



Microstructural path analysis of polycrystalline solidification by using multi-phase-field method incorporating a nucleation model



Yasutaka Nishida ^{a,*}, Fumihiko Aiga ^a, Satoshi Itoh ^b

^a Corporate Research & Development Center, Toshiba Corporation, 1 Komukai-Toshiba-cho, Saiwai-ku, Kawasaki 212-8582, Japan

^b RIKEN Advanced Institute for Computational Science, 7-1-26, Minatojima-minami-machi, Chuo-ku, Kobe, Hyogo 650-0047, Japan

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ABSTRACT

Using the multi-phase-field (MPF) method incorporating a continuous nucleation model, we have revisited polycrystalline solidification described by the KJMA kinetics. Besides the Avrami exponents, the microstructural path functions to quantify the morphological characteristics were calculated within the framework of the MPF method. Our simulation can easily take account of the effects that are difficult to deduce from the conventional KJMA theory such as grain impingement and spatial distribution of crystallite seeds. As a result, quantitative differences among various types of transformation kinetics can be identified.

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1. Introduction

As well as being of fundamental interest in materials science, the kinetics of phase transformation has attracted great interest in regard to industrial processes. In industry, the phase transformation has been applied to various materials for the purpose of improving their physical properties. An important example is the γ - α transformation in steelmaking [1,2], which is the phase transformation from austenite (face-centered cubic structure, γ -Fe) to ferrite (body-centered cubic structure, α -Fe) in cooling processes. It is well known that the mechanical properties of steels are strongly dependent on their microstructure consisting of polycrystal grains produced during cooling processes. Therefore, the material properties of steels can be controlled by cooling processes via the phase transformation. Such a relationship between materials properties and manufacturing processes can be found elsewhere, in magnetic materials [3], shape memory alloys [4], electrode materials [5], etc. From the viewpoint of industrial applications, the phase transformation is important for controlling various properties of engineering materials. Thus, understanding of the kinetics of the phase transformation leads to guidelines of controlled manufacturing processes for desirable products.

Theoretically, the kinetics of the phase transformation is an old problem concerning fundamental phenomena in materials science. The Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory [6–10] is the theory most widely applied to phase transformation. In the KJMA theory, the phase transformation is assumed to proceed via nucleation and subsequent grain growth. In the simplest model of the KJMA theory, spherical nuclei, which are produced and grow at a constant rate, are uniformly distributed in space and the transformed volume fraction is defined as the sum of the volume of the transformed grains divided by the total volume. Then the interaction between grains, such as the grain impingement, is dealt with by an extended volume concept, whereby the grains grow without impingement so that the time evolution of the transformed volume fraction $V_V(t)$ can be related to the extended volume $V_E(t)$ as follows:

$$V_V(t) = 1 - \exp(-V_E(t)). \quad (1)$$

The extended volume $V_E(t)$ is often replaced by Kt^n in a simple assumption where the spherical nuclei are uniformly distributed, and then K is constant and n is the Avrami exponent. Thus, the KJMA formulation provides a simple description and clear explanation about phase transformation kinetics.

However, it is recognized that this theory often fails to explain experimental results for alloys [11,44] because of its simple assumption [12]. There is also some discussion about the validity of the KJMA theory. For example, the effect of the specimen's external surface and inhomogeneity of the germ nuclei are not taken into account in the KJMA theory. In the recrystallization of pure aluminium, Jensen and

* Corresponding author.

E-mail address: yasutaka.nishida@toshiba.co.jp (Y. Nishida).

Godiksen concluded that every single grain has its own kinetics different from the other grains by using 3-dimensional synchrotron X-ray diffraction microscopy [13]. Therefore, to overcome these problems, generalization of the KJMA theory has been developed by several researchers. Theoretically, Cahn [14] demonstrated time cone method to take account of the finite specimen situation analytically. Godiksen approached a continuous distribution of growth velocities using computer simulation [15]. Rios and Villa applied mathematical methods from stochastic geometry theory [16] and derived an analytical expression [17] beyond the original assumption of KJMA theory. In other previous studies, there are some direct computer simulations of phase transformation. Among them, popular approaches are a Cahn–Hilliard model [18], time-dependent Ginzburg–Landau theory [19] and the phase-field model [20–24].

As one way of extending of these early results of KJMA theory, Gokhale and Dehoff [25] and Vandermeer and coworkers [26–31] introduced the concept of the microstructural path method in order to characterize the kinetics of phase transformation. The microstructural path method was developed to describe the time evolution of microstructure during recrystallization, and the following parameters are defined as the microstructural path functions: the recrystallized volume fraction V_v , the interfacial area density between new grains and matrix S_v , and the mean free path of the new grains $\langle \lambda \rangle$. These microstructural path functions can be determined from planar sections using standard stereological techniques [31]. The microstructural method has been extensively used for recrystallized materials. Comparing the computer simulation with the experimental microstructural path functions, the kinetics of phase transformation such as growth rates may be investigated in more detail.

In this study, we used the multi-phase-field (MPF) method [32–34] proposed by Steinbach and Pezzolla [34] for revisiting the transformation kinetics. This method is an extended numerical method of the phase-field model [35,36]. The MPF method is attractive because it can take account of the grain impingement explicitly under the anisotropic grain growth as well as under the isotropic grain growth. Moreover, the microstructural path function proposed by Vandermeer et al. can be calculated in its framework. In this paper, a methodology to calculate the microstructural path functions in the framework of MPF method incorporating with a nucleation model is proposed, so that we can revisit the above-mentioned pioneering work of KJMA theory in detail. Our results suggest a new way to quantify the morphological characteristics of more complex transformation that are difficult to deduce from the conventional KJMA theory.

This paper is organized as follows: in Section 2, we review the MPF method and modeling of the transformation kinetics. In Section 3, we perform a test calculation to check the validity of numerical simulation. In Section 4, we present the results and discussion of our study of the phase transformation. Finally, we summarize the results in Section 5.

2. Multi-phase-field modeling

2.1. Multi-phase-field method

We briefly introduce the formulation of the multi-phase-field (MPF) method by Steinbach and Pezzolla [34]. The MPF method [32–34] is based on the phase-field (PF) method [35,36] that is typically applied to a dual-phase system such as a solid-liquid phase change. An extension of the phase-field method, the MPF method is applicable to a system consisting of many numbers of different grains (or phases) such as grain growth of a polycrystalline system. In this approach, an individual order parameter ϕ_i is

introduced to distinguish each grain, where ϕ_i indicates the probability of finding the i th grain at point \vec{r} and time t , so that the microstructural change of the system is described by the time evolution of each ϕ_i .

Here, we set a polycrystalline system Ω containing N grains. Then an individual ϕ_i is not independent and it must satisfy the following relation at the arbitrary point \vec{r} and in time t :

$$\sum_{i=1}^N \phi_i = 1. \quad (2)$$

The total free energy of the polycrystalline system G_{sys} is defined by

$$G_{\text{sys}} = \int_{\Omega} d\Omega \left\{ \sum_{i=1}^N \sum_{j=i+1}^N \left(-\frac{\varepsilon_{ij}^2}{2} \nabla \phi_i \nabla \phi_j + W_{ij} \phi_i \phi_j \right) + g_{\text{chem}} \right\}, \quad (3)$$

where ε_{ij} is the gradient coefficient, W_{ij} is the height of the energy barrier between grains i and j , and g_{chem} is the Gibbs free energy density in the grains. Assuming that G_{sys} decreases monotonically with time, the equation of the time evolution for ϕ_i is obtained by

$$\frac{\partial \phi_i}{\partial t} = - \sum_{j=1}^m \frac{M_{ij}^{\phi}}{m} \left(\frac{\delta G_{\text{sys}}}{\delta \phi_i} - \frac{\delta G_{\text{sys}}}{\delta \phi_j} \right), \quad (4)$$

$$m = \sum_{j=1}^N s_j, \quad (5)$$

where M_{ij}^{ϕ} is the phase field mobility, s_j is the step function that satisfies $s_j=1$ when $0 < \phi_j(\vec{r}, t) \leq 1$ and $s_j=0$ otherwise, and hence m is the number of locally coexisting grains. Substituting Eq. (3) into Eq. (4), we obtain the following equation:

$$\frac{\partial \phi_i}{\partial t} = \sum_{j=1}^m \frac{M_{ij}^{\phi}}{m} \left[\sum_{k=1}^m \left\{ \frac{1}{2} (\varepsilon_{jk}^2 - \varepsilon_{ik}^2) \nabla^2 \phi_k + (W_{jk} - W_{ik}) \phi_k \right\} - \left(\frac{\partial g_{\text{chem}}}{\partial \phi_i} - \frac{\partial g_{\text{chem}}}{\partial \phi_j} \right) \right]. \quad (6)$$

In Eq. (6), we assume that the partial derivative $\partial g_{\text{chem}} / \partial \phi_i$ satisfies the following relation:

$$\frac{\partial g_{\text{chem}}}{\partial \phi_i} - \frac{\partial g_{\text{chem}}}{\partial \phi_j} = -\frac{8}{\pi} \sqrt{\phi_i \phi_j} \Delta g_{ji}, \quad (7)$$

where $\Delta g_{ji} \equiv g_{\text{chem}}^j - g_{\text{chem}}^i$ is the difference in Gibbs free energy between i - j grains and $8/\pi$ is obtained from $\int_0^1 \sqrt{\phi_1 \phi_2} d\phi = \int_0^1 \sqrt{\phi(1-\phi)} d\phi = \pi/8$. As shown in Appendix A, the parameters included in Eq. (6) are related to the interfacial energy σ_{ij} , the interfacial thickness η_{ij} , and interface mobility μ_{ij} as follows:

$$M_{ij}^{\phi} = \frac{\pi^2 \mu_{ij}}{4\eta_{ij}}, \quad \varepsilon_{ij}^2 = \frac{8\eta_{ij} \sigma_{ij}}{\pi^2}, \quad W_{ij} = \frac{4\sigma_{ij}}{\eta_{ij}}. \quad (8)$$

By using (Eqs. (7)–(8)), we finally obtain the following equation:

$$\frac{\partial \phi_i}{\partial t} = \sum_{j=1}^m \frac{\mu_{ij}}{m} \left[\sum_{k=1}^m \left\{ (\sigma_{jk} - \sigma_{ik}) \nabla^2 \phi_k + (\sigma_{jk} - \sigma_{ik}) \frac{\pi^2}{\eta^2} \phi_k \right\} + \frac{2\pi}{\eta} \sqrt{\phi_i \phi_j} \Delta g_{ji} \right]. \quad (9)$$

Eq. (9) describes the time evolution of the phase field variables ϕ_i according to dissipative dynamics driven by the Gibbs free energy minimization, so that the time evolution of the microstructure change can be traced through the change of ϕ_i . In a 1-dimensional case where we assume that two grains locally coexist, i.e., $m=2$ $i=1, j=2$ and $\mu_{12}=\mu_{21}=\mu$, $\sigma_{12}=\sigma_{21}=\sigma$, $\eta_{12}=\eta_{21}=\eta$ and $\Delta g_{12} = -\Delta g_{21} = -\Delta g$ for simplicity, we obtain the particular solution, $\phi(x, t) = \phi_1(x, t) = 1 - \phi_2(x, t) = \frac{1}{2}[1 - \sin\{\pi/\eta(x - \mu \Delta g t)\}]$. This solution means that a smooth function of sine form at the grain boundary whose width is η , and it proceeds to the right on the x axis with the velocity $\mu \Delta g$.

Hereafter in this paper, we use a simple multi-phase-field model to simulate a phase transformation where new stable grains ϕ_i ($i \neq 1$)

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