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Extended higher-order multi-phase-field model for three-dimensional anisotropic-grain-growth simulations

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ABSTRACT

Based on the multi-phase-field (MPF) model reported by Steinbach et al., we constructed a higher-order MPF model in a previous study that contains a higher-order term and an additional kinetic parameter to represent the properties of triple junctions (TJs); this model was observed to be suitable for the simulation of 2D grain growth with anisotropic grain-boundary (GB) energy and mobility, which are strongly dependent on the misorientation angle ($\Delta\theta$). In the current study, we attempt to improve the accuracy of 3D MPF simulations of anisotropic grain growth by extending this higher-order MPF model such that it accounts for the properties of quadruple junctions as well as those of TJs. In addition, using the extended higher-order MPF model, a series of grain-growth simulations are performed for a 3D columnar structure while considering the anisotropic GB properties, through which the accuracy of the model is examined in detail. The results confirm that the extended higher-order MPF model enables the anisotropic GB properties to be handled accurately for wider-ranging $\Delta\theta$ than in previous models.

1. Introduction

During the heat treatment of a polycrystalline material, the internal microstructure evolves through several thermodynamic phenomena including multiple phase transformations, recrystallization, and grain growth [1–3]. Control over the microstructural evolution enables superior materials to be produced because the physical and mechanical properties of polycrystals are greatly dependent on the microstructure. In general, the fundamental process underlying the microstructural evolution is the migration of grain boundaries (GBs), or grain growth in a broad sense. Thus, with the aim of systematically predicting the evolution of microstructure with heat treatment, numerical approaches have been developed using mesoscale grain-growth models including the Monte-Carlo model [4–7], cellular automaton model [8–10], vertex model [11–14], surface-evolver model [15], front-tracking model [16–18], level-set model [19,20], and phase-field model [21–25].

Recently, the multi-phase-field (MPF) model proposed by Steinbach et al. [26,27] has been frequently used as a prominent model to simulate polycrystalline grain growth. This model enables the quantitative prediction of complicated microstructural evolution in time and space. Additionally, the computation speed of the model can be significantly increased by using the active parameter tracking algorithm [28–30] that was proposed by Vedantam and Patnaik [28], Gruber et al. [31], and Kim et al. [32] independently. However, the original MPF model has one drawback: in real materials, the properties (energy and mobility) of GBs exhibit strong anisotropies, with their variations depending primarily on the misorientation angle ($\Delta\theta$) between the neighboring grains [1,33–36]. These anisotropic properties affect both the kinetics and morphological aspects of grain growth [36–40] and, thus, might be important factors to consider in grain-growth simulations. However, it is difficult to introduce the anisotropic properties in the MPF model for wide-ranging $\Delta\theta$ because when GB properties with large differences are introduced in MPF simulations, unnecessary phases ('ghost phases [41]') leak from multiple junctions into GBs, and consequently, the GB behaviors become unstable. To address this issue, Garcke et al. [42,43] and Hirouchi et al. [44] have proposed modified models, which are known as higher-order MPF models. In these models, the formation of ghost phases is suppressed using a higher-order term representing the free energy of triple junctions (TJs). However, the coefficient of the higher-order term used for the models, which strongly affects the simulation results, has not been optimized. Moreover, the models do not account for the decrease in the accuracy due to the strong anisotropy in GB mobility. Therefore, we developed a novel

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higher-order MPF model [45] by optimizing the coefficient of the higher-order term and introducing the TJ mobility; the validity of the model was confirmed via a series of 2D grain-growth simulations with anisotropic GB properties. However, 3D simulations are essential for simulating actual grain growth [32,33,46], on which quadruple junctions (QJs) as well as TJs might have a considerable effect [33]. Recently, 3D MPF simulation is becoming easy to perform by virtue of parallel computing [47–49] and general-purpose computing on graphics processing units (GPUs) [50–57]. Thus, the improvement of the accuracy of 3D MPF simulation is believed to be an urgent issue.

In this study, we attempt to improve the accuracy of 3D grain-growth simulations with anisotropic GB properties by introducing the properties of QJs to the higher-order MPF model that was proposed in our previous study [45]. First, in Section 2, the higher-order MPF model is extended to account for the QJ properties. Next, in Section 3, the appropriate ways to determine the simulation parameters used for the extended higher-order model are examined. Finally, in the same section, the accuracy of the extended model using the determined parameters is tested using grain-growth simulations with $\Delta\theta$-dependent GB properties.

2. Extended higher-order MPF model considering QJ properties

We derive the governing equation of the extended higher-order MPF model that accounts for the QJ properties. The MPF model represents a polycrystalline system consisting of N grains using N phase-field variables; the ith grain is represented by the phase field ϕ_i, which takes a value of 1 in the ith grain, 0 in the other grains, and $0 < \phi_i < 1$ at the GBs. The sum of the phase fields at any spatial point in the system must be conserved:

$$\sum_{i=1}^{n}\phi_i = 1, \tag{1}$$

where n is the number of coexisting phases at the point.

When the additional free energy of the TJs and QJs are considered, the total free energy of the system can be expressed as

$$F = \int_V \sum_{i=1}^{n}\sum_{j=i+1}^{n}\left\{W_{ij}\phi_i\phi_j + \sum_{k=j+1}^{n}(W_{ijk}\phi_i\phi_j\phi_k + \sum_{l=k+1}^{n}W_{ijkl}\phi_i\phi_j\phi_k\phi_l) - \frac{a_{ij}^2}{2}\nabla\phi_i\cdot\nabla\phi_j\right\}\mathrm{d}V, \tag{2}$$

where W_{ij} and a_{ij} are the barrier height and gradient coefficient of the GB between the ith and jth grains, respectively. The second and third terms on the right-hand side in Eq. (2) are the higher-order terms representing the energetic contributions of the TJs [42–44,58,59] and QJs, respectively. These terms play a role in penalizing ghost phases at the GBs around the junctions. The coefficients W_{ijk} and W_{ijkl} are the barrier heights of TJs and QJs, respectively. A suitable way of determining W_{ijkl} is examined in Section 3; W_{ijk} is expressed by the formula developed in our previous study [45]:

$$W_{ijk} = \begin{cases} k_{\mathrm{TJ}}\left(W_{\mathrm{GB,max}} - \frac{W_{\mathrm{GB,median}}+W_{\mathrm{GB,min}}}{2}\right) & \text{for } 2W_{\mathrm{GB,median}} \leqslant W_{\mathrm{GB,max}} + W_{\mathrm{GB,min}}, \\ 0 & \text{for } 2W_{\mathrm{GB,median}} > W_{\mathrm{GB,max}} + W_{\mathrm{GB,min}}, \end{cases} \tag{3}$$

where $W_{\mathrm{GB,max}}$, $W_{\mathrm{GB,median}}$, and $W_{\mathrm{GB,min}}$ are the maximum, median, and minimum barrier heights of the GBs adjoining the TJ, respectively, and k_{TJ} is a constant. The optimum value of k_{TJ} for 3D simulations is examined in Section 3.

The time-evolution equation for ϕ_i satisfying Eq. (1) is given by

$$\frac{\partial\phi_i}{\partial t} = -\frac{2}{n}\sum_{j=1}^{n}M_{ij}^{\phi}\left(\frac{\delta F}{\delta\phi_i} - \frac{\delta F}{\delta\phi_j}\right), \tag{4}$$

where M_{ij}^{ϕ} is the phase-field mobility of the GB between the ith and jth grains. The functional derivative of Eq. (2) can be calculated as

$$\frac{\delta F}{\delta\phi_i} = \sum_{k=1}^{n}\left\{W_{ik}\phi_k + \sum_{l=1}^{n}\left(W_{ikl}\phi_k\phi_l + \sum_{m=1}^{n}W_{iklm}\phi_k\phi_l\phi_m\right) + \frac{a_{ik}^2}{2}\nabla^2\phi_k\right\}. \tag{5}$$

Finally, the time-evolution equation reduces to

$$\frac{\partial\phi_i}{\partial t} = -\frac{2}{n}\sum_{j=1}^{n}M_{ij}^{\phi}\sum_{k=1}^{n}\left[\frac{1}{2}(a_{ik}^2 - a_{jk}^2)\nabla^2\phi_k + (W_{ik} - W_{jk})\phi_k + \sum_{l=1}^{n}\left\{(W_{ikl} - W_{jkl})\phi_k\phi_l + \sum_{m=1}^{n}(W_{iklm} - W_{jklm})\phi_k\phi_l\phi_m\right\}\right]. \tag{6}$$

W_{ij}, a_{ij}, and M_{ij}^{ϕ} can be related to the thickness (δ), energy (γ_{ij}), and mobility (M_{ij}) of the GB through the following equations:

$$W_{ij} = \frac{4\gamma_{ij}}{\delta}, \quad a_{ij} = \frac{2}{\pi}\sqrt{2\delta\gamma_{ij}}, \quad M_{ij}^{\phi} = \frac{\pi^2}{8\delta}M_{ij}. \tag{7}$$

When M_{ij}^{ϕ} defined in Eq. (7) is substituted into Eq. (6), the migration of the TJ, ijk, is determined by the linear superposition of the GB mobilities, M_{ij}, M_{jk}, and M_{ki}. Thus, when one of the mobilities in the TJ is much higher or lower than the others, it dominates the migration of the TJ, resulting in the occurrence of artificial junction drag on the GBs. To avoid this issue, we modify the definition of M_{ij}^{ϕ} in TJs ($n = 3$) as follows by introducing the TJ mobility M_{ijk} [45]:

$$\left.\begin{aligned} M_{ij}^{\phi} = M_{jk}^{\phi} = M_{ki}^{\phi} &= \tfrac{\pi^2}{8\delta}M_{ijk} \\ M_{ijk} &= M_{ij}\omega_{ij} + M_{jk}\omega_{jk} + M_{ki}\omega_{ki} \end{aligned}\right\} \text{only for } n = 3, \tag{8}$$

where ω_{ij} is the weight function defined as follows using a constant m_{TJ} and the average of the GB mobilities $M_{\mathrm{GB,ave}} = (M_{ij} + M_{jk} + M_{ki})/3$:

$$\omega_{ij} = \frac{1}{2}\left(1 - \frac{|M_{ij} - M_{\mathrm{GB,ave}}|^{m_{\mathrm{TJ}}}}{|M_{ij} - M_{\mathrm{GB,ave}}|^{m_{\mathrm{TJ}}} + |M_{jk} - M_{\mathrm{GB,ave}}|^{m_{\mathrm{TJ}}} + |M_{ki} - M_{\mathrm{GB,ave}}|^{m_{\mathrm{TJ}}}}\right). \tag{9}$$

m_{TJ} represents the strength of the weighting; when m_{TJ} is set to zero, M_{ijk} is equal to $M_{\mathrm{GB,ave}}$. Further, to accurately express the QJ behaviors, the QJ mobility, M_{ijkl}, is introduced by extending the formulation of M_{ijk} as follows:

$$\left.\begin{aligned} M_{ij}^{\phi} = M_{jk}^{\phi} = M_{kl}^{\phi} = M_{li}^{\phi} &= \tfrac{\pi^2}{8\delta}M_{ijkl} \\ M_{ijkl} &= M_{ijk}\omega_{ijk} + M_{jkl}\omega_{jkl} + M_{kli}\omega_{kli} + M_{lij}\omega_{lij} \end{aligned}\right\} \text{only for } n = 4, \tag{10}$$

$$\omega_{ijk} = \frac{1}{3}\left(1 - \frac{|M_{ijk} - M_{\mathrm{TJ,ave}}|^{m_{\mathrm{QJ}}}}{|M_{ijk} - M_{\mathrm{TJ,ave}}|^{m_{\mathrm{QJ}}} + |M_{jkl} - M_{\mathrm{TJ,ave}}|^{m_{\mathrm{QJ}}} + |M_{kli} - M_{\mathrm{TJ,ave}}|^{m_{\mathrm{QJ}}} + |M_{lij} - M_{\mathrm{TJ,ave}}|^{m_{\mathrm{QJ}}}}\right), \tag{11}$$

where m_{QJ} is a constant and $M_{\mathrm{TJ,ave}} = (M_{ijk} + M_{jkl} + M_{kli} + M_{lij})/4$ is the average of the TJ mobilities. The optimum values of m_{TJ} and m_{QJ} for 3D simulations are determined in Section 3.

3. Determination of the parameters and their validations

3.1. Coefficients of the higher-order terms: W_{ijk} and W_{ijkl}

We examine the optimum values of the coefficients of the higher-order terms in Eq. (6), W_{ijk} and W_{ijkl}, for 3D problems, by evaluating the accuracy of the extended higher-order MPF model. As the simulation model, we employ a simple 3D system, illustrated in Fig. 1, that contains TJs and QJs; the steady-state boundary velocity, V, is compared with the theoretical value. The domain