Multi-Phase-Field Study for Pearlite Transformation with Grain Boundary Diffusion

Akinori Yamanaka[1], Takashi Yamamoto[2], Tomohiro Takaki[3], Yoshihiro Tomita[2]

[1]Graduate School of Science and Technology, Kobe University,
1-1, Rokkodai, Nada, Kobe, Hyogo, Japan, yamanaka@solid.mech.kobe-u.ac.jp;
[2]Graduate School of Engineering, Kobe University,
1-1, Rokkodai, Nada, Kobe, Hyogo, Japan;
[3]Graduate School of Science and Technology, Kyoto Institute of Technology,
Matsugasaki, Sakyo, Kyoto, Japan

ABSTRACT

In order to investigate the effect of grain boundary diffusion (GBD) of carbon on growth velocity of pearlitic microstructure, pearlitic transformation accompanying with the GBD in Fe-C-Mn alloy is simulated by multi-phase-field (MPF) method. The results show that the growth velocity of pearlite decreases with increasing lamellar spacing of pearlite, as suggested by numerical studies using the Zener-Hillert model and experimental studies. And, the present MPF simulation also reveals that the GBD considerably enhances carbon diffusion from ferrite (α) phase to cementite (θ) and assists cooperative growth of α phase and θ. From these results, it can be mentioned that the rate of the GBD largely governs the growth velocity of pearlite.

1. Introduction

Microstructure in steels consists of α phase, pearlite, bainite and martensite phase. In particular, pearlite exhibits lamellar structure of α phase and θ, and possesses good balance between strength and toughness. Therefore, pearlite is widely used as constituent phase in many steels such as ferrite-pearlite (FP) steel. Recently, authors have developed the integrated simulation model for predicting microstructure formation and mechanical properties of steel using the phase-field (PF) method and the homogenization method [1]. Using this model, the mechanical properties of the FP steel depending on the FP microstructure was clarified. However, in order to predict the mechanical properties of the FP steel precisely, morphology of pearlite is needed to be predicted in the PF simulation. For this issue, Steinbach et al. [2] and Nakajima et al. [3] proposed MPF models for the pearlitic transformation and simulated the formation of pearlitic microstructure based on the volume diffusion-controlled mechanism. However, many studies suggest that the GBD of carbon is an essential phenomenon controlling the pearlitic transformation [4]. Thus, the effects of the GBD should be considered in MPF simulation of the pearlitic transformation. Therefore, in this study, the pearlitic transformation is simulated by the MPF method considering both volume diffusion and the GBD of carbon. Furthermore, the role of the GBD on the growth of pearlite is investigated.

2. Multi-Phase-Field Model

In order to simulate the pearlitic transformation in Fe-C-Mn alloy, the generalized multi-phase-field (GMPF) method proposed by Steinbach et al. [5] is used. In the GMPF method, the system of N grains can be considered. Thus, we use N phase field variables, ϕ_i (i = 1, 2, … , N). ϕ_i describes volume fraction of the i th grain and varies smoothly across an interface from $\phi_i = 1$ in the i th grain to $\phi_i = 0$ in other grains. Hereafter, we consider a $\alpha + \gamma + \theta$ three-grain (phase) system for simple description. By using these phase field variables, the total Gibbs free energy of the system, G, is defined by the Ginzburg-Landau type Gibbs free energy functional,

$$G = \int_V \left\{ \sum_{i=1}^{3} \sum_{k=i+1}^{3} \left(-\frac{a_{ik}^2}{2} \nabla\phi_i \cdot \nabla\phi_k + W_{ik}\phi_i\phi_k \right) + g_e \right\} dV , \tag{1}$$

where a_{ij} and W_{ij} are the gradient coefficient and potential height, respectively. The evolution equation of the phase field variable is derived by assuming that the total free energy decreases monotonically with time.

$$\frac{\partial\phi_i}{\partial t} = -\sum_{j=1}^{n} \frac{2M^{\phi}}{n} \left[\sum_{k=1}^{n} \left\{ \left(W_{ik} - W_{jk}\right)\phi_k + \frac{1}{2}\left(a_{ik}^2 - a_{jk}^2\right)\nabla^2\phi_k \right\} - \frac{8}{\pi}\sqrt{\phi_i\phi_j}\,\Delta G_{ij} \right]. \tag{2}$$

Here, n is the number of phase fields in the arbitrary point and is given by $n = \sum_{i=1}^{3} \xi_i$. ξ_i is a step function, which is expressed as $\xi_i = 1$ in a region $0 < \phi_i < 1$ and $\xi_i = 0$ in other region. The third term on the right-hand side of Eqn. (2) is the phenomenological thermodynamic driving force and ΔG_{ij} is its magnitude. To simulate the carbon diffusion during the pearlite transformation in a multiphase system, the total carbon concentration C is defined as a linear function of the local carbon concentration C_{λ}^{i} and the phase-field variables ϕ_i. Therefore, when ϕ_1, ϕ_2 and ϕ_3 correspond to α, γ and θ phases, respectively, the total carbon concentration C is written as $C = \phi_1 C_{\alpha}^{1} + \phi_2 C_{\gamma}^{2} + \phi_3 C_{\theta}^{3}$. The evolution equation of the total carbon concentration C is expressed by the sum of diffusion fluxes of carbon, J_i, in individual grains as [6],

$$\frac{\partial C}{\partial t} = \nabla \cdot \left(\phi_1 J_1 + \phi_2 J_2 + \phi_3 J_3 \right) = \nabla \cdot \left\{ \phi_1 D_{\alpha}^{1} \nabla C_{\alpha}^{1} + \phi_2 D_{\gamma}^{2} \nabla C_{\gamma}^{2} + \phi_3 D_{\theta}^{3} \nabla C_{\theta}^{3} \right\}. \tag{3}$$

Here, D_{λ}^{i} denotes diffusion coefficient of carbon atoms in the i th grain (λ phase). The local concentration C_{λ}^{i} is related to the partition coefficient of carbon atoms k_{jr}. The partition coefficient k_{jr} and the driving force ΔG_{ij} are calculated with a linearized phase diagram [7].

3. Computational Model

The growth of a single pearlite lamellar during isothermal pearlitic transformation in Fe-C-Mn alloy is simulated in two-dimensions. Because the diffusion of manganese atoms is much slower

than that of carbon atoms, it is not considered. In this study, the effects of the lamellar spacing λ and the GBD on the growth of pearlite are investigated. When the effect of λ is studied, we use a rectangular computational domain. The size of computational domain along x direction DX, which corresponds to λ, is changed from 0.24 μm to 0.48 μm. And, when the effect of the GBD is studied, λ is set to be constant at 0.24 μm and a $DX \times DY = 0.24 \times 0.48$ μm^2 rectangular computational domain is used. The initial α phase and θ is set at the bottom of the computational domain. Temperature is set to be constant at $T_0 = 973$ K. The interfacial energy of all interfaces is assumed to be constant at 0.5 J/m^2. The initial carbon concentrations of both α phase and θ are in the equilibrium values. The governing equations, Eqns. (2) and (3), are solved by the finite difference method with periodic boundary condition for x direction and zero Neumann boundary condition for y direction. And, the GBD is described by considering k (k = 1, 2, 3, 4) times larger diffusion coefficient than that of bulk phase in the grain boundary region defined as $0 < \phi_i < 1$.

4. Results and Discussions

Figure 1 shows the evolution of carbon concentration field during the growth of pearlite for different λ. From these results, it can be confirmed that the growth velocity of pearlite V decreases with increasing λ, because the increase of λ promotes long diffusion distance of carbon atom from α phase to θ. This dependency of V upon λ is qualitatively identical with the numerical results obtained by the Zener-Hillert model and experiments [7].

Figure 2 shows the distribution of carbon concentration during the pearlitic transformation accompanying with the GBD. It is found that as the carbon partitioning from α phase into θ becomes fast by the GBD, V increases. In the case of k = 4, V equals to 3.0 μm/s. Furthermore, according to Ridley [8], λ and V satisfies the following relationship: λV^m = constant. Here, m is a constant taking the value of m = 2 ~ 3 in the range of the obtained V. Figure 3 shows the relationship between λ and V obtained by the present MFP simulation. It is clarified that the relationship, λV^m = constant, is also satisfied in the present study and the value of m becomes 1.2 ~ 1.4. Although m is smaller than the conventional values (m = 2 ~ 3), m tends to increase

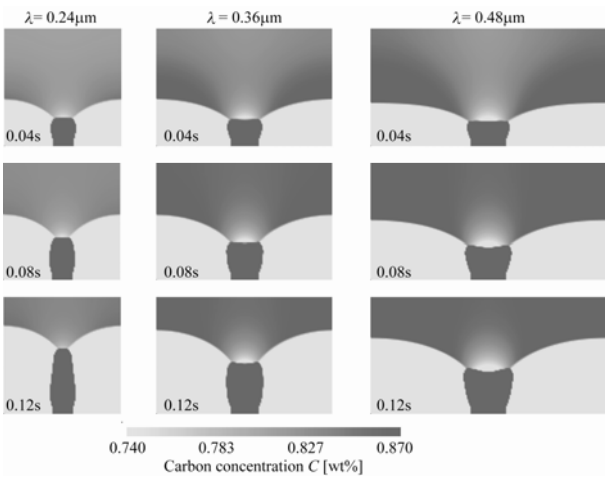

Figure 1. Distribution of carbon concentration during growth of pearlite for different λ.

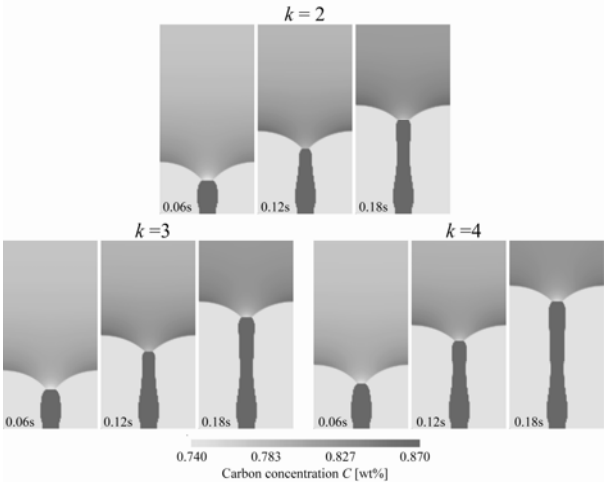

Figure 2. Distribution of carbon concentration during growth of pearlite with GBD.

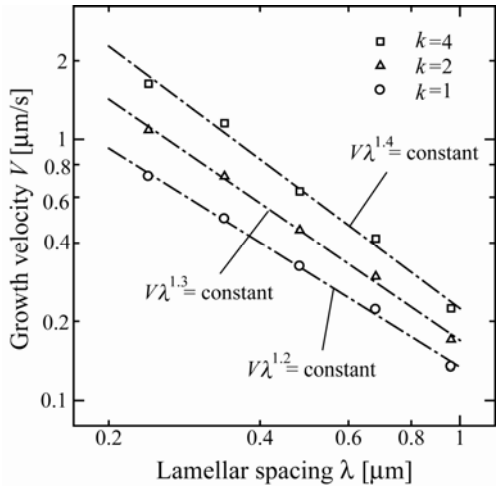

Figure 3. Relationship between lamellar spacing λ and growth velocity of pearlite V.

with increasing the rate of the GBD (the value of k). Therefore, it can be concluded that the growth of pearlite observed in real system can be simulated by considering quite fast GBD.

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