Accuracy Evaluation of Phase-field Models for Grain Growth Simulation with Anisotropic Grain Boundary Properties

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The phase-field method has been widely employed recently for simulating grain growth. Phase-field grain growth models are classified into two types according to their conservation constraints for phase-field variables: the multi-phase-field model and the continuum-field model. In addition, within the multi-phase-field model framework, three models with different formulations exist. These models are reported to accurately simulate grain growth under conditions of isotropic or weakly anisotropic grain boundary energy and mobility. However, for cases of strongly anisotropic grain boundary properties, the accuracy of these models has not yet been examined in detail. In this study, using the continuum-field model and three different multi-phase-field models, systematic grain growth simulations with anisotropic grain boundary energies and mobilities are performed. Through the detailed investigation of the accuracy of the simulated results, the suitability of each model for anisotropic grain growth simulations is revealed. Furthermore, based on the higher-order terms, accuracy improvement of the phase-field models is attempted.

KEY WORDS: phase-field model; grain growth; microstructure; grain boundary energy; grain boundary mobility.

1. Introduction

The process of competitive grain growth under curvature-driven boundary migration is one of the most important microstructural evolution phenomena in the manufacturing of polycrystalline materials because it determines the final microstructures and resultant physical properties of materials.^{1–3)} However, the experimental study of grain growth is severely limited by the high temperatures at which it occurs and the optical opacity of polycrystalline samples. Therefore, to systematically examine grain growth phenomena, numerical approaches have been developed using continuum-based grain growth models,⁴⁾ including the Monte-Carlo,^{5–8)} cellular automaton,^{8–11)} vertex or front-tracking,^{12–17)} surface evolver,^{18–20)} and phase-field^{7,21–26)} models. In particular, the phase-field method has become common because it can accurately address curvature-driven grain boundary migration without explicit boundary tracking. With the benefit of rapid developments in high-performance computing, recent phase-field simulations have enabled significant contributions toward elucidating various metallurgical processes, including grain

growth.^{27–34)}

Most phase-field studies on grain growth have focused on ideal grain growth under the conditions of isotropic grain boundary energy and mobility. However, in actual materials, these grain boundary properties are usually strongly anisotropic, with largely different values for each grain boundary.^{1,35–37)} Theoretical, experimental, and numerical studies have suggested that grain boundary property anisotropy is a dominant factor of important metallurgical phenomena related to grain growth, *e.g.*, nucleation of recrystallized grains,^{38–40)} texture development,^{41–43)} preferential selection of specific grain boundaries,^{44–46)} and deviation of grain growth kinetics from the ideal parabolic law.^{47,48)} Therefore, to achieve more realistic prediction of microstructural evolutions, a phase-field model must be developed that can accurately simulate anisotropic boundary properties.

The most frequently used phase-field grain growth models are so-called multi-order-parameter models, which represent polycrystalline systems by assigning phase-field variables to each grain. These models can be classified into two types. One is the continuum-field (CF) model, in which the sum of the phase fields at each spatial point is non-conserved. This model originates from the works of Chen *et al.*,^{49–51)} and was improved by Kazaryan *et al.*⁵²⁾ and Moelans *et al.*^{53,54)}

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to quantitatively relate the model parameters to material properties. The other is the multi-phase-field (MPF) model with the constraint of phase-field conservation, which was first reported by Steinbach *et al.*⁵⁵⁾ and then reformulated by Garcke *et al.*⁵⁶⁾ and Steinbach and Pezzolla⁵⁷⁾ to accommodate the treatment of multiple-grain interactions at multi-junctions. In addition, a simplified version of the MPF model,⁵⁸⁾ referred to as the anti-symmetric MPF (ASMPF) model, has been widely employed for its computational convenience. Furthermore, within the framework of the MPF model, a recent work by Tóth *et al.*⁵⁹⁾ proposed a generalized MPF (XMPF) model based on a unique formulation. All of these phase-field models are reportedly capable of accurate simulation of grain growth under isotropic or weakly anisotropic grain boundary properties (e.g., the ratio of the maximum and minimum boundary energies is less than two^{60–63)}). However, for cases with strong anisotropy in grain boundary properties, the accuracy of the models has not yet been tested in detail.

Based on the above background, this study performs a detailed evaluation of the accuracies of the four different phase-field models (CF, MPF, ASMPF, and XMPF), elucidating the applicability of each model to the simulation of grain growth with strongly anisotropic grain boundary energy and mobility. The rest of this paper is outlined as follows: first, Section 2 briefly describes the formulations of the phase-field grain growth models. Next, Section 3 examines the effects of large differences in boundary properties on the accuracy of the models by performing a series of grain growth simulations for an idealized tri-crystal system. Finally, in the same section, we discuss a way to improve the accuracy based on the higher-order modification.^{63–68)}

2. Phase-field Grain Growth Models

All of the CF, MPF, ASMPF, and XMPF models represent polycrystalline systems consisting of N grains through N phase-field variables ϕ_i ($i = 1, 2, \dots, N$), which take a value of 1 in the i th grain, 0 in the other grains, and $0 < \phi_i < 1$ at the grain boundaries. The free energy functional of the system is defined as:

$$F = \int_V [f_{\text{barr}}(\phi) + f_{\text{grad}}(\phi, \nabla \phi)] dV, \dots (1)$$

where f_{barr} and f_{grad} indicate the barrier term and gradient term, respectively. Based on this free energy functional, in all models, the migration of grain boundaries is reproduced by calculating the time evolution of ϕ_i for each spatial point under the constraints of free energy minimization. However, the specific forms of f_{barr} and f_{grad} and the derivation of the time-evolution equation differ significantly for each model, as described below.

2.1. CF Model

In the CF model,⁵³⁾ the barrier term f_{barr} and gradient term f_{grad} are given as:

$$f_{\text{barr}} = m \left\{ \sum_{i=1}^N \left(\frac{\phi_i^4}{4} - \frac{\phi_i^2}{2} \right) + \sum_{i=1}^N \sum_{j>i}^N w_{ij} \phi_i^2 \phi_j^2 + \frac{1}{4} \right\}, \dots (2)$$

$$f_{\text{grad}} = \sum_{i=1}^N \frac{\kappa}{2} (\nabla \phi_i)^2, \quad \kappa = \sum_{i=1}^N \sum_{j>i}^N \varepsilon_{ij} \phi_i^2 \phi_j^2 / \sum_{i=1}^N \sum_{j>i}^N \phi_i^2 \phi_j^2,$$

where m is a parameter and w_{ij} and ε_{ij} denote the barrier height and gradient coefficient of the grain boundary between the i th and j th grains, respectively. Here, f_{barr} is formulated based on the so-called “multi-well” potential. The time-evolution equation of ϕ_i is derived as follows without the constraint of phase-field conservation:

$$\frac{\partial \phi_i}{\partial t} = -L \frac{\delta F}{\delta \phi_i},$$

$$\frac{\delta F}{\delta \phi_i} = m \left(\phi_i^3 - \phi_i + 2\phi_i \sum_{j \neq i}^N w_{ij} \phi_j^2 \right) - \kappa \nabla^2 \phi_i, \dots (3)$$

$$L = \sum_{i=1}^N \sum_{j>i}^N L_{ij} \phi_i^2 \phi_j^2 / \sum_{i=1}^N \sum_{j>i}^N \phi_i^2 \phi_j^2,$$

where L_{ij} is the phase-field mobility of the i - j grain boundary. The model parameters m , w_{ij} , ε_{ij} , and L_{ij} can be related to the width (δ_{MW} , where the subscript MW indicates the multi-well potential), energy (σ_{ij}), and mobility (M_{ij}) of the grain boundary by using the numerical algorithm proposed by Moelans *et al.*⁵³⁾ While the original algorithm of Moelans *et al.* uses the fixed grain boundary width δ_{MW} for all boundaries, Tang *et al.*⁶⁹⁾ proposed a modification that varies δ_{MW} for each boundary depending on its energy σ_{ij} . From our preliminary tests, the modified algorithm yielded better computational accuracy for the cases where two high-energy boundaries and one low-energy boundary are connected at the triple junction (corresponding to the conditions of the energy ratio $\sigma_A/\sigma_B < 1$ in **Fig. 1**; see Section 3 for details). Therefore, for such cases, we employ the algorithm of Tang *et al.*

2.2. MPF and ASMPF Models

The MPF model⁵⁷⁾ has the following forms of f_{barr} and f_{grad} :

$$f_{\text{barr}} = \sum_{i=1}^N \sum_{j>i}^N w_{ij} \phi_i \phi_j, \quad f_{\text{grad}} = - \sum_{i=1}^N \sum_{j>i}^N \frac{\varepsilon_{ij}^2}{2} \nabla \phi_i \cdot \nabla \phi_j. \dots (4)$$

Fig. 1. Tri-crystal system for evaluating the accuracy of the phase-field grain growth models: (a) initial state and (b) steady state. The system consists of three grains represented by the phase-field variables ϕ_1 , ϕ_2 , and ϕ_3 . In each panel, grains are distinguished by different colors. (Online version in color.)

The barrier term f_{barr} in Eq. (4) is generally referred to as the “double-obstacle” potential. In this model, the sum of the phase-field variables at any spatial point in the system must be conserved as $\sum_{i=1}^N \phi_i = 1$. Under this constraint, the time-evolution equation is derived as:

$$\frac{\partial \phi_i}{\partial t} = -\frac{2}{n} \sum_{j=1}^n L_{ij} \left(\frac{\delta F}{\delta \phi_i} - \frac{\delta F}{\delta \phi_j} \right), \quad \frac{\delta F}{\delta \phi_i} = \sum_{k=1}^n \left(w_{ik} \phi_k + \frac{1}{2} \varepsilon_{ik}^2 \nabla^2 \phi_k \right), \quad \dots \dots \dots (5)$$

where n is the number of nonzero phase fields at a given point. In this study, the n values for each point are evaluated using the iterative algorithm of Takaki *et al.*⁷⁰⁾ Our preliminary tests showed that this algorithm significantly improves the numerical accuracy and stability of MPF simulations. The parameters w_{ij} , ε_{ij} , and L_{ij} can be directly related to the grain boundary properties through the following analytical equations:

$$w_{ij} = 4 \frac{\sigma_{ij}}{\delta_{\text{DO}}}, \quad \varepsilon_{ij}^2 = \frac{8}{\pi^2} \delta_{\text{DO}} \sigma_{ij}, \quad L_{ij} = \frac{\pi^2}{8} \frac{M_{ij}}{\delta_{\text{DO}}}, \quad \dots \dots (6)$$

where δ_{DO} indicates the grain boundary width for the double-obstacle potential-based models.

The time-evolution equation for the ASMPF model⁵⁸⁾ is obtained by applying the “antisymmetric approximation”^{58,71)} to the MPF Eq. (5), in which all terms of $k \neq i, j$ indices are neglected:

$$\frac{\partial \phi_i}{\partial t} = \sum_{j=1}^n L_{ij} \{ w_{ij} (\phi_i - \phi_j) + \varepsilon_{ij}^2 (\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j) \}. \quad \dots (7)$$

2.3. XMPF Model

In the XMPF model,⁵⁹⁾ f_{barr} and f_{grad} are defined as:

$$f_{\text{barr}} = \omega \left\{ \sum_{i=1}^N \left(\frac{\phi_i^4}{4} - \frac{\phi_i^3}{3} \right) + \frac{1}{2} \sum_{i=1}^N \sum_{j>i}^N \phi_i^2 \phi_j^2 + \frac{1}{12} \right\},$$

$$\omega = \frac{\sum_{i=1}^N \sum_{j>i}^N w_{ij} \phi_i^2 \phi_j^2}{\sum_{i=1}^N \sum_{j>i}^N \phi_i^2 \phi_j^2}, \quad \dots (8)$$

$$f_{\text{grad}} = \sum_{i=1}^N \frac{\kappa}{2} (\nabla \phi_i)^2, \quad \kappa = \frac{\sum_{i=1}^N \sum_{j>i}^N \varepsilon_{ij}^2 \phi_i^2 \phi_j^2}{\sum_{i=1}^N \sum_{j>i}^N \phi_i^2 \phi_j^2}.$$

Here, the multi-well-type potential is used for f_{barr} . With the constraint of phase-field conservation and the Bollada–Jimack–Mullis mobility matrix,⁶⁵⁾ Γ , the time-evolution equation of ϕ_i is derived as:

$$\frac{\partial \phi_i}{\partial t} = -\sum_{j=1}^N \Gamma \left(\frac{\delta F}{\delta \phi_i} - \frac{\delta F}{\delta \phi_j} \right),$$

$$\frac{\delta F}{\delta \phi_i} = \omega \frac{\partial f_{\text{barr}}}{\partial \phi_i} + \frac{\partial \omega}{\partial \phi_i} f_{\text{barr}} - \kappa \nabla^2 \phi_i$$

$$+ \sum_{k=1}^N \left[\frac{1}{2} \frac{\partial \kappa}{\partial \phi_i} \nabla \phi_k - \frac{\partial \kappa}{\partial \phi_k} \nabla \phi_i \right] \cdot \nabla \phi_k, \quad \dots \dots \dots (9)$$

$$\Gamma(\phi_i, \phi_j) = L_{ij} \left| \frac{\phi_i}{1 - \phi_i} \right| \left| \frac{\phi_j}{1 - \phi_j} \right|.$$

The analytical relations between the model parameters and grain boundary properties are given as:

$$w_{ij} = 24 \frac{\sigma_{ij}}{\delta_{\text{MW}}}, \quad \varepsilon_{ij}^2 = \frac{3}{2} \delta_{\text{MW}} \sigma_{ij}, \quad L_{ij} = \frac{1}{3} \frac{M_{ij}}{\delta_{\text{MW}}}. \quad \dots (10)$$

2.4. Grain Boundary Width in Each Model

Although the above phase-field models all treat the grain boundaries as diffuse interfaces, the phase-field profiles at the interfaces differ for each model depending on the form of the barrier term f_{barr} . In the MPF and ASMPF models, which use the double-obstacle potential for f_{barr} , the one-dimensional equilibrium profile of a phase field, $\phi_i(x)$, is given by a sine curve:

$$\phi_i(x) = \frac{1}{2} \left[1 - \sin \left(\pi \frac{x}{\delta_{\text{DO}}} \right) \right]. \quad \dots \dots \dots (11)$$

In this case, the grain boundary width can be clearly defined as δ_{DO} , within which $\phi_i(x)$ has a value of $0 < \phi_i < 1$. On the other hand, for the multi-well-potential-based CF and XMPF models, the phase-field profiles $\phi_i(x)$ have infinite tails; the boundary width, δ_{MW} , for these models is typically defined by the gradient of ϕ_i at the center ($x = 0$) of the boundary:

$$\delta_{\text{MW}} = \frac{1}{\left| (\partial \phi_i / \partial x)_{x=0} \right|}. \quad \dots \dots \dots (12)$$

Using this definition of δ_{MW} , the one-dimensional equilibrium profile of ϕ_i can be expressed by a hyperbolic tangent function:

$$\phi_i(x) = \frac{1}{2} \left[1 - \tanh \left(2 \frac{x}{\delta_{\text{MW}}} \right) \right]. \quad \dots \dots \dots (13)$$

Note that when the grain boundary properties are anisotropic, the curves of the phase-field profiles of the CF model deviate from the hyperbolic tangent curve, becoming more asymmetric in shape.⁵³⁾

3. Accuracy Evaluation of the Phase-field Models

3.1. Computational System and Parameters

By performing grain growth simulations with anisotropic grain boundary energies and mobilities, we evaluate the accuracy of the above-described phase-field models. Here, time, spatial length, boundary energy, and mobility in the simulations are all given in dimensionless units scaled by typical orders of 1 s, 10^{-6} m, $1 \text{ J} \cdot \text{m}^{-2}$, and $10^{-12} \text{ m}^4 \cdot \text{J}^{-1} \cdot \text{s}^{-1}$, respectively. As the simulation model, an idealized tri-crystal system depicted in Fig. 1(a) is employed; the steady-state grain boundary velocity, V , shown in Fig. 1(b), is compared to the theoretical value. The computational system consists of three grains represented by different phase fields ϕ_1 , ϕ_2 , and ϕ_3 that are under zero-Neumann boundary conditions in all directions. The domain with a height $H = 128$ and width $W = 256$ is divided into square regular grids of size Δx . The theoretical value of V , V_{th} , is given as:^{40,60,72)}

$$V_{\text{th}} = M_B \frac{\sigma_A}{H}, \quad \dots \dots \dots (14)$$

where σ_A is the energy of grain boundary A and M_B is the mobility of boundary B. In the simulations, the energy of grain boundary B, σ_B , and the mobility of boundary A, M_A , are fixed to 1, while σ_A and M_B are varied. In the conditions

of $\sigma_A/\sigma_B \geq 2$, steady-state grain boundary migration cannot occur because grain boundary A splits into two boundaries under the occurrence of solid-state wetting.⁷³⁾ Therefore, we limit the σ_A value such that $\sigma_A/\sigma_B \leq 1.9$. The time-evolution equations are numerically solved using the first-order forward difference scheme and the second-order central difference scheme for time and space, respectively. The time increment Δt is taken as large as possible so as to satisfy the stability condition of the explicit scheme.

In general, the computational accuracy of a phase-field model is affected by the grid resolution and the grain boundary width. Herein, to determine the appropriate settings to evaluate the accuracies of the phase-field models, we first performed grain growth simulations while varying the resolution, $H/\Delta x$, and grain boundary width, through which the variations in the relative error $(V - V_{th})/V_{th}$ were determined for each model. Here, the grain boundary properties were set to be isotropic ($\sigma_A = \sigma_B$ and $M_A = M_B$). Note that, as described in Section 2.4, the definition of the grain boundary width is different for the MPF/ASMPF models (δ_{DO}) and the CF/XMPF models (δ_{MW}). To directly compare the results for each model, we here employed the following quantity, δ , as a unified measure of the boundary width:

$$\delta = \delta_{DO} = \frac{\pi}{2} \delta_{MW}. \quad (15)$$

When the same value is set to δ , the gradients of phase fields at the centers of the grain boundaries are identical in each model. Here, we want to briefly note the actual grain boundary width⁷⁴⁾ of each model, within which two or more phase fields take values larger than a small threshold value λ . It can be analytically shown from Eqs. (11) and (13) that, at the same value of δ , the actual boundary width for the CF/XMPF models is always larger than that for the MPF/ASMPF models;⁷⁴⁾ for instance, the ratio of the former and the latter is 1.185, 1.677, and 2.291 for the threshold values $\lambda = 0.1, 0.01$, and 0.001 , respectively. When we use the efficient numerical algorithm (so-called “active parameter tracking”^{22,70,75,76)}) storing and solving only phase-field variables larger than λ , such difference in actual boundary width could lead to a significant difference in the computational costs of the models, especially in simulations for three-dimensional complicated microstructures. The efficiencies of the models for such applications will be addressed in detail elsewhere.

The simulation results for different $H/\Delta x$ and δ values

are shown in **Fig. 2**, from which we can see that $\delta = 4\Delta x$ yields more than 10% error for any $H/\Delta x$ and any phase-field model. In the cases of $\delta = 8\Delta x$ and $10\Delta x$ for $H/\Delta x = 128$, the XMPF model shows good accuracy with less than 1% error. However, for the CF, MPF, and ASMPF models, these δ values yield errors of 3–5% even for $H/\Delta x = 128$ and, therefore, are considered to be too large compared to the grid resolution of the system. In this case, although the errors decrease with the increase in $H/\Delta x$, it is expected that a very high resolution is necessary to decrease the errors to approximately zero. In contrast, the results obtained for $\delta = 6\Delta x$ are visibly more accurate, and the errors of the phase-field models all become less than ~1% at $H/\Delta x = 128$. Therefore, to optimize the computational accuracy and cost, we used $\delta = 6\Delta x$ and $H/\Delta x = 128$ for the following simulations.

3.2. Effect of Anisotropic Grain Boundary Energy

To examine the effects of anisotropic grain boundary energy on the accuracies of the phase-field models, simulations were performed under the above-described conditions while varying the energy ratio σ_A/σ_B , with M_B/M_A fixed to 1. **Figure 3** shows the relative errors $(V - V_{th})/V_{th}$ of different models as functions of σ_A/σ_B . As shown in the figure, for the range of $\sigma_A/\sigma_B \geq 0.2$, although the error of the MPF model almost monotonically increases on the positive side as σ_A/σ_B deviates from 1, the error remains less than ~10%.

Fig. 3. Variations in relative error $(V - V_{th})/V_{th}$ depending on boundary energy ratio σ_A/σ_B , as calculated from different phase-field models. (Online version in color.)

Fig. 2. Variations in relative error $(V - V_{th})/V_{th}$ depending on grain boundary width δ as calculated from different phase-field models for grid resolutions of (a) $H/\Delta x = 64$, (b) $H/\Delta x = 96$, and (c) $H/\Delta x = 128$. (Online version in color.)

At $\sigma_A/\sigma_B = 0.1$, the error jumps to the negative side, reaching 20%. Therefore, if an error of $\sim 10\%$ is acceptable, the MPF model is considered suitable for modeling grain growth under energy anisotropy within the ratio of the minimum-to-maximum boundary energy of 0.2. Note that the accuracy of the MPF model obtained here is visibly better than that in our previous study,⁶⁸⁾ this is because, as described in Section 2.2, the iterative algorithm of Takaki *et al.*⁷⁰⁾ was employed in the present MPF simulations, which significantly improves the computational accuracy. In Fig. 3, the CF model shows the similar degree of accuracy (magnitude of error) as that of the MPF model for $\sigma_A/\sigma_B < 1$. However, for $\sigma_A/\sigma_B > 1$, the decrease in the accuracy is relatively large, and the error is maximized at $\sim 20\%$. In actual grain growth processes, triple junctions comprising one high-energy grain boundary and two low-energy boundaries, like the case of $\sigma_A/\sigma_B > 1$ in Fig. 3, are rarely formed.^{77–79)} Thus, in many cases, it is expected that the CF model can address anisotropic boundary energy with the similar degree of accuracy as that offered by the MPF model. In the ASMPF model, the increase in error is significant for both the ranges of $\sigma_A/\sigma_B > 1$ and $\sigma_A/\sigma_B < 1$. Because the formulation of this model is simplified by ignoring the interactions of three or more grains, it is considered that the energy balance of grain boundaries at the triple junctions cannot be reproduced correctly. As an example, Fig. 4 shows the steady-state configurations of grain boundaries simulated by each phase-field model for the conditions $\sigma_A/\sigma_B = 0.5$ and $\sigma_A/\sigma_B = 1.5$. Unlike the cases with other models, the grain boundary angles in the ASMPF model are almost unchanged for the different energy ratios. Therefore, the ASMPF model is considered to be unsuitable for problems where grain boundary energy anisotropy is important. The XMPF model maintains less than 10% error in the range of $\sigma_A/\sigma_B \geq 0.7$. On the other hand, the error suddenly jumps to exceed 60% at $\sigma_A/\sigma_B = 0.5$. This sudden jump is attributed to the “ghost phase” problem,^{60,63)} via which unnecessary phases leak from the triple junction into the grain boundaries, thus inducing behavioral instabilities in the boundaries. As an example, Fig. 5 depicts the distributions of the values of phase field

ϕ_2 for $\sigma_A/\sigma_B = 0.5$, as obtained from the simulations using each phase-field model. As shown, for the XMPF model, the leakage of ϕ_2 into the ϕ_1 – ϕ_3 boundary is clearly observed.

3.3. Introduction of Higher-order Term

Tóth *et al.*⁶³⁾ reported that the ghost phase problem of the XMPF model can be resolved by introducing a higher-order (triplet) term, f_{ho} , into the free energy functional:

$$F = \int_V [f_{barr}(\phi) + f_{grad}(\phi, \nabla \phi) + f_{ho}(\phi)] dV, \quad \dots (16)$$

$$f_{ho} = \sum_{i=1}^N \sum_{j>i}^N \sum_{k>j}^N C_{ijk} \phi_i \phi_j \phi_k,$$

where C_{ijk} is a coefficient. The higher-order term energetically penalizes ghost phases, and is often used to improve the accuracy of other phase-field models.^{63–68)} Herein, by using the higher-order term, we investigate the possibility of improving the accuracies of the CF, MPF, and XMPF models. Note that the ASMPF model is not considered here because, in principle, this model cannot introduce the

Fig. 5. Distributions of the values of phase field ϕ_2 for the condition of $\sigma_A/\sigma_B = 0.5$: (a) CF model, (b) MPF model, (c) ASMPF model, and (d) XMPF model. In panel (d), the leakage of ϕ_2 into the ϕ_1 – ϕ_3 boundary (*i.e.*, ghost phase) is observed. (Online version in color.)

Fig. 4. Steady-state grain boundary configurations for the conditions of $\sigma_A/\sigma_B = 0.5$ and $\sigma_A/\sigma_B = 1.5$: (a) CF model, (b) MPF model, (c) ASMPF model, and (d) XMPF model. In all panels, grains are distinguished by different colors. (Online version in color.)

higher-order term because of the antisymmetric approximation.

The accuracy of the phase-field models with the higher-order term is largely dependent on the value of its coefficient,⁶⁸⁾ C_{ijk} . However, a way of setting C_{ijk} to the appropriate value is not yet established. Therefore, to examine the optimum values of C_{ijk} , we first performed simulations using the system of Fig. 1 and each phase-field model for various energy ratios σ_A/σ_B , with $M_A = M_B$. For each σ_A/σ_B value, C_{ijk} was varied by 0.01, through which the variations in the relative error $(V - V_{th})/V_{th}$ were determined. As an example, Fig. 6(a) shows the results of the XMPF model for $\sigma_A/\sigma_B = 1$ and 0.5. As shown, in both cases the

relative error $(V - V_{th})/V_{th}$ decreases almost monotonically with increases in C_{ijk} . For $\sigma_A/\sigma_B = 0.5$, the magnitude of the relative error, $|(V - V_{th})/V_{th}|$, approaches zero at $C_{ijk} = 0.48$. For $\sigma_A/\sigma_B = 1$, $|(V - V_{th})/V_{th}|$ does not become zero, but is minimized at $C_{ijk} = 0$. These values of C_{ijk} , which minimize $|(V - V_{th})/V_{th}|$, are defined as the optimum values. The optimum values obtained for each model are summarized in Fig. 6(b) as functions of σ_A/σ_B .

Next, we compared the accuracy of the models with and without the higher-order term via accuracy evaluation simulations, in the same manner as described in Section 3.2. Here, the coefficients of the higher-order terms use the optimal values shown in Fig. 6(b). The results are given in Fig. 7.

Fig. 6. Determining the optimum values of C_{ijk} . (a) Variations in $(V - V_{th})/V_{th}$ depending on C_{ijk} , as calculated from the XMPF model for $\sigma_A/\sigma_B = 1$ and $\sigma_A/\sigma_B = 0.5$. (b) Variations in the optimum value of C_{ijk} for minimizing $|(V - V_{th})/V_{th}|$ for different σ_A/σ_B values. (Online version in color.)

Fig. 7. Variations in $(V - V_{th})/V_{th}$ with and without the higher-order term for different σ_A/σ_B values: (a) CF model, (b) MPF model, and (c) XMPF model. The right panel of (c) depicts the distributions of the values of phase field ϕ_2 for $\sigma_A/\sigma_B = 0.5$ and $\sigma_A/\sigma_B = 0.3$, as calculated using the XMPF model with the higher-order term. The coefficients of the higher-order terms use the optimal values shown in Fig. 6 (b). (Online version in color.)

Fig. 8. Variations in relative error $(V - V_{th})/V_{th}$ depending on boundary mobility ratio M_B/M_A , as calculated from different phase-field models. (Online version in color.)

As can be seen from Fig. 7(a), the accuracy improvement for the CF model is small. In Fig. 7(b), The MPF model can reduce the error for $\sigma_A/\sigma_B > 1.3$ and $\sigma_A/\sigma_B = 0.1$ to almost zero by including the higher-order term, but there is no improvement for other ranges of σ_A/σ_B . In Fig. 7(c) for the XMPF model, the higher-order term suppresses the error to almost zero for most of the grain boundary energy ratios, exhibiting a drastic improvement in accuracy. However, even though the coefficient C_{ijk} is set to the optimum value (Fig. 6(b)), the ghost phase problem still occurs in the range of $\sigma_A/\sigma_B \leq 0.3$, as depicted in the right panel of Fig. 7(c). By increasing C_{ijk} from the optimum value for $\sigma_A/\sigma_B = 0.3$, the disappearance of the ghost phase is observed at C_{ijk} approximately twice the optimum value; nevertheless, the error $(V - V_{th})/V_{th}$ reaches 40%, resulting in the decrease of the computational accuracy for the grain boundary velocity. To fully achieve both accuracy and ghost phase suppression, additional improvement of the model might be required.

3.4. Effect of Anisotropic Grain Boundary Mobility

Finally, we evaluated the accuracy of the phase-field models while considering anisotropic grain boundary mobilities. Here, grain growth simulations using the system of Fig. 1 and different phase-field models were performed for various mobility ratios M_B/M_A , with σ_A/σ_B fixed to 1. The results are shown in Fig. 8, where the relative errors $(V - V_{th})/V_{th}$ are plotted as functions of M_B/M_A . As shown in the figure, the MPF, ASMPF, and XMPF models maintain almost constant errors of less than 2% for the very wide-ranging mobility ratio range of $0.01 \leq M_B/M_A \leq 100$, exhibiting high degrees of accuracy. Compared to these models, the increase in the error of the CF model is relatively large, especially for $M_B/M_A < 1$; however, the maximum error remains within 4%. These results enable us to conclude that, if we accept an error of several percent, all of the phase-field models allow for the introduction of arbitrarily strong anisotropy in grain boundary mobility.

4. Conclusions

This study was conducted to elucidate the applicability of four different phase-field models in simulating grain growth

under conditions of strongly anisotropic grain boundary energy and mobility. To this end, the accuracies of the phase-field models were systematically evaluated by performing a series of anisotropic grain growth simulations. In addition, based on the higher-order modification, accuracy improvement of the models was attempted. The main findings are summarized as follows:

(1) All of the phase-field models can be used for grain growth simulations with almost arbitrarily strong mobility anisotropy.

(2) If an error of around 10% is accepted, the CF and MPF models without the higher-order term can adequately simulate energy anisotropies within the ratio of the minimum-to-maximum boundary energies $\sigma_{\min}/\sigma_{\max} = 0.2$. Although the usage of the higher-order term improves the accuracy of the MPF model for simulations with stronger energy anisotropy, errors near 10% are not fully resolved.

(3) By using the higher-order term, the XMPF model achieves high accuracy with almost no error for any grain boundary energy ratio. However, to achieve both accuracy and ghost phase suppression for the range of $\sigma_{\min}/\sigma_{\max} \leq 0.3$, further improvement of the model is required.

(4) The ASMPF model is not suitable for simulations with anisotropic boundary energy. However, because of its simple formulation and resultant computational efficiency, this model is a promising choice for conditions of only anisotropic mobility.

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