the average grain diameters often observed in real steel sheets are on the order of several ten \( \mu \)m. In actual grain growth, both the grain boundaries and the triple junctions migrate simultaneously. However, we focused on only the migration of the grain boundaries for the sake of simplicity. We used a circular arc grain boundary with a radius of 10 and both ends fixed in Fig. 3. The white circles represent fixed junctions,

---

**Fig. 2.** Generation and annihilation of virtual vertex (double junction).
which are pinned, and the black circles represent virtual vertices. We used the fixed junctions as triple junctions, and thus, the evaluation was performed on the migration of the grain boundaries (virtual vertices) in case that the triple junctions do not migrate. At this time, the positions of the fixed junctions were set such that the circular arc length was 1/2 to 1/12 of the circumference length. In addition, it was assumed that the virtual vertices in the initial state were arranged at even distances on the circular arc such that the virtual vertices divided the circular arc into 2 to 96 segments. The number of such segments was always an even number, and we evaluated the migration of the virtual vertex that was located at the very center of two fixed junctions and was located at the farthest position from the chord that connects the two fixed junctions. For example, the distance between two adjacent virtual vertices is 14.14 when the division number is 2 and 0.33 when the division number is 96.

**Figure 4** shows the evaluation results of the time evolution of the position and speed of the centered virtual vertex on a half circular arc. Figure 4 also shows the migration of an isolated grain boundary in the shape of a complete circle that is not pinned. The speeds of the centered virtual vertices at all distances at the start of grain boundary migration were the same. As the centered virtual vertices in a semicircular grain boundary with both ends fixed are not affected by pinning in the early stage of migration, this result is regarded as appropriate. Based on the positions and speeds in case of the shortest virtual vertex distance of 0.33 (96 divisions), the differences of the positions and speeds of the centered virtual vertices in case that the division number is changed in the range from 2 to 96 to make the distance between the virtual vertices smaller are defined as errors. **Figure 5**

![Figure 3](image1.png) **Fig. 3.** Arc grain boundary for accuracy validation. (a) Half circular arc divided into 8 segments by 7 virtual vertices. (b) One-sixth circular arc divided into 6 segments by 5 virtual vertices.

![Figure 4](image2.png) **Fig. 4.** Grain boundary migrations of half circles calculated by the local curvature multi-vertex model and of isolated full circle calculated by conventional curvature model. (a) Time evolution of position. (b) Time evolution of speed. The radius of the initial circle is 10.

![Figure 5](image3.png) **Fig. 5.** Calculation errors of the position and speed of grain boundary migration as a function of the initial distance between adjacent vertices on half circular arc, on the basis of the initial distance 0.33. (a) Position error. (b) Speed error. The radius of the initial circle is 10.
shows the maximum errors in the positions and speeds as a function of the initial vertical vertex distance. On the half circular arc, it is found that the virtual vertex distance should be approximately 4.2 or less (7 divisions or more) in order to keep the maximum error in the position to 1% or less and approximately 2.4 or less (12 divisions or more) in order to keep the maximum error in the speed to 1% or less.

The above results are for a case where the circular arc length is 1/2 of the circumference length. Similar simulations were performed for cases where the circular arc length was from 1/3 to 1/12 of the circumference length. Figure 6 shows the evaluation results of both the initial division numbers of the virtual vertices and the initial distance of the virtual vertices in case that the maximum errors in the positions and speeds were 1% and 2%, respectively, as a function of the division number of the circumference. It was found that the maximum error did not depend much on the division number of the circumference, even when the initial grain diameter was the same, but there were differences in the distance between the fixed vertices and the migration distance of the centered virtual vertex. We found that in order to keep the maximum position error to 1% or less, the division number between two fixed junctions, or two triple junctions, should be about 6 or more. Also, we found that in order to keep the maximum speed error to 1% or less, the division number should be about 10 or more. In two dimensions, under the condition that the grain boundary characteristics (grain boundary energies and grain boundary mobilities) are uniform, the grain size generally becomes large when the number of the triple junctions on one grain or the division number of the circumference is 7 or more, and the grain size generally becomes small when the number is 5 or less.13 Therefore, we consider that the specific virtual vertex distance should be decided with a circumference division number of 6, which is the mean value of the above numbers. Specifically, if the calculation accuracy of the position needs to be 1%, the virtual vertex distance should be approximately 2.0 or less (virtual vertex division number of 6 or more) as shown in Fig. 6. In order to achieve calculation accuracies of 2% and 1% for the speed, the virtual vertex distances need to be approximately 1.6 or less (virtual vertex division number of 7 or more) and approximately 1.2 or less (virtual vertex division number of 9 or more), respectively.

As is clear from the above discussion, the calculation accuracy is roughly determined by the relative virtual vertex distance of the two triple junctions, which is the division number, rather than the absolute value of the virtual vertex distance. However, as described in Section 2.5, when the optimization of the virtual vertex distance and time interval are comprehensively considered, the absolute value of the virtual vertex distance becomes important, rather than the relative value of the virtual vertex distance. For these reasons, both the division number and the absolute value of the virtual vertices need to be taken into consideration.

2.4. Optimization of the Time Interval in the Local Curvature Multi-vertex Model

The impact of the time interval in the local curvature multi-vertex model on the accuracy of the calculation time was studied. The time evolution of the vertex \( p_i \) on the grain boundary can be calculated by the following Eqs. (8) and (9),

\[
\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \Delta \vec{v}_i(t) \quad \text{(8)}
\]

\[
\Delta \vec{v}_i(t) = \vec{v}_i(t)\Delta t \quad \text{(9)}
\]

where \( t \) is the time; \( \Delta t \) is the time interval; \( \vec{r}_i(t) \) is the position vector of the vertex \( p_i \) on the grain boundary at time \( t \); \( \Delta \vec{v}_i(t) \) is the change in the position vector of the vertex \( p_i \) on the grain boundary at time \( t \); and \( \vec{v}_i(t) \) is the speed of the vertex \( p_i \) on the grain boundary at time \( t \). As \( \vec{v}_i(t) \) is subjected to Eq. (1) for the double junction and Eq. (3) for the triple junction, we compared the double junction to the conventional curvature model and the triple junction to the conventional vertex model in this study. In order to simplify the study, the time obtained by multiplying time \( t \) by \( M_{p_1p_2}G_{ij} / \mu_1 \) or \( M_{p_2p_3}G_{ij} / \mu_2 \) was regarded as the time in consideration of grain boundary characteristics for the curvature model or the vertex model.

2.4.1. Optimization of the Time Interval in the Curvature Model

First, we evaluated the time evolution of an isolated circular grain and studied the calculation time accuracy of the curvature model. Assuming that the initial grain radius was 10, the time evolution of the grain radius was calculated using Eqs. (1), (2), (5), (8) and (9), which are related to the curvature model. Figure 7 shows the calculation results and analysis solution of the curvature model. While the grains were annihilated at time \( t = 50 \) in the analysis solution, the simulation made the errors different depending on the time interval \( \Delta t \). Figure 8 shows the errors against the grain annihilation time \( t = 50 \) obtained from the analysis solu-

![Fig. 6. Calculation error against initial virtual vertex condition. (a) Errors of position and speed are presented as a function of the division number of the circle and division number of the circular arc. (b) The errors are presented as a function of the division number of a circle and the initial distance between adjacent vertices.](image)
2.4.2. Optimization of the Time Interval in the Vertex Model

The time evolution of the triple junction in Fig. 9(a) was evaluated, and the calculation time accuracy of the vertex model was studied with the assumption that the characteristics of all three grain boundaries were equal. In this case, all crossing angles of the triple junction are 120 degrees in the final state, which is in equilibrium (Fig. 9(b)). We assumed that all distances between the triple junction in equilibrium and its adjacent vertices were 10 and that the adjacent vertices were fixed. Then, the time evolution of the triple junction was calculated using Eqs. (3), (4), (8) and (9), which are related to the vertex model. Figure 10 shows the calculation results. As it is difficult to obtain the analysis solution of the time evolution of the triple junction shown in Fig. 9(a), the calculations were performed until the time interval $\Delta t = 0.001$. Then, after approximate convergence of the time evolution was confirmed, we started consideration based on this time evolution. It was found that the error differed depending on the time interval $\Delta t$ in the simulation, as is the case in the curvature model. As it is considered that infinite time can be required to reach the equilibrium state, the valuation was performed employing the time required for the triple junction to migrate to the position where the distance from the equilibrium state is 0.05, which is 1% of the distance of 5 between the initial state and equilibrium state. Figure 11 shows the errors of the migration time based on the time interval $\Delta t = 0.001$. As is the case of the curvature model, it can be concluded that the calculation time accuracy of 1% or less is possible if the time interval $\Delta t$ is approximately 0.2 or less.

From the above examination, it was confirmed that in case that the initial grain radius was assumed to be on the order of 10 $\mu$m, when grain growth simulation was performed using the proposed model, it was possible to obtain a calculation time accuracy on the order of 1% with the enough computation rate secured by setting the time interval to approximately 0.2 or less.

2.5. Comprehensive Optimization of the Adjacent Vertex Distance and Time Interval in the Local Curvature Multi-vertex Model

In this section, the optimization of both the distance discussed in Sections 2.3 and the time interval discussed in Sections 2.4 is comprehensively studied.

2.5.1. Topological Transformations in Grain Growth and Transformation Conditions

Topological transformations are required in the processes of the discrete time evolution in grain growth. Following the study by Weygand et al., who have already established the topological transformations in the vertex model, we employ the topological transformations in the proposed model.

Fig. 7. Time evolution of isolated circle.

Fig. 8. Calculated error in time evolution of grain growth with an isolated circle shape.

Fig. 9. Time evolution of triple junction. Solid circles are triple junctions. Open circles are fixed. (a) Initial stage. (b) Final stage.

Fig. 10. Time evolution of triple junction calculated by vertex model.

Fig. 11. Calculation error in time evolution of triple junction.
Figure 12(a) shows the switching of two triple junctions, and Figs. 12(b) and 12(c) show the annihilations of grains. In order to reproduce the continuous actual phenomena by discrete simulations, it is necessary to set the critical grain boundary lengths used in the topological transformations of triple junction switching and grain annihilations. In the following subsections, we discuss the relationships between the critical grain boundary lengths and time interval, which are required for performing the stable simulations. We also discuss the relationship between the virtual vertex distances and time interval.

2.5.2 Study on the Restrictions of the Triple Junctions in the Vertex Model

Using Eqs. (3), (4), (8) and (9), we examine the switching conditions of the triple junctions, the annihilation conditions of the grains and the conditions to prevent the triple junctions from overrunning the equilibrium positions.

2.5.2.1 Switching Conditions of the Triple Junctions

We consider the migration of two triple junctions in a nonequilibrium state in Fig. 12(a). The critical grain boundary length \( L_{cr,sw} \) of triple junction switching must satisfy Eq. (10) in Table 1, where \( M_{tp,\text{max}} \) is the maximum triple junction mobility and \( \gamma_{\text{max}} \) is the maximum grain boundary energy per unit length. It can be said that Eq. (10) is the most stringent condition in which only the energy of the grain boundary between the subject triple junctions is taken into account and the other grain boundary energies are set to 0. Further, as it is desirable that no virtual vertex exists on the grain boundary between two triple junctions when switching, Eq. (11) in Table 1 can be obtained.

2.5.2.2 Annihilation Conditions of the Grains

When a grain annihilates, the grain shrinks into a final form of a triangle and vanishes in many cases (Fig. 12(b)). As the grain annihilation conditions, we assume that all three grain boundary lengths are the critical grain boundary length or less.

We consider the case where the form of the grain immediately before vanishing is an equilateral triangle. Because it is necessary to prevent each triple junction of the grain from migrating over the center of the circumscribed circle of the equilateral triangle, the critical grain boundary length \( L_{cr,an} \) for grain annihilation must satisfy Eq. (12) in Table 1. As with Eq. (10), it can be said that Eq. (12) provides the most stringent condition that only the energies of the grain boundaries surrounding the subject grain are considered and the other grain boundary energies are set to 0. Moreover, as is the case with triple junction switching, it is desirable that no virtual vertex exists on the grain boundary between two triple junctions when the grain is annihilated. Accordingly, Eq. (13) in Table 1 is obtained. If the subject grain is not in the shape of an equilateral triangle, Eqs. (12) and (13) meet the annihilation conditions for such grains.

If one side of the triangle grain is shorter than the critical grain boundary length \( L_{cr,sw} \) of triple junction switching, triple junction switching is performed to convert the grain

![Fig. 12. Topological transformations. (a) Switching of triple junctions. (b) Annihilation of triangle grain. (c) Annihilation of a grain with two triple junctions.](image-url)

| Constraint items | Condition of vertex model | Condition of curvature model | Parameters |
|------------------|---------------------------|----------------------------|-----------|
| Triple junction switching | \( 2M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{cr,sw} \) (10) | | \( \Delta t, L_{cr,sw}, L_{\text{max}} \) |
| | \( L_{cr,sw} < L_{\text{max}} \) (11) | | |
| Annihilation of grain with three triple junctions | \( 3M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{cr,an} \) (12) | \( \sqrt{2} \sqrt{M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{cr,an}} \) (17) | \( \Delta t, L_{cr,an}, L_{\text{max}} \) |
| | \( L_{cr,an} < L_{\text{max}} \) (13) | \( L_{cr,an} < L_{\text{max}} \) (18) | |
| Annihilation of grain with two triple junctions | \( 2M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{cr,an2} \) (14) | | \( \Delta t, L_{cr,an2}, L_{\text{max}} \) |
| | \( L_{cr,an2} < L_{\text{max}} \) (15) | | |
| Prevention of virtual vertex overrun from equilibrium position | \( 2M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{\text{min}} \) (16) | \( 2M_{tp,\text{max}}\gamma_{\text{max}}\Delta t < L_{\text{min}} \) (19) | \( \Delta t, L_{\text{min}} \) |
| Generation and annihilation of double junction | \( L_{\text{min}} < L < L_{\text{max}} \) | \( 2L_{\text{min}} < L_{\text{max}} \) | \( L, L_{\text{min}}, L_{\text{max}} \) |

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into a grain with two triple junctions in Fig. 12(c). The grain boundary is depicted by curved lines for convenience sake. In this case as well, the grain is annihilated by the topological transformation in Fig. 12(c). The critical grain boundary length \( L_{cr,ant} \) of grain annihilation must satisfy Eq. (14) in Table 1. As it is desirable that no virtual vertex exists on the grain boundary between two triple junctions when the grain is annihilated, Eq. (15) in Table 1 is obtained.

### 2.5.2.3. Conditions for Preventing the Triple Junctions from Overrunning the Equilibrium Positions

In order to calculate the triple junction migration in a stable manner, it is desirable to prevent the triple junctions from overrunning the equilibrium positions. Even if an overrun takes place, the distance between the post-overrun position and equilibrium position of the triple junction must be prevented from being longer than the distance between the ante-overrun position and equilibrium position.

The triple junction migration from a nonequilibrium position to the equilibrium position when the energies of the three grain boundaries are equal, as shown in Fig. 13(a), is considered. The driving force \( F_{\gamma,i} \) that acts on the triple junction at the nonequilibrium position can be approximated as \( F_{\gamma,i} \approx (3\Delta L_1/2L)\gamma_i \), where \( L \) is the distance between adjacent vertices; \( \Delta L_1 \) is the distance between the nonequilibrium position and the equilibrium position; and \( \gamma_i \) is the grain boundary energy. The more stringent condition of the overrun prevention is \( M_{\gamma,i}(3\Delta L_1/2L)\gamma_i \Delta t \leq \Delta L_1 \). We also consider the triple junction migration from a nonequilibrium position to the equilibrium position when the energy of one grain boundary is 0 and the energies of the other two grain boundaries are equal but not 0 as shown in Fig. 13(b). The driving force \( F_{\gamma,i} \) that acts on the triple junction at the nonequilibrium position can be approximated as \( F_{\gamma,i} \approx (2\Delta L_2/L)\gamma_i \), where \( \Delta L_2 \) is the distance between the nonequilibrium and the equilibrium positions. The more stringent condition of the overrun prevention is \( M_{\gamma,i}(2\Delta L_2/L)\gamma_i \Delta t \leq \Delta L_2 \). From the above discussion, Eq. (16) in Table 1 is obtained from the latter condition which is more stringent.

### 2.5.3. Study of the Restrictions in the Curvature Model

Using Eqs. (1), (2), (5), (8) and (9), we examine both the annihilation condition of an isolated grain and the conditions for preventing the virtual vertices from overrunning the equilibrium position.

#### 2.5.3.1. Annihilation Conditions of an Isolated Grain

An isolated grain in the proposed model consists of only virtual vertices. We study the relationship between the critical grain boundary length and time interval for the annihilation of an isolated grain that consists of three virtual vertices. Again in this case, as one of the grain annihilation conditions, all three grain boundaries are assumed to have critical grain boundary lengths or less. However, it is assumed that the annihilations of virtual vertices do not occur in isolated grains with three virtual vertices or less.

In order to ensure the annihilation of an isolated grain, it is desirable to prevent the virtual vertices from overrunning the center of the circumscribed circle. Even if such an overrun takes place, the radius of the circumscribed circle of the post-overrun triangle grain must be shorter than that of the ante-overrun triangle grain. The latter condition is employed because there is no problem of grain boundary intersects in the case of isolated grains. The radius \( R_{cr,iso} \) of the critical circumscribed circle of grain annihilation must satisfy \( M_{\gamma}((\gamma/R_{cr,iso})\Delta t < 2R_{cr,iso}, i.e., \sqrt{2M_{\gamma,\delta}/\Delta t/2} \leq R_{cr,iso} \). 3\sqrt{R_{cr,iso}} = L_{cr,iso} \) holds when the grain is an equilateral triangle, and \( 2R_{cr,iso} = L_{cr,iso} \) holds when one side of the triangle is much longer than the others, where \( L_{cr,iso} \) is the critical grain boundary length of isolated grain annihilation. With the latter condition, which is more stringent, the critical grain boundary length \( L_{cr,iso} \) of the isolated grain annihilation and the calculation time interval \( \Delta t \) must satisfy Eq. (17) in Table 1. Moreover, because it is desirable that the triangle is composed of three virtual vertices when the grain vanishes, Eq. (18) in Table 1 can be derived.

#### 2.5.3.2. Conditions for Preventing the Virtual Vertices from Overrunning the Equilibrium Positions

In order to calculate the virtual vertex migration in a stable manner, it is desirable to prevent the virtual vertex from overrunning the equilibrium position. We consider the migration of the virtual vertex in Fig. 14. Both of the two vertices adjacent to the virtual vertex are fixed. To prevent the virtual vertex from overrunning the equilibrium position, \( M_{\gamma,\delta}(\gamma/R)\Delta t \leq \delta \) must be satisfied. From Fig. 14, we obtain the relational expressions \( \delta = R - Rcos(\theta/2) \) and \( L = 2Rsin(\theta/4) \). As the condition for stable calculation, the minimum length \( L_{min} \) of the adjacent vertex distance and calculation time interval \( \Delta t \) must satisfy Eq. (19) in Table 1.

The results of the comprehensive study on the optimization of adjacent vertex distance and time interval in the local curvature multi-vertex model as explained above are summarized in Table 1. These are the restrictions on the time interval, adjacent vertex distance, critical grain boundary...
ary length of triple junction switching and the critical grain boundary length of grain annihilation that are required to perform the simulation in a stable manner.

3. Verification of the Proposed Model for Grain Growth Time Evolution

The newly developed local curvature multi-vertex model was used for grain growth simulations. The simulation parameters were set to satisfy the restrictions discussed in the above sections. Specifically, the parameters were set targeting a position calculation accuracy of about 1% and a speed calculation accuracy of about 2% in the case of the average grain diameter of 10. Thus, the parameters were set as follows:

\[ M_\gamma \Delta = 0.2, \quad L_{\min} = 0.7, \quad L_{\max} = 1.5, \]

\[ L_{\gamma,sw} = L_{\gamma,am} = L_{\gamma,av2} = 0.7 \]

This parameter set satisfies all of the conditions shown in Table 1. The grain structure used in the simulation for validating the model was artificially prepared. The size of the specimen was 210 μm × 216 μm, in which 5,040 grains made up of rough squares of approximately 3 μm × 3 μm were two-dimensionally arranged. More precisely, the position of each corner of a quadrangle was randomly displaced from the position of each corner of a square on a minute scale. The grain orientation is randomly decided. In this study, the energies and mobilities of the grain boundaries were assumed to be constant independent of the difference in grain misorientation. The grain boundary mobility was applied for the mobility of the double junction. On the other hand, although the triple junction mobility, which is involved in three grains with different orientations, differs from grain boundary mobility, we assumed the value of triple junction mobility was the mean value of the mobilities of the three grain boundaries connected to the triple junction due to a lack of sufficient data on triple junction mobility. Because there was no grain misorientation dependency of mobility in this case, the value of triple junction mobility was set to the same as that of grain boundary mobility. Further consideration on triple junction mobility is necessary. The initial grain shape was set to a quadrangle because it was easier to create random, artificial data. In the first time step of the simulation, a quadruple junction needed to be divided into two triple junctions, which is the reason why the grain form was not set to not square. The quadruple junction was divided into triple junctions according to a rule equivalent to that of the topological transformation of triple junctions.10)

Figure 15 shows examples of both the initial structure after the division of the quadruple junction and the results of the grain growth simulations performed using the proposed model. Grain growth is calculated in a stable manner, and it is revealed that the average grain area, or the square of the average grain diameter, is nearly proportional to the time. This result simulates grain growth under the condition that the grains are unpinned. In fact, the simulations were performed using several types of initial structures that were artificially prepared by changing the displacement of each corner of the quadrangle in the specimen, and the similar results as those above were obtained. The slope of the average grain area against the time was 0.99 ± 0.02, which is regarded to have the intended accuracy. Accordingly, it is confirmed that the proposed model, which includes the generation and annihilation of virtual vertices, can be used for grain growth. We will report in the future on the application of this model for the growth of the observed recrystallized grains; the construction of a model that takes account of the grain misorientation dependency of energy and mobility of grain boundary; and the application of the model to the

![Fig. 15.](image-url) Grain growth simulation by the local curvature multi-vertex model showing time evolutions of grains. The initial number of grains is 5,040. The average grain areas are (a) 9.0 (initial), (b) 50.6 and (c) 324.0. (d) Time evolution of average grain area.
secondary recrystallization process.

Furthermore, grain growth in three dimensions exhibits differences in appearance from that in two dimensions, which demands three-dimensional models in order to increase the accuracy. Three-dimensional models can be far more complicated than two-dimensional models. However, by expressing a plane in triangle meshes and calculating the curvature in two orthogonal directions at each vertex of the meshes, the migration of each vertex on meshes, that is a plane, can be calculated.

4. Conclusions

We developed a two-dimensional local curvature multi-vertex model. It is a two-dimensional topological network model to straightforwardly express grain growth based on the physical principles that take account of the grain boundary curvature and the grain boundary tension at the triple junction. In the proposed model, the driving force of the grain boundary is calculated from the local curvature of the grain boundary by arranging several virtual vertices along the grain boundary, and the driving force of the triple junction is calculated from the tensions of the grain boundaries which connect to the triple junction. This allows the proposed model to predict grain growth more accurately than the conventional curvature models and vertex models. In addition, the virtual vertices can be appropriately arranged by being generated and annihilated in the course of grain growth. Further, we have confirmed that it is possible to secure the calculation accuracies of positions and speeds by optimizing the virtual vertex distance according to the average grain diameter. By optimizing the time interval according to the average grain diameter, the accuracy of the calculation time is secured along with securing the computation rate. While grain topology transformation becomes necessary in the course of grain growth, the calculation is performed in a stable manner by appropriately setting the critical grain boundary length of triple junction switching and grain annihilation, adjacent vertex distance and time interval. Based on the results of this study, we have presented a simulation parameter set such that a position calculation accuracy of approximately 1% and speed calculation accuracy of approximately 2% are expected.

A simulation of the grain growth with 5 040 grains, which were artificially prepared, was performed by the proposed model using these optimized parameters. It was confirmed that the grain growth calculation was stable and the average grain area during the grain growth was nearly proportional to the time. We also confirmed that the proposed model, which performs the generation and annihilation of virtual vertices, applies to grain growth.

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Appendix

The units of the proposed two-dimensional local curvature multi-vertex model are considered. Table 2 shows the definitions and units of each character in Eqs. (1)–(4). The driving force acting on the grain boundary in Eq. (2) is defined by the force acting on the grain boundary per unit length. The driving force acting on the triple junction in Eq. (4) is defined by force. Because the units for the migration velocities are same, the units of grain boundary mobility and triple junction mobility in Eqs. (1) and (3) are different.

| Table 2. Definitions and units of physical properties related to triple junction and grain boundary in the two-dimensional model. |
| --- |
| **Triple junction of grain boundary (point)** | **Grain boundary (line)** |
| Symbol [Unit] | Definition | Symbol [Unit] | Definition |
| $\gamma$ [J/m] | Grain boundary energy per unit length. | $\gamma$ [J/m] | Grain boundary energy per unit length. |
| $F_{tr,j}$ [N/m] | Driving force acting on triple junction. | $F_{gr,b}$ [N/m] = [J/m] | Driving force per unit length, acting on grain boundary. |
| $M_{tr,j}$ [(m/s)/N] | Mobility of triple junction. Speed of triple junction applying the driving force of 1N on it. | $M_{gr,b}$ [(m/s)/(N/m)] | Mobility of grain boundary. Speed of grain boundary applying the driving force of 1N on the grain boundary of unit length. |
| $v_{tr,j}$ [m/s] | Velocity of triple junction. | $v_{gr,b}$ [m/s] | Velocity of grain boundary. |