Phase-field Analysis of Austenite to Ferrite Transformation and Partitioning of Carbon in Fe-C Alloy

A. Yamanaka¹, T. Takaki², Y. Tomita¹

Summary

Phase field simulations during the austenite-to-ferrite transformation of Fe-C alloy are performed to analyze the partitioning of carbon from a supersaturated plate of ferrite. The results demonstrate that the carbon buildup at the interface suppresses the interface velocity due to the reduction of the chemical driving force for the transformation, and the composition on both sides of the interface approaches their equilibrium state.

Introduction

In tempered martensitic steels and bainitic steels (if bainitic ferrite grows with full or partial supersaturation of carbon [1]), the behavior of carbon diffusion seems to determine the microstructure and the kinetics of transformation in steels. Therefore, it is important to understand the partitioning of carbon from supersaturated plates of ferrite to retain austenite. Although numerous studies of partitioning concepts have been carried out for several decades, a consensus has not yet been achieved [2] [3]. In this paper, to investigate both the partitioning of carbon from supersaturated ferrite and interface migration, we employ the phase-field method.

Phase-field model

The total free energy of Fe-C alloy is expressed by the Gibbs free energy functional:

\[ G = \int \left[ g(\phi, y_c, T) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right] dV \]  

(1)

where \( \phi \) is the phase field taking \( \phi = 1 \) in ferrite and smoothly changing to \( \phi = 0 \) in austenite, the temperature \( T \) is assumed to be constant due to isothermal transformation, and \( y_c \) is related to the normal fraction of carbon \( x_c \), i.e., \( y_c = x_c/(1-x_c) \). The Gibbs free energy density of the alloy \( g(\phi, y_c, T) \) is postulated as a function of the phase field variable, concentration, and temperature.

\[ g(\phi, y_c, T) = p(\phi)g^\alpha(y_c, T) + (1-p(\phi))g^\prime(y_c, T) + W(\phi) \]  

(2)

¹ Graduate School of Science and Technology, Kobe University, Nada, Kobe, 657-8501, Japan
² Department of Marine Engineering, Kobe University, Higashinada, Kobe, 658-0022, Japan
where $g^w(y_c, T)$ and $g^f(y_c, T)$ are the Gibbs free energy of ferrite and austenite, respectively. $p(\phi) = \phi^2(10 - 15\phi + 6\phi^2)$ is a monotonically increasing function that satisfies $p(0) = 0$, $p(1) = 1$, and $dp(\phi)/d\phi = 30\phi^2(1-\phi)^2$. $q(\phi) = \phi^2(1-\phi)^2$ is the double-well potential. $W$ and $\varepsilon$ are the well height and kinetic parameter, respectively, and related to the surface energy $\sigma$ and the interface thickness $\delta$ by the means of $W = 6\sigma b / \delta$ and $\varepsilon^2 = 3\sigma\delta / b$. Assuming that the interface region is $\lambda < \phi < 1 - \lambda$, we obtain $b = 2\tanh^{-1}(1 - 2\lambda)$ [4].

The evolution of the phase field is governed by the Cahn-Allen equation, and Eqs. (1) and (2) give the phase field equation.

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\partial G}{\partial \phi} = M_\phi \left[ \varepsilon^2 \nabla^2 \phi + 4W \phi (1-\phi) \left\{ \frac{15}{2W} \phi (1-\phi) \Delta g^m + \phi - \frac{1}{2} \right\} \right]$$

where $\Delta g^m$ is the free energy change accompanying the austenite-to-ferrite transformation. $M_\phi$ is the kinetic parameter related to the interfacial mobility $M$ and the interfacial thickness $\delta$, i.e., $M_\phi = bM / 3\delta$ [5].

The equation describing the evolution of concentration is developed from the mass conservation equation. Assuming the molar volume of substitutional atoms $v_m$ to be constant, the normal diffusion equation can be written as

$$\frac{1}{v_m} \frac{\partial y_c}{\partial t} = -\nabla \cdot J$$

where the diffusional flux $J$ is assumed proportional to the gradient of the variational derivative of $G$ with respect to $y_c$. Considering Eqs. (1) and (2), we obtain

$$J = -Lv_m \nabla \left( \frac{\partial G}{\partial y_c} \right) = -Lv_m \frac{\partial^2 g}{\partial y_c^2} \nabla y_c - Lv_m \frac{\partial^2 g}{\partial y_c \partial \phi} \nabla \phi$$

where the first and second terms correspond to the normal Fick’s law and Darken’s thermodynamic factor, respectively. The kinetic parameter $L$ is related to the diffusional mobility $M_C$, i.e., $L = y_c y_v M_C / v_m$ [6]. $y_v$ is the fraction of vacant interstitials represented as $1 - y_v / 3$ for ferrite and $1 - y_v$ for austenite. If $y_v$ depends on the phase field variable, it
is represented as \( y_c = p(\phi)(1 - y_c/3) + (1 - p(\phi))(1 - y_c) \). The diffusional mobility in two phases could differ by several orders of magnitude, so \( M_c \) is postulated to be a function of phase field as follows [5]:

\[
M_c = \left( M_c^a \right)^{\gamma(\phi)} \left( M_c^p \right)^{1-\gamma(\phi)}
\]

(6)

where \( M_c^a \) and \( M_c^p \) are the mobilities of ferrite and austenite, respectively. Combining Eqs. (4)~(6) gives the diffusion equation

\[
\frac{\partial y_c}{\partial t} = \nabla \cdot \left[ L'(\phi, y_c, T) \left( \frac{\partial^2 g}{\partial y_c^2} \nabla y_c + \frac{\partial^2 g}{\partial y_c \partial \phi} \nabla \phi \right) \right],
\]

(7)

\[
L'(\phi, y_c, T) = v_m y_c \left[ p(\phi) \left( 1 - y_c/3 \right) + (1 - p(\phi))(1 - y_c) \right] \left( M_c^a \right)^{\gamma(\phi)} \left( M_c^p \right)^{1-\gamma(\phi)}
\]

Numerical simulation

In the present study, Eqs. (3) and (7) are solved on a one-dimensional uniform grid using a second-order central in space, and a first-order forward in time-finite difference approximations to the derivative. Zero Neumann boundary conditions are applied to both variables. The initial state of the system is shown in Fig.1. As mentioned previously, we have studied the partitioning process of carbon from a supersaturated ferrite during the isothermal transformation. The ferrite plate of its half-thickness \( h \) is placed on the left side of the system. The phase field is initially set as 1 in ferrite phase and 0 in austenite phase, and varied smoothly over the interface region. The initial distribution of carbon concentration is set as uniform in the computational domain, i.e., \( y_c^0 = y_c^i = y_c \). The temperature is assumed constant all over the whole system, i.e., \( T = 673K \). We perform simulations at a number of carbon supersaturations. Here, the carbon supersaturation \( \Omega \) is denoted as

\[
\Omega = \frac{y_c^{\alpha} - y_c}{y_c^{\alpha} - y_c^{\alpha^i}}
\]

where \( y_c^{\alpha^i} \) and \( y_c^{\alpha^a} \) are the equilibrium compositions of ferrite and austenite, respectively, and can be determined by constructing a tangent common to both the free-energy curve, i.e., \( g^a(y_c, T) \) and \( g^i(y_c, T) \). In this study, \( y_c^{\alpha^i} = 0.001 \) and \( y_c^{\alpha^a} = 0.195 \).
To perform quantitative evaluations in phase-field analysis, the selected interface thickness $\delta$ should be physically realistic values that are in the regime of 0.5-1.5 nm [5]. In the present study, we chose an interface thickness $\delta$ of 1.0 nm. In the interfacial region, the concentration gradients were too large that we applied $\delta$ to eight grids, i.e., $\delta=8dx$.

The physical data, namely, the phase-field parameters mentioned above, are as follows [5] [6]: $\sigma=1.0$ J/m$^2$, $v_m=7.0\times10^{-6}$ m$^3$/mol, $e=3.695\times10^{-5}$ (J/m)$^{0.5}$, $W=1.318\times10^{10}$ J/m$^3$, $M_\phi=9.709\times10^{-5}$ m$^3$/Js, $DX=0.25$ µm, $dx=1.25\times10^{-4}$ µm, and $dt=0.01$ µs.

**Results and Discussion**

The partitioning processes of carbon from supersaturated ferrite with 0.1 µm thick (i.e., $h=0.1\mu$m) were simulated for various carbon supersaturations. In this paper, we show the results only at three different supersaturations, i.e., at $\Omega=0.95$, 0.90, and 0.85, the corresponding mole fractions of carbon $y_c$ are 0.01, 0.02, and 0.03, respectively.

Figure 2(a) presents the profile of carbon evolved with time at $\Omega=0.90$. The ferrite-austenite interface migrates accompanying the partition of excess carbon from ferrite into austenite. Because the solubility of carbon is much greater in austenite and carbon diffusion in ferrite is much faster than that in austenite, carbons in ferrite escaped to austenite on the order of a few milliseconds. However, in austenite, the carbon that escaped from ferrite is piled up ahead of the interface, and a pile of excess carbons develops during interface migration.

The time variations in interface ($\phi=0.5$) velocity are shown in Fig.2(b). The decrease in $\Omega$ (the increase in the initial carbon concentration in the alloy) causes a higher amount of excess carbon to partition from ferrite to austenite and the carbon concentration at the austenite side to increase. Consequently, the interface velocity decreases with decreasing

![Fig.1 Computational model and initial conditions.](image)
carbon supersaturation because the chemical driving force for the transformation decreases. The carbon concentration profiles at 0.02s in $\Omega=0.95$, 0.90, and 0.85 are presented in Fig.3(a). The decrease in $\Omega$ suppresses the migration of the interface, and as the interface migration is suppressed, the carbon concentration at the ferrite-austenite interface gradually approaches the equilibrium.

Fig.2 Partitioning of carbon and its effect on interface velocity. (a) Profiles of carbon evolved with time at $\Omega=0.90$. The corresponding times are 0.0001 s, 0.005 s, 0.015 s, and 0.03 s. (b) Time variations in interface velocity at $\Omega=0.95$, 0.90, and 0.85.

Fig.3 Influence of supersaturation on carbon partitioning. (a) Carbon concentration profiles at 0.02 s. (b) Time variations in carbon concentration at the center of the ferrite plate at $\Omega=0.95$, 0.90, and 0.85.
Figure 3(b) shows the time variation in carbon concentration at the center of the plate of ferrite in which cementite is likely to form. At all degrees of supersaturation, the concentration rapidly decreases to about 0.025 at 0.03s. Cementite formation would be evaluated accurately by comparing the time required to reject excess carbon from supersaturated ferrite with the time required for cementite precipitation [1].

Conclusions

In the present study, it is confirmed by phase field analysis that the ferrite-austenite interface migrates with the partitioning of carbon, raising the stability of austenite in the interface region and reducing the interface velocity due to a decrease in the chemical driving force required for transformation. The carbon concentration at the interface approaches the equilibrium level as the interface velocity decreases. Simulations in a two-dimensional geometry will enable us to describe bainitic ferrite formation.

Reference


