Phase-field Simulations of Grain Growth in Two-dimensional Systems Containing Finely Dispersed Coarsening Particles

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In this study, we have performed phase-field simulations of grain growth in two-dimensional systems containing finely dispersed coarsening particles. In particular, the effects of the Ostwald ripening of particles on the grain growth kinetics and the morphology of the matrix grains have been investigated. After reaching a steady state, not only does the growth of the particles obey power-law kinetics, but also the growth of the matrix grains, with an exponent of 3. In the case of systems having a small fraction of immobile particles, the grain size distributions (GSDs) of the matrix grains become broader with a small fraction of particles. For systems containing particles that coarsen with simulation time, the GSDs become narrower with an increase in the area fraction of the particles, \( fp(0) \). We have applied both active parameter tracking (APT) algorithms and parallel coding techniques to the multi-phase-field (MPF) model to accelerate the computations and to embody large-scale calculations.

KEY WORDS: computer simulation; phase-field modeling; Zener pinning; grain growth; Ostwald ripening.

1. Introduction

The grain size of polycrystalline materials is the key microstructural length scale indicating their mechanical properties. A classical method used by metallurgists to control the texture and length scale of such microstructures is the addition of solute elements with low solubility, which results in the precipitation of second-phase particles to pin the grain boundaries.

Over sixty years ago, Smith and Zener proposed an equation for grain growth in a system containing a random dispersion of rigid and immobile particles with radius \( r \).17 The maximum attainable mean grain size \( \langle R(st) \rangle \) can be expressed as:

\[
\langle R(st) \rangle = a \frac{r}{f_p b} \quad \text{............... (1)}
\]

where \( f_p \) is the volume fraction of the particles and \( a \) and \( b \) are constants. Under the Smith-Zener assumptions, \( a = 4/3 \) and \( b = 1.21 \) A number of subsequent researchers have proposed modifications to this approach.

Experimental data on Zener pinning is too limited to ascertain the difficulty of different assumptions.12 Therefore, the pinning effect of second-phase particles is frequently studied by means of computer simulations based on Monte Carlo Potts (MC),13-18 front-tracking (or vertex),19,20 phase-field (PF),21-24 and finite element (FE) models.25 The main advantage of these techniques is that the entire microstructure — namely, the shape and position of the grain boundaries — is calculated as a function of time. Furthermore, as compared to experimental studies, the materials and process parameter can be varied relatively easily and independently in computer simulations. A serious drawback of these techniques is that the simulations for grain growth require massive computer resources, particularly in the case of three-dimensional (3D) simulations. For two-dimensional (2D)13,15,16,18,19,21,23 systems, the simulations show that most particles are in contact with a grain boundary and the final mean grain radius at the pinned structure \( \langle R(st) \rangle \) obeys a relationship having the form of Eq. (1) with \( b = 0.5 \). In 3D systems,14,17,24,25 it is clear that the fraction of particles in contact with a grain boundary is lower than that in 2D systems, however, no agreement on the parameter values in Eq. (1) has been obtained.

As mentioned above, a number of simulations with finely dispersed “immobile” particles have been performed. However, there are many situations in which the particles are unstable. In particular, an important situation is that in which the grain growth has stagnated due to particle dispersion, but coarsening of particles controlled by the Ostwald ripening mechanism occurs.12 Systematic investigations of systems containing coarsening particles are feasible, provided that the volume (area) fraction of the particles is relatively high \( (i.e. f_p > 0.1) \).21,26,27 However, in such dual-phase structures, the mean size as well as the volume fraction of the matrix grains and second-phase particles becomes compatible with an increase in the value of \( f_p \). Furthermore, these particles in the dual-phase structures are more effective in retarding grain growth compared to the effect predicted by Zener’s relationship.21,28 Therefore, dual-phase structures should be classified into a different class from the system containing finely dispersed particles.

In cases where the value of \( f_p \) is small, almost no system-
atic investigation has been performed, even using 2D systems. Although simulation results obtained from the MC model have been reported,\(^{29}\) we have to simultaneously involve both the site reorientation and exchange events in this model in order to handle both grain growth and the Ostwald ripening phenomenon. It is fairly difficult to set an appropriate frequency between reorientation and exchange when considering the physical boundary mobility and diffusivity of the solute. Meanwhile, in PF models, simultaneously describing the grain growth and Ostwald ripening by combining the kinetic equations for the orientation field variables, which describe the evolution of grain boundaries, is straightforward with the diffusion equation for the concentration field.\(^{21,30}\) However, it is well known that the particle growth speed becomes drastically slower with a decrease in the value of \(f_p\).\(^{31}\) Moreover, the system size needed to obtain statistically meaningful results becomes larger with a decrease in the value of \(f_p\) due to the smaller pinning pressure of the particles.

The purpose of this study is to investigate grain growth in systems containing finely dispersed coarsening particles, where we mainly consider systems with \(f_p < 0.1\). In particular, the effects of the Ostwald ripening of particles on the grain growth kinetics and the morphology of the matrix grains are investigated. Numerical simulations are performed in 2D systems by using the multiphase-field (MPF) model proposed by Steinbach et al.\(^{32}\) We apply both active parameter tracking (APT) algorithms\(^{33–36}\) as well as parallel coding techniques, to the MPF model to accelerate computations and to embody large-scale calculations such as those having 2,048\(^2\) grid points.

### 2. Method

#### 2.1. PF Model

In order to represent the temporal evolution of polycrystalline material with finely dispersed secondphase particles, we utilize the MPF model proposed by Steinbach, et al.\(^{32}\)

In this paper, a set of continuous field variables \(\phi_i(r,t), \phi_2(r, t), \ldots, \phi_N(r, t)\) is defined to distinguish the type of constituents (matrix grains and particles) and their orientations, where \(\phi_i(r, t)\) represents the existence ratio of each constituent at a position \(r\) and time \(t\). In order to avoid coalescence between constituents having the same field number \(i\), we apply a different number to each different constituent (i.e., \(N\) is assumed to be the total number of constituents). Here, we outline the equations from the MPF model, which are essential for this study. The model details are described in Refs. 32, 36, 37:

The sum of each PF at any position in the system is conserved.

\[
\sum_{i=1}^{N} \phi_i(r, t) = 1 \quad (2)
\]

The free-energy functional of a system of volume \(V\) is given by:

\[
F = \int V \left[ f^T + f^P + \lambda_e \left( \sum_{i=1}^{N} \phi_i - 1 \right) \right] dV \quad (3)
\]

where \(\lambda_e\) is the Lagrange multiplier accounting for the constraint in Eq. (2), and \(f^P\) can be defined as

\[
f^P = \sum_{j=1}^{N} \sum_{i=1}^{N} \left[ -\frac{\varepsilon_{ij}^2}{2} \nabla \phi_i \cdot \nabla \phi_j + \omega_{ij} \phi_i \phi_j \right] \quad (4)
\]

as in Steinbach and Pezzolla,\(^{32}\) where \(\varepsilon_{ij}\) is the gradient energy coefficient and \(\omega_{ij}\) is the height of the double-well potential. The double obstacle potential \(\phi_i \phi_j\) is defined in the boundary region only where \(0 < \phi_i < 1\) and \(0 < \phi_j < 1\). For the thermodynamic potential \(f^T\), we assume a rule of mixture:

\[
f^T = \sum_{i=1}^{N} \phi_i f_i(c_i) \quad (5)
\]

where \(f_i(c)\) is the free-energy density of phase \(i\) with composition \(c_i\). Any point \(r\) in the system is assumed to be a mixture of \(N\) phases with the fraction of \(\phi_i\) for phase \(i\). However, the compositions of the phase coexisting at a given point are not independent of each other, but constrained by the following condition:\(^{38}\)

\[
f_i(t, r) = f_j(t, r) = \ldots = f_N(t, r) = f_0(t, r) ... \quad (6)
\]

where the subscripts \(c_i\) under the free-energy densities denote the derivatives with respect to \(c_i\). This condition enforces the coexisting phases to have an equal chemical potential, which is defined by the difference in the chemical potential between the solute and the solvent. With the imposed equal chemical potential condition (Eq. (6)), the extra chemical double-well potential at the boundary region can be removed, resulting in a relaxation of the boundary width limitation. The average composition of the mixture is also given by the mixture rule:

\[
c(r, t) = \sum_{i=1}^{N} \phi_i c_i \quad (7)
\]

With the restrictions of Eqs. (2), (6), and (7), the compositions \(c(i = 1, 2, \ldots, N)\) of each phase can be expressed as functions of \(c\) and \(\phi_i\).

Finally we get the PF equation:

\[
\frac{\partial \phi_i}{\partial t} = -\frac{2}{n} \sum_{j=1}^{N} s_{ij} M_{\phi} \left[ \frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j} \right] \quad (8)
\]

where:

\[
\frac{\partial F}{\partial \phi_i} = \sum_{j=1}^{N} \left[ \frac{\varepsilon_{ij}^2}{2} \nabla^2 \phi_j + \omega_{ij} \phi_j \right] + f_i(c_i) - c_i f_i \quad (9)
\]

with \(\omega_{ij} = \omega_{ji}\) and \(\varepsilon_{ij} = \varepsilon_{ji}\). Further, the number of phases coexisting at a given point \(n(r, t)\) can be expressed as:

\[
n(r, t) = \sum_{i=1}^{N} s_{i}(r, t) \quad (10)
\]

where \(s_i(r, t)\) is a step function that satisfies \(s_i(r, t) = 1\) if \(\phi_i > 0\), and \(s_i(r, t) = 0\) otherwise. It should be emphasized that Eq. (9) was derived under the condition of the chemical potential among the coexisting phases given by Eq. (6).

The diffusion equation where the mass should be conserved is expressed as:

\[
\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \frac{\partial F}{\partial c} \quad (11)
\]
where $M_r$ is the mobility of the diffusion field. If we put $M_r = D/f_{c\ell}$, where $D$ is the diffusivity dependent on the PFs, then the diffusivity in a bulk phase can be maintained as a constant and the diffusion Eq. (11) becomes:

$$\frac{\partial c}{\partial t} = \nabla \cdot D \sum_i \phi \nabla c_i \quad \text{................. (12)}$$

For the purpose of a numerical simulation, the set for PF Eq. (8) and diffusion Eq. (12) have to be numerically solved by discretizing them in space and time. The second-order central difference method and the simple explicit Euler equation are used for this discretization with respect to space and time, respectively.

In this paper, we utilize the APT algorithm for the temporal evolution of $\{\phi(r, t)\}$ ($i = 1, \ldots, N$) in order to perform simulations along with avoiding coalescence between the grains that have the same field number.33–36 For the purpose of further accelerating the calculation speed, we combine the APT algorithm with parallel coding techniques. The parallelization of the APT algorithm is fairly easy compared to that of the dynamic grain-orientation reassignment (DGR) algorithm.39,40 The only requirement is that the data arrays located along the surfaces of each adjacent message-passing interface (MPI) domain have to communicate with each other at every time step.

2.2. Model Parameters and Simulation Procedure

All the calculations are performed on a 2D lattice with periodic boundary conditions. For simplicity, we assume that we have only one type of orientation for both the matrix grains (M$k = 1$) and particles (P$k = 2$). If two constituents have the same value of $k$, they belong to the same class of constituents (M or P), and all the constituents ($i = 1, \ldots, N$) belong to one of each constituent class ($k = 1, 2$). (Hereafter, we use the word “phase” instead of “constituent class” for simplicity.) The target materials are not specified in this paper. However, in order to express the simulation results in actual units, we use the word “phase” instead of “constituent class” for simplicity.

In order to simplify the calculation of the compositions $c(i = 1, 2, \ldots, N)$ with the restrictions of Eq. (6), the chemical free-energy density of each phase is approximated as parabolic functions:41

$$f^k = K_k (c_i - \sigma_k^0)^2 \quad (k = 1, 2; i = 1, 2, \ldots, N) \quad \text{............. (13)}$$

where the coefficients $K_k$, which determines the stability of each phase, is set to $K_1 = 5.0 \times 10^3$ ($k = 1, 2$)[J/mol], and the equilibrium concentration of each phase is $\sigma_k^0 = 0.1$ and $\sigma_k^0 = 0.9$, respectively. We consider the isotropic boundary energy condition as $\sigma_{kl} = \sigma = 1.0$[J/m$^2$], where $\sigma_{kl}$ is the boundary energy between phases $k$ and $l$. The molar volume is set to $7.0 \times 10^{-7}$[m$^3$/mol]. The lattice step size $\Delta t$ is set to $1.0 \times 10^{-7}$[m], and the boundary width is assumed to be $7.0 \times \Delta t$. From the definition of $D$, the mobility of the diffusion field in the phase $k$, $M_{r,k}$, is calculated as $M_{r,k} = D/\kappa_{k}$, where the value of $M_{r,k}$ as well as $D$ are maintained as constants in the simulation run. This means that we perform the simulation with the ratio of the mobilities, $M_{r,k}/M_{r,\alpha} \Delta t$, between 0 to $8.75 \times 10^{-5}$.

Hereafter, the length and area are expressed in [m] and [m$^2$], respectively; further, we do not express the unit of the diffusivity explicitly for simplicity. Then the parameters $\varepsilon_{kl}$ and $\omega_{kl}$ are calculated as $\varepsilon_{kl} = 4\pi(3.5\Delta x\sigma_{kl})^{0.5}$ and $\omega_{kl} = 2\sigma_{kl}(3.5\Delta x)^{3.5}$.

3. Results and Discussion

3.1. Verification of Simulation Model

In this section, we utilize immobile and insoluble particles in order to investigate the effects of the size of dispersed particles on the microstructure in the steady state; in the system containing immobile particles, the phrase “steady state” means the structure in which all the boundaries are pinned by the particles and no further evolution is observed. Thus, $D$ is set to zero throughout this section. According to the Zener relationship in Eq. (1), the grain size in the steady state is proportional to the particle size for a given area fraction. Consequently, it is better not to assume an excessively large value for the particle size so that the system size is restricted. On the other hand, the particles should have a minimum size that depends on the grain boundary thickness to obtain realistic grain boundary-particle interactions. Furthermore, the stability of the particles against the Gibbs-Thomson effect should be taken into account in the case when we utilize mobile and soluble particles. Therefore, particles with a radius in the range of $3.5 \times 10^{-7} \sim 6.5 \times 10^{-7}$ have been considered. The initial configurations have been constructed as follows: first, a polycrystalline microstructure was created by simulating the normal grain growth mechanism in which one group of orientation was assigned for the entire system. Next, particles with a uniform radius of $r(\theta) = r(0)$ were superimposed on the matrix grains so that they were located at a pre-set minimum distance $\ell_{lim}$. In this section, the area fraction of the particles, $f_p$ was maintained constant at $f_p(0) = 0.02$. Due to the zero value of $D$, the mean particle radius $r(\theta)$ and the area fraction $f_p(\theta)$ are maintained as constants as $\sigma(t) = r(0)$ and $f_p(\theta) = f_p(0)$ in the simulation run.

The temporal evolutions of the microstructure on the condition of $\sigma(t) = 3.5 \times 10^{-7}(a, b, c)$ and $r(0) = 6.5 \times 10^{-7}(d, e, f)$ are shown in Fig. 1. In order to save page space, only the upper left portions of the entire system are included. Both in the upper (a, b, and c) and the lower (d, e, and f) columns, the simulated microstructures reach their steady state in the right row; no further evolution of the microstructures was observed. The ratio of the mean radius of the matrix grains ($\sigma(t)$) to the value of $\sigma(t)$, ($\sigma(t)/\sigma(t)$), are plotted for various values of $r(0)$ in Fig. 2. According to the Zener-type relationship, namely, $\sigma_r(r)/\sigma(r) = a/r^b$, the value of $\sigma_r(r)/\sigma(t)$ should maintain the same value regardless of $r(0)$, where $a$ and $b$ are constants and $\sigma_r(t)$ and $\sigma(t)$ are the values of $\sigma(r)$ and $\sigma(t)$ in the steady state. However, the simulation results show that this ratio...
The ratio of the mean radius of the matrix grains \( \langle R \rangle(0) \) to the value of \( \langle r \rangle \), \( \langle R(\text{st})/r(\text{st}) \rangle \), are plotted for various values of \( \langle r \rangle \). According to the Zener-type relationship, i.e., \( \langle R(\text{st})/r(\text{st}) \rangle = a/b \), the value of \( \langle R(\text{st})/r(\text{st}) \rangle \) should maintain the same value regardless of \( \langle r \rangle \), where \( a \) and \( b \) are constants, and \( \langle R(\text{st}) \rangle \) and \( \langle r(\text{st}) \rangle \) are the values of \( \langle R(t) \rangle \) and \( \langle r(t) \rangle \) in the steady state. However, the simulation results show that the ratio has a different value depending on the value of \( \langle r \rangle \), although the ratio seems to approach a fixed value as \( \langle r \rangle \) increases.

In order to comprehend this phenomenon, the locations of the particles in the steady state for various values of \( \langle r \rangle \) are plotted in Fig. 3. In the simulation, the fractions \( \Phi_4(\text{st}) \) of the particles in the matrix grain, as well as the fractions on the boundary between the two grains \( \Phi_3(\text{st}) \) at a triple junction among three grains \( \Phi_3(\text{st}) \), and at a junction among more than four grains \( \Phi_4(\text{st}) \), were determined.

of \( \langle r \rangle \) as follows.

It is well known that in a single polycrystalline structure without particle and textures (i.e., boundary properties are equivalent throughout the system), a quadruple junction is unstable and will become dissociated into two stable triple junctions. However, if the particle plays a combining role and the boundary segments on the joint do not interact with each other, the quadruple junction can be stabilized. In PF models, due to their finite boundary width, boundary segments on the particles can easily interact with each other provided that the size of the particles is not greater than the width of the boundaries; this sometimes leads to the unpinning of boundaries. Therefore, the value of \( \Phi_4(\text{st}) \) is almost zero in the case of \( \langle r \rangle = 3.5 \times 10^{-7} \), although it has a finite value in the case of \( \langle r \rangle = 6.5 \times 10^{-7} \). In addition, in 2D systems, the boundary segment — which was captured between two particles — cannot spontaneously escape from...
the particles due to zero curvature of the segment. Therefore, the interaction between the boundaries on a particle plays an important role in the mechanism of the unpinning phenomenon. For example, let us consider the situation described in Fig. 4(a). Theoretically, in 2D systems, the value of $\theta$ should be zero to unpin the boundary segments. However, the boundary segments can interact with each other and unpin with a finite value of $\theta$, provided that the boundary width is comparable to the particle size. The possibility of this unpinning due to the interaction on the particle becomes smaller with an increasing value of $\langle r(0) \rangle$. Thus, the value of $\Phi_1(\theta)$ becomes smaller with an increasing value of $\langle r(0) \rangle$. (Similarly, this explanation can be used to describe the decrease in the value of $\Phi_2(\theta)$ with an increasing value of $\langle r(0) \rangle$, as described in Fig. 4(b)).

In 2D systems, the value of $\Phi_1$ at the initial stage, $\Phi_1(0)$, also influences the value of $\Phi_1(\theta)$. As expected, the value of $\Phi_1(0)$ decreased with an increasing value of $\langle r(0) \rangle$. When $\langle r(0) \rangle = 3.5 \times 10^{-7}$, the value of $\Phi_1(\theta)$ increased with the simulation time due to the unpinning described above. In contrast to the abovementioned phenomenon, $\Phi_1(\theta)$ was almost constant in the case of $\langle r(0) \rangle = 6.5 \times 10^{-7}$. Practically, the value of $\langle r(0) \rangle$ is quite large compared to the width of the boundaries. In the following sections, we set the value of $\langle r(0) \rangle$ as $5.5 \times 10^{-7}$ out of consideration for the computational costs as well as the realistic grain boundary-particle interactions.

### 3.2. Effects of Solute Diffusivity

In this section, let us consider the effects of the value of $D$ on the growing kinetics of the matrix grains and particles and also their steady states; in the system containing coarsening particles, the phrase “steady state” means the structure in which the ratio $\langle R(t) \rangle/\langle r(t) \rangle$ is maintained as a constant. We set the value of $D$ as $0, 1.0 \times 10^{-14}$, and $1.0 \times 10^{-13}$; the area fraction of the particles at the initial configuration $f_p(0)$ between 0.02 and 0.08 at an interval of 0.02 was considered. A single run of the simulation was performed for each different simulation condition. In the case of $D = 1.0 \times 10^{-13}$ and $f_p(0) = 0.02$, however, we performed two simulation runs with each different initial configuration. This is because in this case, the number of matrix grains and particles became too small in the steady-state condition to obtain statistical values such as grain size distributions.

Before performing the PF simulations, we estimate the decrease in the area fraction of the particles due to the Gibbs-Thomson effect in our simulation systems. From the definition of the chemical free-energy density of each phase (as described by Eq. (13)), we can easily calculate the concentration of the matrix at the surface of a circular particle with radius $r$, $C_m$, the concentration of the particle at the surface, $C_p$, as $C_m = \alpha_1 + \sigma V_m/2Kr(\alpha_2 - \alpha_1)$ and $C_p = \alpha_2 + \sigma V_m/2Kr(\alpha_2 - \alpha_1)$; here, we assumed the uniformity of the coefficient $K$ as $K_3 = K_2 = K$ and $\alpha_1$ and $\alpha_2$ are the equilibrium concentrations for a flat surface. If we consider a particle with a radius of $5.0 \times 10^{-7}$, the value of $C_m$ can be estimated as $C_m = 0.10175$, where the values of $\alpha_1$ and $\alpha_2$ are set to 0.1 and 0.9, respectively. Then, a decrease in the area fraction of the particle, $\Delta f_p$, is roughly estimated as $\Delta f_p \approx (C_m - \alpha_1)/f_p(0) (\alpha_2 - \alpha_1)$. Consequently, the value of $\Delta f_p$ exceeds 0.1 in the case of $f_p(0) = 0.02$, provided that the particles do not coarsen and the matrix grains have sufficiently larger radii.

#### 3.2.1. Microstructure

The microstructures at $t = 13500$[s] for $D = 1.0 \times 10^{-14}$ for various values of $f_p(0)$ are shown in Fig. 5. Similarly, the microstructures at $t = 13500$[s] for $D = 1.0 \times 10^{-13}$ for various values of $f_p(0)$ are shown in Fig. 6. As expected, the larger value of $\langle R(13500) \rangle$ is observed with an increase in
the value of $D$ if the value of $f_p(0)$ is equivalent. As far as the particles are concerned, the shape is far from the circular shape seen in all the microstructures. For $D = 1.0 \times 10^{-13}$, ripening of the particles is observed and all the particles are located on the boundary or at the junction (i.e., $\Phi_t(13\,500) = 0$) regardless of the value of $f_p(0)$.

3.2.2. Relationship between $\langle R(st) \rangle$ and $\langle r(st) \rangle$

The temporal evolutions of the value of $\langle R(t) \rangle$ and $\langle r(t) \rangle$ for various values of $D$ and $f_p(0)$ are shown in Fig. 7. The temporal evolutions of the ratio $\langle R(t) \rangle / \langle r(t) \rangle$ for various values of $D$ and $f_p(0)$ are also shown in Fig. 8. Furthermore, the temporal evolutions of the value of $f_p(t)$ normalized by $f_p(0)$ for various values of $D$ and $f_p(0)$ are shown in Fig. 9. Figure 8 shows that all the simulated microstructures reached their steady states within a simulation run. However, for simplicity in the visualization, we do not show the results for $D = 0$; the ratio obtained in these simulations reached a constant 1.0 during the simulation period. In the case of $D = 1.0 \times 10^{-13}$, the value of $f_p(t)$ decreases due to a larger value of $f_p(0)$ for various values of $D$ and $f_p(0)$. This leads to an increase in the ratio of $\langle R(t) \rangle / \langle r(t) \rangle$. With this increase in the ratio, the value of $f_p(t)$ decreases due to a larger Gibbs-Thomson effect. Consequently, it accelerates the increase in the ratio of $\langle R(t) \rangle / \langle r(t) \rangle$. After reaching the maximum value, the preferential growth of the particles located at energetically favorable sites (i.e., junctions) dominates which reduces the ratio of $\langle R(t) \rangle / \langle r(t) \rangle$. In the case of $D = 1.0 \times 10^{-14}$, the decreases in the value of $f_p(t)$ are large as compared to those in the case of $D = 1.0 \times 10^{-13}$. This is because there is no preferential growth of the particles located at energetically favorable sites. In order to perform the simulations of the ripening process of particles along with preventing a decrease in the value of $f_p(t)$, we have to utilize a larger $K_i$ value, which requires a much larger computational power.

The relationship between the ratio $\langle R(st) \rangle / \langle r(st) \rangle$ and the value of $f_p(st)$ for the various values of $D$ are shown in Fig. 10; for $D = 1.0 \times 10^{-13}$ and $D = 1.0 \times 10^{-14}$, the ratio $\langle R(13\,500) \rangle / \langle r(13\,500) \rangle$ decreases due to a larger value of $f_p(0)$ for various values of $D$ and $f_p(0)$. This leads to an increase in the ratio of $\langle R(t) \rangle / \langle r(t) \rangle$. After reaching the maximum value, the preferential growth of the particles located at energetically favorable sites (i.e., junctions) dominates which reduces the ratio of $\langle R(t) \rangle / \langle r(t) \rangle$. In the case of $D = 1.0 \times 10^{-14}$, the decreases in the value of $f_p(t)$ are large as compared to those in the case of $D = 1.0 \times 10^{-13}$. This is because there is no preferential growth of the particles located at energetically favorable sites. In order to perform the simulations of the ripening process of particles along with preventing a decrease in the value of $f_p(t)$, we have to utilize a larger $K_i$ value, which requires a much larger computational power.

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In this section, we evaluate the growth kinetics of matrix grains controlled by Ostwald ripening of the second-phase particles by focusing on the results obtained for $D = 1.0 \times 10^{-13}$. According to the LSW theory, during bulk-diffusion-controlled coarsening, the mean particle size should increase as a power law in time, $(r(t))^{m} - (r(0))^{m} = k_{\text{particle}}t$, with an exponent $m = 3$ and a particle size distribution function - which scaled by the mean particle size - is independent of time, where $k_{\text{particle}}$ is the growth constant of the particles. In Fig. 11, the temporal evolutions of $(R(t))^{3}$ and $(r(t))^{3}$ are plotted for various values of $f_p(0)$. This figure indicates that the value of $(R(t))^{3}$ as well as that of $(r(t))^{3}$ is proportional to the simulation time after reaching their steady states. Therefore, the growth kinetics of matrix grains is considered to be controlled by the Ostwald ripening of particles. Although the shape of the particles deviated considerably from a circle due to the existence of a boundary between the matrix grains, the growth kinetics follows a cubic law. The value of $(k_{\text{matrix}}/k_{\text{particle}})^{1/3}$ should be equal to the ratio $(R(t))/r(t)$, where $k_{\text{matrix}}$ is the growth constant of the matrix grains. However, the difference between the two values is found to be at most 4%. This is because we have included the region at which the growth kinetics has not truly reached the steady state to obtain the values of $k_{\text{matrix}}$ and $k_{\text{particle}}$, although $(R(13\,500))/r(13\,500)$ was used as the ratio of $(R(t))/r(t)$. As expected, $k_{\text{matrix}}$ increases with a decrease in the value of $f_p(0)$. Conversely, $k_{\text{particle}}$ increases with an increase in the value of $f_p(0)$.

The temporal evolutions of the fraction of three types of grain boundaries, namely the $\text{MM}$, $\text{MP}$, and $\text{PP}$ boundaries, are plotted in Fig. 12, where the value of $D$ and $f_p(0)$ are $D = 1.0 \times 10^{-13}$ and $f_p(0) = 0.08$. This figure indicates that the fraction of the $\text{MM}$ boundary decreases with the simulation time. This can be attributed to the fact that $\text{MM}$ and $\text{PP}$
boundaries can move faster than MP boundaries; the fraction of MM boundaries decreases rapidly with the growth of matrix grains at an early stage of the simulation. The fractions for all types of boundaries are almost constant value by the end of the simulation. In addition, this figure indicates that the fraction of PP boundaries is quite small compared to the other boundaries. This is because the fraction of particles $f_p$ is relatively small in this study. Therefore, the coarsening of the particles is mainly controlled by long-distance diffusion via the MP boundaries and the role of the PP boundaries is negligible. However, if the value of $f_p$ is comparable to the area fraction of the matrix grains, we have to take into account the effect of the PP boundary. In such a regime with a high $f_p$ value, further investigation is needed to validate whether the particles and the matrix grains still obey the cubic growth law or not. In some simulation studies, values for $m$ other than 3 have been reported.\(^{27}\) However, to perform a power-law approximation, determination of the value of $b_0$ is essential. Furthermore, when we inappropriately determine the $b_0$ value, the value of $m$ can deviate from the value of 3 even if we assume spatially homogeneous diffusivity and eliminate the possibility of growth kinetics controlled by boundary diffusion.

### 3.3.2. Morphological Evolution

Let us consider the morphological evolution of the matrix grains and particles. Initially, we refer to the results related to the grain size distribution (GSD). In order to compare our results with those obtained in previous simulations, the temporal evolution of the GSD in the case of $D = 0$ and $f_p(0) = 0.02$ is shown in Fig. 13, where GSDs are normalized by the mean grain radius, $\langle R(t) \rangle$. In this case, the number of grains existing at the end of the simulation ($t = 6000$ [s]) is 596. For comparative purposes, the steady-state distribution in a polycrystalline structure without precipitation is also plotted; in this single-phase structure, the phrase “steady state” means a structure in which the GSD becomes time-invariant. This figure indicates that the peak top shifts to the smaller side as compared to the GSD in the single-phase structure. This is because, in 2D systems, a boundary segment is easily pinned by two particles and becomes flat, and such segments cannot vanish even in the later stages of the simulation. Therefore, a grain composed of such segments can exist even if the grain is much smaller than a grain with the size of $\langle R(t) \rangle$. The shift in the peak top is also reported in Ref. 23).

However, in 3D systems, the situation is completely different. In this figure, the steady-state GSD in 3D systems with $f_p(0) = 0.04$ is also plotted; the GSD was produced from the results in Ref. 24). This GSD is obviously narrower than that in 2D systems. This phenomenon can be explained as follows: the driving force for grain growth can be approximated as the difference in the curvature between a specific grain and its surroundings.\(^{47}\) At the initial stage, all the grains that are larger than their surroundings can grow while the smaller ones can shrink, because the size of the grains is small enough to overcome the pinning force. At a later stage, significantly smaller grains can still shrink because of the large driving force; this differs from the situation in 2D systems. Further, some larger grains, which are adjacent to such significantly smaller grains, can grow. Consequently, there is no smaller grain that can shrink and this leads to the narrower GSD. At the end of the simulation, grains smaller than $0.3 \langle R(st) \rangle$ vanished completely. The simulation results based on the mean field theory revealed similar GSDs.\(^{48,49}\)

The temporal evolution of the GSDs and PSDs in the case of $D = 1.0 \times 10^{-13}$ are shown in Figs. 14 and 15, respectively. Figure 14 shows that the GSDs become narrower when compared with those obtained in the case of $D = 0$. In particular for $f_p(0) = 0.08$, the GSDs are narrower than the steady-state distribution in the single-phase structure. The reason is considered as follows: when the system reaches its steady state, the growth kinetics of the matrix grains are controlled by Ostwald ripening of the particles, as mentioned in Sec 3.3.1. In the case of $D = 0$, the grain composed of pinned segments cannot vanish throughout a simulation. However, in the case of $D = 1.0 \times 10^{-13}$, if the particles, which pin the segments, are located close to each other, almost all of them vanish due to Ostwald ripening and the small grains pinned by such particles also vanish. Thus, the...
dependent of the value of that the steady-state values of the ratio of the values of $R_{\text{st}}(0)$ to $R_{\text{st}}(t)$ respond to the case where grain growth follows homogeneously throughout the system. As a consequence, the preferential growth of particles located at energetically favorable sites occurs. Therefore, smaller grains do not always have larger curvatures. This leads to a broadening of the PSDs. Furthermore, the dragging of the particles by the MM boundaries may also affect the growth exponent of the particles and the PSD.\textsuperscript{51)}

\section{3.4. Effects of $(R(0))/(\langle r(0) \rangle)$ on Steady State}

In this section, the role of the mean radius of the matrix grain at the initial condition $\langle R(0) \rangle$ is considered. Grain nucleation and initial grain growth occurred first without the particles. In the case where the mean grain size is equivalent to the specified initial grain $(R(0))$, the particles were randomly distributed throughout the system. As a consequence, many particles lie within the grains. These simulations correspond to the case where grain growth follows homogeneous precipitation or recrystallization.\textsuperscript{52)} In the case of $D = 0$, the value of $\langle R(0) \rangle$ or the ratio of $\langle R(0) \rangle/(\langle r(0) \rangle)$ has a significant effect on the value of $(\langle R(st) \rangle)/(\langle r(st) \rangle)$, as pointed out by Moelans \textit{et al.}\textsuperscript{23)} We shall only consider a system with $D = 1.0 \times 10^{-13}$ and $f_p(0) = 0.08$ to emphasize the effects of the coarsening of particles. We set the values of $(\langle R(0) \rangle)$ as $7.4 \times 10^{-7}$, $1.6 \times 10^{-6}$, and $2.1 \times 10^{-6}$.

The temporal evolutions of the ratio $(R(t))/(\langle r(t) \rangle)$ for various values of $(R(0))$ are shown in Fig. 16. This figure shows that the steady-state values of the ratio $(\langle R(st) \rangle)/(\langle r(st) \rangle)$ are independent of the value of $(\langle R(0) \rangle)$.

\section{4. Concluding Remarks}

We investigated the grain growth in 2D systems containing finely dispersed coarsening particles. The numerical simulations were performed using an MPF model. In order to accelerate the computation, we applied both the APT algorithm and parallel coding techniques to the MPF model. The following results were obtained:

- If the size of the second-phase particles is not large enough in comparison to the width of the boundaries, the ratio $(\langle R(st) \rangle)/(\langle r(st) \rangle)$ is dependent on the value of $(\langle r(0) \rangle)$, even if the area fraction of the particles, $f_p(0)$ is maintained to be equivalent. This is because, in PF simulations, the possibility of unpinning due to the interaction of the boundaries on a particle reduces with an increasing value of $(\langle r(0) \rangle)$.

- In all the calculations, the ratio $(R(t))/(\langle r(t) \rangle)$ became almost constant at $(R(st))/(\langle r(st) \rangle)$ during the simulation period. For $D = 0$, the simulated results fitted the Zener type relation as $(R(st))/(\langle r(st) \rangle) = 1.03/f_p(st)$.\textsuperscript{51)} The value of 0.51 is in good agreement with those obtained in previous simulations. Although the relationships obtained for $D = 1.0 \times 10^{-14}$ and $D = 1.0 \times 10^{-13}$ deviated slightly from that in the case of $D = 0$, almost the same exponents were obtained.

- In the case of $D = 1.0 \times 10^{-13}$, after reaching a steady state, not only does particle growth obey the power-law kinetics, but so too does the growth of the matrix grains, with an exponent of 3. This fact indicates that in the steady state, the growth of the matrix grains is controlled by Ostwald ripening of the particles.

- For $D = 0$, the GSDs become broader in systems containing a small fraction of particles. On the other hand, for $D = 1.0 \times 10^{-13}$, the GSDs become narrower with an increase in the value of $f_p(0)$. This is because, if the particles, which pin the segments, are located close to each other, almost all of them vanish due to Ostwald ripening; furthermore, small grains pinned by such particles also vanish. Thus, the minimum distance between the particles is also controlled by the Ostwald ripening of particles.

- In the case of $D = 1.0 \times 10^{-13}$, the PSDs are broader than those in the system without the matrix grains. This is because the particles cannot maintain their circular shape due to the existence of boundaries between the matrix grains. In addition, the preferential growth of[right]
particles located at energetically favorable sites occurs. Therefore, a smaller grain does not always have a larger curvature and driving force for shrinkage.

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