Computational Materials Science 112 (2016) 44–51

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Validation of a novel higher-order multi-phase-field model for grain-growth simulations using anisotropic grain-boundary properties

Eisuke Miyoshi [a], Tomohiro Takaki [b,*]

[a] Department of Mechanical and System Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo, Kyoto 606-8585, Japan
[b] Faculty of Mechanical Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo, Kyoto 606-8585, Japan

ARTICLE INFO

Article history:
Received 13 July 2015
Received in revised form 8 October 2015
Accepted 11 October 2015
Available online 19 November 2015

Keywords:
Multi-phase-field model
Microstructural evolution
Grain growth
Grain boundary
Triple junction

ABSTRACT

The multi-phase-field (MPF) model proposed by Steinbach et al. has several advantages when it comes to numerically simulating the grain growth, recrystallization, and multiple phase transitions. In this study, in order to improve the accuracy of MPF simulations using the anisotropic grain-boundary energy and mobility, which depend strongly on the misorientation angles, we account for the triple-junction properties in the MPF model. Further, two-dimensional simulations of grain-boundary migrations in three-grain systems as well as simulations of abnormal grain growth in a polycrystalline system are performed using the proposed model, in order to confirm its validity. The results show that the proposed model allows for the introduction of the anisotropic energy and mobility with high accuracy for a wider range of misorientations, in contrast to the conventional model.

1. Introduction

When a metallic polycrystalline material is heat treated, its microstructure changes drastically through several phenomena such as multiple phase transitions, recrystallization, and grain growth [1,2]. The ability to predict and control the microstructure formed during the heat-treatment process is crucial for developing materials with desirable mechanical properties. In general, the microstructural evolution is accompanied by the migration of grain boundaries, a phenomenon that can be regarded as grain growth in a broad sense. Therefore, in order to predict the heat-treated microstructure systematically, numerical simulations based on a grain-growth model are usually performed [2].

The Monte-Carlo model [3], the cellular automaton model [4], the vertex model [5,6] and the phase-field (PF) model [7–11] are frequently used for numerically modeling grain growth [12]. The PF model can successfully simulate complicated microstructural evolutions on real-time and real-space scales. In addition, because this model takes into account the effects of the grain-boundary curvature, which affects the grain-growth behavior, the curvature does not have to be calculated. Hence, the PF model is considered the most suitable one for simulating grain growth. The following are the commonly used polycrystalline-grain-growth models within the framework of the PF model: the KWC model [13–16] proposed by Kobayashi, Warren, and Carter and the multi-phase-field (MPF) models reported by Steinbach et al. [17,18] and Chen et al. [19,20]. The KWC model can express an arbitrary number of crystal orientations using only two order parameters [21]. In addition, the coalescence of the grains, owing to their rotation, is also taken into consideration. However, the time-evolution equations of the order parameters are singular diffusion equations and thus the time increment for the numerical simulations must be kept very small. Furthermore, using this model, it is difficult to express the grain growth quantitatively while taking into account the misorientation-dependent grain-boundary energies. In contrast, the MPF model developed by Steinbach et al. [17,18] exhibits numerous advantages, in that the coefficients of the time-evolution equation are related directly to the material parameters. Thus, a quantitative evaluation of the evolution of the microstructure is possible. Moreover, it is easy to introduce the active parameter tracking algorithm [22–24] proposed by Kim et al. in this model [25]; this increases the computation speed significantly. Thus, the MPF model is more suitable as a grain-growth model, as it lowers the computational cost and allows for accurate simulations of the microstructural evolution during heat treatments [26–30].

The dependencies of the grain-boundary energy and mobility on the misorientation angle [1,31–34] have a significant effect on

* Corresponding author. Tel./fax: +81 75 724 7317.
E-mail address: takaki@kit.ac.jp (T. Takaki).

http://dx.doi.org/10.1016/j.commatsci.2015.10.010
0927-0256/

both the growth kinetics and the morphology of the grains [34]. Thus, it is important to take into account the misorientation-dependent properties in the MPF model. However, the MPF model developed by Steinbach et al. does not allow for the introduction of the misorientation dependencies with high accuracy. This is because the model becomes numerically unstable in the case of calculations where the energies of the grain boundaries adjoining a triple junction exhibit large differences. To overcome this issue, Garcke et al. [35,36] and Hirouchi et al. [37] proposed a modified model having a higher-order term representing the free energy of the triple junction. However, this model, which is referred to as the higher-order MPF model, exhibits a few problems. For instance, the correct way of determining the coefficient of the higher-order term has not been established. While some groups set the coefficient as a constant [35,36,38], Hirouchi et al. determined it using an assumed equation [37]. However, as discussed in Section 3, the accuracy of the higher-order model depends on the value of the coefficient. In addition, the optimum value of the coefficient varies with the conditions. Thus, it is believed that the coefficient must be modeled through minute evaluations of the accuracy. Further, the limits of the applicability of the model, that is, the range of differences in the grain-boundary energies for which the model can be used, have not been elucidated. Finally, the accuracy of the model in the case where the mobilities of the different boundaries exhibit large differences remains untested.

The purpose of this paper is to propose the appropriate values for the parameters of the higher-order MPF model and to show the accuracy as well as the limits of applicability of the model for two-dimensional cases with respect to predicting heat-treated microstructures. First, in Section 2, we suggest a higher-order MPF model based on the model reported by Steinbach et al. [17,18]. Next, the coefficient of the higher-order term is modeled in Section 3. In this section, we also determine the effects of large differences in boundary mobilities on the accuracy of the MPF model and attempt to improve the accuracy of the model by introducing a triple-junction mobility. Finally, in Section 4, through a series of grain-growth simulations based on the modeled parameters, we investigate the accuracy and the limits of applicability of the proposed higher-order model.

2. Higher-order multi-phase-field model

On the basis of the MPF model proposed by Steinbach et al. [17,18], we derive the time-evolution equation for the higher-order MPF model. Let us consider a polycrystalline system consisting of N grains. In the MPF model, such a system is represented by the phase-field variables ϕ_α ($\alpha = 1, 2, \ldots, N$); these take a value of 1 in the αth grain, 0 in the other grains, and $0 < \phi_\alpha < 1$ at the grain boundaries. Here, none of the variables is independent, and each must satisfy the following condition:

$$\sum_{\alpha=1}^{N} \phi_\alpha = 1. \tag{1}$$

The free-energy functional of the system can be written as follows using ϕ_α:

$$F = \int_V \sum_{\alpha=1}^{N} \sum_{\beta=\alpha+1}^{N} \left(W_{\alpha\beta}\phi_\alpha\phi_\beta + \sum_{\chi=\beta+1}^{N} W_{\alpha\beta\chi}\phi_\alpha\phi_\beta\phi_\chi - \frac{a_{\alpha\beta}^2}{2}\nabla\phi_\alpha \cdot \nabla\phi_\beta \right) dV, \tag{2}$$

where $W_{\alpha\beta}$ and $a_{\alpha\beta}$ are the height of the energy barrier and the gradient coefficient of the boundary between the αth and βth grains, respectively. The second term on the right-hand side in Eq. (2) is the higher-order term representing the additional free energy of the triple junctions [35–40]. The time-evolution equation of the phase field ϕ_i ($i = 1, 2, \ldots, n$) satisfying Eq. (1) is given by [18]

$$\frac{\partial\phi_i}{\partial t} = -\frac{2}{n}\sum_{j=1}^{n} M_{ij}^{\phi}\left(\frac{\delta F}{\delta\phi_i} - \frac{\delta F}{\delta\phi_j}\right), \tag{3}$$

for each spatial point, where n is the number of nonzero phase fields at the point and M_{ij}^{ϕ} is the phase-field mobility of the boundary between the ith and jth grains. The functional derivative of Eq. (3) can be calculated as

$$\frac{\delta F}{\delta\phi_i} = \sum_{k=1}^{n}\left(W_{ik}\phi_k + \sum_{l=1}^{n} W_{ikl}\phi_k\phi_l + \frac{a_{ij}^2}{2}\nabla^2\phi_k \right). \tag{4}$$

Finally, the time-evolution equation reduces to

$$\frac{\partial\phi_i}{\partial t} = -\frac{2}{n}\sum_{j=1}^{n} M_{ij}^{\phi}\left[\sum_{k=1}^{n}\left\{ (W_{ik} - W_{jk})\phi_k + \sum_{l=1}^{n}(W_{ikl} - W_{jkl})\phi_k\phi_l + \frac{1}{2}\left(a_{ik}^2 - a_{jk}^2\right)\nabla^2\phi_k \right\}\right]. \tag{5}$$

W_{ij}, a_{ij}, and M_{ij}^{ϕ} are related to the grain-boundary thickness, δ; the grain-boundary energy, γ_{ij}; and the grain-boundary mobility, M_{ij} by

$$W_{ij} = \frac{4\gamma_{ij}}{\delta}, \tag{6}$$

$$a_{ij} = \frac{2}{\pi}\sqrt{2\delta\gamma_{ij}}, \tag{7}$$

$$M_{ij}^{\phi} = \frac{\pi^2}{8\delta}M_{ij}. \tag{8}$$

Note that δ can be varied for each grain boundary similar to γ_{ij} and M_{ij}. In this study, however, we kept it constant to simplify the numerical calculations.

3. Modeling of parameters

3.1. Coefficient of higher-order term: W_{ijk}

When grain-boundary energies with large differences are introduced in the conventional MPF model, unnecessary phases (i.e., "ghost phases" [38]) leak from the triple junctions into the grain boundaries, making the behavior of the boundaries unstable. The higher-order term in the time-evolution equation (5) is employed as a penalty term to prevent the ghost phases from leaking [35–38]. However, since the coefficient of the higher-order term W_{ijk} has a significant effect on the simulation results [35], W_{ijk} must be set with care. Therefore, to determine the most suitable way of determining W_{ijk}, we examine the optimum values of W_{ijk} by evaluating the accuracy of the higher-order MPF model. For this

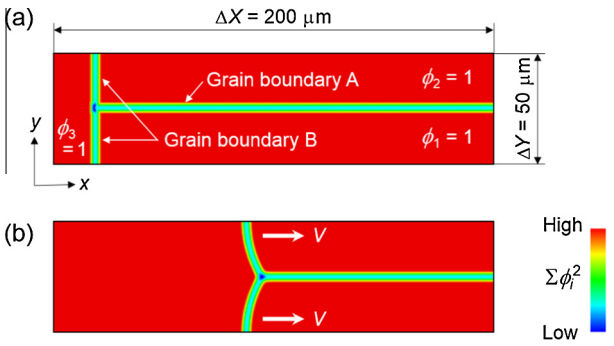

Fig. 1. Three-grain system used for evaluating the accuracy of the higher-order MPF model: (a) initial state and (b) steady state.