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The study of Widmanstätten ferrite in Fe–C alloys by a phase field model coupled with anisotropic elasticity

Li Zhang [a], Yao Shen [a, *], Haibo Wan [a, b], Xiaochuan Xiong [c], Lanting Zhang [a]

[a] China State Key Lab of Metal Matrix Composites, School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
[b] Shanghai Power Equipment Research Institute, Shanghai 200240, China
[c] General Motors Global Research & Development, China Science Laboratory, Shanghai 201206, China

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ABSTRACT

A phase field model accounting for anisotropic elastic energy has been formulated to investigate the morphology and growth kinetics of a Widmanstätten microstructure during the isothermal austenite to ferrite transformation in binary Fe–C. Physically realistic parameters are employed, for which the thermodynamic functions and the diffusional mobilities are from the literatures that were assessed via the Calphad technique and from experimental results respectively. The simulation results suggest that the anisotropy of elastic energy, resulting from the lattice distortion between the ferrite precipitate and the austenite matrix in the phase transformation, is sufficient to generate a plate-like Widmanstätten structure. The growth of the ferrite precipitate follows completely different dynamic laws in different directions, i.e., parabolic thickening in the direction of the plate thickness and linear lengthening in the direction toward the plate tip. The chief reason for the former is that the moving of the plate broad sides may be regarded as a migration of straight interfaces in the diffusion-controlled phase transformation; the latter is because that the plate tip can maintain a constant radius of curvature during the phase transition after a transient initial stage. Furthermore, the aspect ratio and the lengthening rate of the Widmanstätten ferrite plate simulated by our analyses are in good agreement with the experimental observations.

1. Introduction

The FCC-austenite (γ) to BCC-ferrite (α) transformation upon cooling is one of the most important microstructure transitions in physical metallurgy. The grain size and morphology of the α precipitate have a great effect on the mechanical properties of steels. Based on its technological importance and theoretical significance, the $\gamma \rightarrow \alpha$ transformation has been widely studied [1,2]. Different morphologies of ferrite might be produced during heat treatments, such as grain boundary allotriomorphic ferrite, intragranular ferrite idiomorph, acicular ferrite and plate-like Widmanstätten ferrite. In particular, Widmanstätten ferrite, which is often observed at temperatures between Ae_3 and Ae_1, has a significant influence on the mechanical performance of steels, especially the toughness. Therefore, numerous research studies have been performed to probe its formation mechanism and growth kinetics [3,4].

In fact, the $\gamma \rightarrow \alpha$ transformation is a very complicated process that is accompanied by a competition between phase interface migration and solute atom diffusion. Hence, it is difficult to clearly investigate the formation of Widmanstätten ferrite by experimental methods alone. There are many theoretical treatments for the lengthening of Widmanstätten ferrite plates based on the diffusion-controlled scheme, such as the Ivantsov model [5], Zener–Hillert model [6], Trivedi model [7], Enomoto model [8] and Townsend–Kirkaldy model [9]. These analytical solutions seem capable of providing good agreement with the experimentally observed growth rates when the effect of capillarity of the plate tip is taken into account. However, various assumptions have been proposed in these models in order to conveniently solve the diffusional problem with a migrating interface, such as the local equilibrium (LE) condition of the concentrations at the interface and the use of a parabolic cylinder or a ledge for depiction of the plate-like shape. As a consequence, these models are only suitable for investigating simple morphologies in low-dimensional spaces, and analyses of complicated microstructure evolutions in 2D or 3D require other more sophisticated tools.

* Corresponding author.
E-mail address: yaoshen@sjtu.edu.cn (Y. Shen).

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Over the past two decades, phase field modeling (PFM) has been a powerful framework for studying microstructure evolutions in phase transformations, such as solidification [10,11], solid-state transformation [12,13], crystallization [14], etc. The fundamental idea is to use continuum field variables ϕ_i to identify the nature of the phase, the presence of an interface, the local chemical composition or the strain. The evolution of the microstructure is represented by the temporal evolution of the field variables ϕ_i driven by the reduction in the free energy of the system. The significant computational advantage of this method is that it avoids explicit tracking and setting up rules of evolution for the interfaces [15].

A few PFMs that couple with the anisotropic interfacial energy have been developed for studying the austenite to Widmanstätten ferrite transformation in Fe–C [16–18]. They successfully investigated the evolution of Widmanstätten plates under the influences of the anisotropy of interfacial energy and the degrees of undercooling and supersaturation. As discussed in their papers, the plate-like Widmanstätten structure would only develop if the interfacial energy is very highly anisotropic, i.e., the interfacial energy at the tip position is approximately 5 times as large as that on the broad sides ($\sigma_{(010)}/\sigma_{(100)} \approx 5$). However, such high anisotropy is a lack of experimental evidence in a realistic Fe–C alloy. Qin et al. [19] suggested that the ratio of the maximum value to the minimum one of the interfacial anisotropy in cubic crystals is typically 1–2 by applying the embedded-atom method. Hence, the anisotropy of interfacial property may not be the most relevant factor for determining the morphology and growth kinetics of the Widmanstätten structure, and other sources of anisotropy might need to be taken into consideration.

Indeed, the anisotropy of elastic strain energy plays an important role in the morphology of product precipitates [20], where the elasticity at interfaces between two solid phases results from the mismatch of lattice parameters between the product precipitates and the parent matrix. This is supported by the relevant example that anisotropic and inhomogeneous elasticity has been observed to greatly change the equilibrium shape of precipitates in Ni-based alloys [21]. More recently, Cottura et al. [22] built a phase field model that coupled with the anisotropic elasticity for the growth of the Widmanstätten structure, and their qualitative simulations suggested that the elastic anisotropy is enough to engender plate-like microstructures growing at a stationary rate. As the lattice parameters of austenite and ferrite in a binary Fe–C alloy are obviously distinct, the optimal growth directions would be affected by the elastic energy during the processes of nucleation and growth of Widmanstätten ferrite precipitates.

In the present study, the roles of the anisotropic elasticity during the austenite to Widmanstätten ferrite transformation in binary Fe–C are investigated. We extend the phase field model proposed by Cottura [22], where the realistic thermodynamic functions and diffusional mobilities are applied, including the Gibbs free energy function, lattice parameter, elastic moduli and diffusional mobility. In particular, the processes of the nucleation and growth of Widmanstätten ferrite and the evolution kinetics in different directions are analyzed, and various quantitative comparisons with experimental observations are implemented.

2. Phase field model

In this section, a phase field model that couples with elasticity for the austenite to Widmanstätten-ferrite transformation in a binary Fe–C alloy is derived.

2.1. Free energy functional

The total free energy is the summation of chemical free energy and elastic strain energy as:

$$F = F_{ch}(u_C, \phi, \nabla\phi) + F_{el}\left(\phi, \underset{\sim}{\varepsilon}\right) \tag{1}$$

where the u-fraction is defined as $u_C = x_C/(1 - x_C)$ with the carbon normal mole fraction x_C [16], ϕ is the phase field variable taken as 1 in ferrite and 0 in austenite and $\underset{\sim}{\varepsilon}$ is the strain field. The chemical free energy can be written as:

$$F_{ch}(u_C, \phi, \nabla\phi) = \int_V \left[\frac{G_m(u_C, \phi)}{V_m} + wg(\phi) + \frac{\lambda}{2}|\nabla\phi|^2\right] dV \tag{2}$$

where V_m is the molar volume of substitutional atoms and assumed to be constant. $G_m(u_C, \phi) = p(\phi)G_m^{\alpha}(u_C) + [1 - p(\phi)]G_m^{\gamma}(u_C)$ represents the Gibbs energy, where G_m^{α} and G_m^{γ} denote the normal Gibbs energy of α and γ and are taken from the assessments of Gustafson based on a Calphad type of thermodynamical description [23,24]. $p(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$ is the interpolation function, which should satisfy the following requirements: it is a monotonic function in [0, 1] with $p(0) = 0$ and $p(1) = 1$, and the chemical free energy density should have two minima in the two bulk phases as $\partial p(\phi)/\partial\phi|_{\phi=0,1} = 0$. $g(\phi) = \phi^2(1 - \phi)^2$ is the double-well potential function, which guarantees that the free energy density has two local minima at $\phi = 0$ and $\phi = 1$. w is a coefficient reflecting the energy barrier height between the two minima, λ is an interfacial energy coefficient and these two parameters are analytically related to two physical quantities, the interfacial energy $\sigma = \sqrt{\lambda w/18}$ and the interface thickness $\delta = \sqrt{\lambda/w}$ [19].

Based on the linear elasticity, the elastic strain energy is given by Ref. [25]:

$$F_{el}\left(\phi, \underset{\sim}{\varepsilon}\right) = \frac{1}{2}\int_V \sigma_{ij}\varepsilon_{ij}^{el} dV = \frac{1}{2}\int_V C_{ijkl}\varepsilon_{kl}^{el}\varepsilon_{ij}^{el} dV \tag{3}$$

where the elastic strain is the difference between the total strain, $\varepsilon_{ij}^{tot}(\vec{r})$, and the stress-free strain, $\varepsilon_{ij}^{0}(\vec{r})$:

$$\begin{aligned}\varepsilon_{ij}^{el}(\vec{r}) &= \varepsilon_{ij}^{tot}(\vec{r}) - \varepsilon_{ij}^{0}(\vec{r}) \\ &= \frac{1}{2}\left(\frac{\partial u_i(\vec{r})}{\partial r_j} + \frac{\partial u_j(\vec{r})}{\partial r_i}\right) - p(\phi)\varepsilon_{ij}^{00}\end{aligned} \tag{4}$$

where ε_{ij}^{00} is the eigenstrain corresponding to the precipitate of the α phase. Eigenstrain, which is also known as stress-free transformation strain (SFTS), represents the strain that occurs inside the material in the absence of external constraints during phase transitions. For the Fe–C system, three non-coplanar vectors are chosen as the axes of a reference coordinate, $x_1 : [100]_{\gamma}\left\|[110]_{\alpha}\right.$, $x_2 : [010]_{\gamma}\left\|[\bar{1}10]_{\alpha}\right.$ and $x_3 : [001]_{\gamma}\left\|[001]_{\alpha}\right.$. The lattice correspondences (LC) between the α and γ phases based on the Bain orientation relationship in both three and two dimensions are shown in Fig. 1a and b, respectively. The calculated eigenstrain tensors and other physical parameters used for calculations are presented in Table 1 [26].

2.2. Evolution equations

The governing equations based on the Cahn–Hilliard (CH) [27] and Allen–Cahn (AC) [28] kinetic equations are deduced. The