PHASE-FIELD SIMULATION OF ISOTHERMAL TRANSFORMATION IN Fe-C ALLOY

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ABSTRACT: Phase-field simulations of the isothermal austenite-to-ferrite transformation and the formation of Widmanstätten ferrite in Fe-C alloys are carried out. The effects of the strong anisotropy of interfacial properties on the formation and growth of Widmanstätten ferrite are studied by the regularized gradient coefficient method. The simulation results clarified that Widmanstätten ferrite plates develop due to morphological instability in the early stage of formation and that strong interface anisotropy is required for the formation of Widmanstätten ferrite from allotriomorph ferrite.

INTRODUCTION: The mechanical properties of steels are closely related to the morphology and composition of microstructures produced during the austenite to ferrite transformation. Therefore, it is essential to understand the transformation kinetics and the evolution of microstructures. In particular, the formation of plate or lath like ferrite by high supercooling, such as Widmanstätten ferrite, pearlite and bainite, has been the subject of many studies. However, since the transformation involves a complex competition between interface migration and fast solute diffusion, the formation processes of the microstructures are difficult to investigate only by experiments. In this study, we employ the phase-field model of the transformation in Fe-C alloys and the regularized gradient coefficient method in order to introduce strong interface anisotropy. We clarify the effects of interfacial properties on the formation and growth mechanism of Widmanstätten ferrite through phase-field simulations.

PHASE-FIELD METHOD: The total free energy of Fe-C alloy is defined by the Gibbs free energy functional [Loginova, I. *et al*, 2001]

$$G = \int_V \left\{ g(\phi, u_C, T) + \frac{\varepsilon(\theta)^2}{2} |\nabla\phi|^2 \right\} dV \qquad (1)$$

where ϕ is the phase field taking a value of $\phi = 1$ in ferrite and $\phi = 0$ in austenite. Temperature T is assumed to be constant due to isothermal transformation and u_C is the carbon concentration related to the sub lattice carbon concentration y_C as $y_C = (a/c)u_C$. Here, *a* and *c* are the site numbers of sub-lattice position per Fe atom position defined as

$a = c = 1$ in austenite and $a = 1$, $c = 3$ in ferrite, respectively. The chemical free energy density of Fe-C alloy $g(\phi, u_C, T)$ is postulated to be a function of the phase field, carbon concentration and temperature.

$$g(\phi, u_C, T) = p(\phi)g^\alpha(u_C, T) + \{1 - p(\phi)\}g^\gamma(u_C, T) + Wq(\theta) \qquad (2)$$

Here, $g^\alpha(\phi, u_C, T)$ and $g^\gamma(\phi, u_C, T)$ are the chemical free energy density of pure ferrite and pure austenite phases, respectively. $p(\phi)$ and $q(\phi)$ are the energy density function and double-well potential function, respectively. W is the potential height related to the interfacial energy σ and interface thickness δ by $W = 6\sigma b/\delta$. We assume that the interface region is $\lambda \leqq \phi \leqq 1-\lambda$ and $b = 2\tanh^{-1}(1-2\lambda)$ [Takaki, T. *et al*, 2005].

We assume the interface anisotropy is caused by anisotropic interfacial energy σ and adopt the gradient energy coefficient $\varepsilon(\theta)$ by the following equation:

$$\varepsilon(\theta) = \sqrt{\frac{3\sigma\delta}{b}}\{1 + \gamma\cos k(\theta - \theta_0)\} \equiv \bar{\varepsilon}(\theta) \qquad (3)$$

where γ is the strength of anisotropy, k is the mode number of anisotropy, and θ is defined as the angle between the interface normal and the x-axis. When we introduce strong anisotropy such as $\gamma \geq 1/(k^2 - 1)$, the equilibrium shape cannot be provided in the range of $2\pi i/k - \theta_m \leq \theta - \theta_0 \leq 2\pi i/k + \theta_m$, where θ_m is the first missing orientation. In order to consider such strong anisotropy and provide the equilibrium shape, we employ the following regularized gradient coefficient for missing orientations [Takaki, T. *et al*, 2006]

$$\varepsilon(\theta) = \frac{\bar{\varepsilon}(\theta_m + \theta_0)}{\cos\theta_m}\cos(\theta - \theta_0) \qquad (4)$$

Considering that the total Gibbs free energy G decreases monotonically with time, the time evolutions of the phase-field ϕ and carbon concentration u_c are governed by the Allen-Cahn equation and the Cahn-Hilliard equation, respectively:

$$\frac{\partial\phi}{\partial t} = M_\phi\left\{\nabla\cdot\left(\varepsilon(\theta)^2\nabla\phi\right) - \frac{\partial g}{\partial\phi} - \frac{\partial}{\partial x}\left(\varepsilon(\theta)\frac{\partial\varepsilon(\theta)}{\partial\theta}\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial y}\left(\varepsilon(\theta)\frac{\partial\varepsilon(\theta)}{\partial\theta}\frac{\partial\phi}{\partial x}\right)\right\} \qquad (5)$$

$$\frac{\partial u_C}{\partial t} = \nabla\cdot\left\{D_C(\phi, u_C, T)\left(\frac{\partial^2 g}{\partial u_C^2}\nabla u_C + \frac{\partial^2 g}{\partial u_C\partial\phi}\nabla\phi\right)\right\} \qquad (6)$$

where M_ϕ is the mobility of the phase field related to the mobility of the α/γ interface M and the interface thickness δ as $M_\phi = Mb/3\delta$. $D_C(\phi, u_C, T)$ is the diffusion coefficient of carbon atoms in the Fe-C alloy and is related to the carbon concentration, vacant sub lattice concentration y_v and mobility of carbon atoms in Fe-C alloy Mc, as $D_C = u_C y_v M_C$. In numerical simulations, Eqns.(5) and (6) are solved by the Crank-Nicolson centered finite difference method for time and the adaptive finite element method for space [Takaki, T. *et al*, 2005].

COMPUTATIONAL MODEL AND RESULTS: Figure 1 shows the computational model and initial conditions. Allotriomorph ferrite is set at the bottom of the computational domain and the interface is disturbed by a combination of sinusoidal curves. Temperature is set to be constant at T =1000K. In order to simulate the formation and growth processes of Widmanstätten ferrite, the mode number of anisotropy $k = 2$ and the growth direction $\theta_0 = 60$ degrees are adopted. Figure 2 and Figure 3 show the time evolutions of ferrite and the distribution of carbon concentration with interfacial energy σ =1.0 J/m^2 for γ=0.3 and γ=0.4, respectively. Although the ferrite phase grows into the austenite matrix with carbon diffusion in both cases, Widmanstätten ferrite is not formed in the case of γ=0.3 due to the low strength of anisotropy. On the other hand, the growth process of Widmanstätten ferrite from allotriomorph ferrite is observed for γ=0.4. At the early stage of the growth, initial tips of plate like ferrite are formed on the α / γ interface. Widmanstätten ferrite plates develop competitively after the coalescence of plate tips. These results clarified that in the early stage of formation, the Widmanstätten ferrite is formed from allotriomorph ferrite due to morphological instability and strong interface anisotropy is required for this growth process.
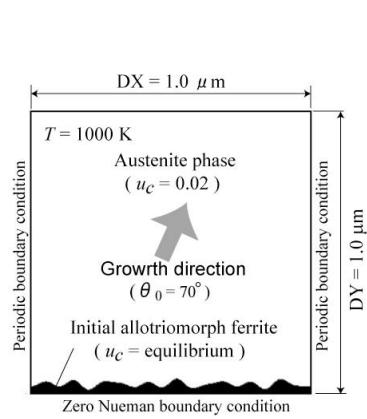

Fig.1. Computational Model and Initial Conditions.
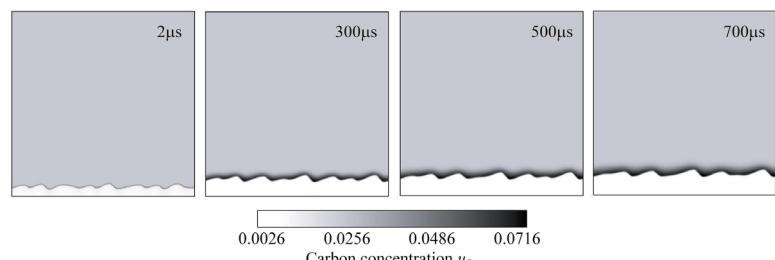
Fig.2. Growth of Allotriomorph Ferrite with $\gamma = 0.3$.
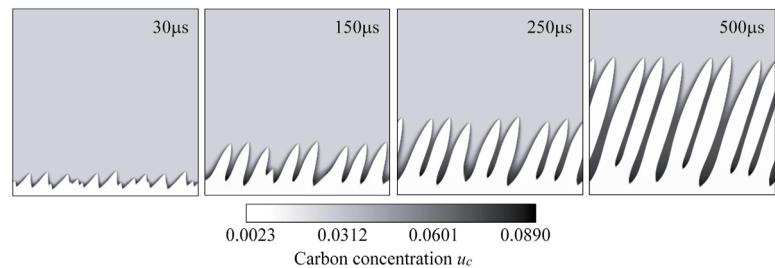
Fig.3. Formation of Widmanstätten Ferrite Plates with $\gamma = 0.4$.

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