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Phase-field modeling of Widmanstätten ferrite formation during isothermal transformation in low carbon steels

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ABSTRACT

The simulation of Widmanstätten ferrite formation, developing from grain-boundary ferrite allotriomorphs during the isothermal austenite to ferrite transformation in binary Fe–C alloys, has been realized using Loginova and KKS phase-field models. It was found that the KKS model can quantitatively predict the transformation kinetics at a larger interfacial thickness comparing with the Loginova model. The plate spacing predicted by the KKS model is more comparable with the experimental result. Both models show that lengthening rates of plates increase linearly with increasing interfacial thickness. The simulation results demonstrate that the formation of Widmanstätten ferrite plates with realistic morphologies requires high anisotropy of interface energy. The increased strength of anisotropy causes a higher lengthening rate of Widmanstätten ferrite plate. A large interfacial energy leads to a high growth velocity of broad sides of Widmanstätten ferrite plate. The disappearance of some plates and the coalescence of two adjacent plates coarsen plate spacing, which is in good agreement with the experimental observation. The lengthening rate increases and the plate spacing decreases with increasing degree of undercooling. As the supersaturation is increased the plate lengthening rate is obviously improved and the spacing of ferrite group is refined.

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1. Introduction

Over the past decades, the austenite–ferrite transformation in steels has attracted lots of interest due to its technological relevance in controlling and tailoring steel properties. Different morphologies of ferrite can be obtained by controlling processing parameters of heat treatment. An interesting and important one is Widmanstätten ferrite. Widmanstätten ferrite often forms within appropriate ranges of temperature and composition and is seriously detrimental to the ductility of steels, so the formation mechanism of Widmanstätten ferrite draws considerable attention during the past decades. Many experiments [1–5] and phenomenological models [6–9] have been performed to investigate the formation mechanism and/or growth kinetics of Widmanstätten ferrite.

Based on thermodynamic calculations, there are various theoretical treatments for the diffusion-controlled lengthening of Widmanstätten ferrite plates during precipitation from a supersaturated solid solution. Zener [9] proposed the Gibbs–Thomson equation to analyze the growth dynamics of a precipitated plate and came up with a critical radius below which the tip cannot grow and a radius at which the tip grows with the maximum growth velocity. Hillert et al. [10] found that Ivantsov model [11] can perfectly predict the dramatic increase of growth velocity of the plate, while it ignores the effect of tip capillarity. Considering both the interface kinetics and the surface tension, Trivedi's theory [8] gives the best account of lengthening rates of Widmanstätten ferrite plates. The primary Widmanstätten ferrite directly grows from the austenite grain boundary, whereas the secondary Widmanstätten ferrite develops from ferrite allotriomorphs which already exist in the microstructure. For the transition from allotriomorphic to plate-like growth different viewpoints have been proposed. Townsend and Kirkaldy [1] developed a theory which combined the Zener–Hillert equation with the perturbation theory of Mullins and Sekerka [12] to explain various characteristics of Widmanstätten ferrite formation, such as the interplate spacing and the lengthening rate. Assuming the plate tip consisting of a pair of ledges, Enomoto [13] demonstrated that the reported lengthening kinetics of ferrite plates can be well explained by the diffusion-controlled motion of these ledges. Aaronson et al. [14] suggested that Widmanstätten ferrite forms atop the grain boundary allotriomorph through an edge-to-face sympathetic nucleation process, which is supported by the experimental evidence obtained in low carbon steels [15].

Actually, the formation of Widmanstätten microstructure is a very complicated process which is closely related to physical

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properties of the interface and the solute diffusion. Therefore, clear understanding of the evolution process of such a microstructure is difficult only by analytical or experimental method. In recent years, it is possible to investigate the complex microstructure evolution in time and space due to the convenience of the numerical calculation. Thus, the computer simulation is helpful in studying the growth dynamics of Widmanstätten ferrite and revealing its formation mechanism. As one of numerical approaches to address microstructure formations, the phase-field modeling has recently emerged as a powerful computational approach to modeling and predicting arbitrarily morphological and complex microstructure evolution in materials, such as solidification [16–20], solid–solid phase transformations [21–23], crystal nucleation [24], grain growth [25,26] and thin film growth [27]. An important advantage of the phase-field method is that, due to the diffuse-interface description, there is no need to track the interfaces during microstructure evolution. Therefore, evolution of complex grain morphologies can be predicted without any prior assumptions on the shape of the grains.

Few studies show the application of the phase-field model in simulating the austenite–Widmanstätten ferrite transformation. Loginova et al. [28] investigated the growth of Widmanstätten plates emanating from an austenite grain boundary in a Fe–0.22 wt% C alloy by developing a phase-field model which is called "Loginova model" in the present work. They introduced a highly anisotropic function related to the anisotropy strength of the interfacial energy and interface thickness. The results demonstrated that Widmanstätten plates would only develop if the anisotropy strength is larger than the critical value. More recently, Yamanaka et al. [29] proposed an alternative anisotropy function by employing the regularized gradient energy coefficient. The distribution of Widmanstätten plates depends on the initial shape of allotriomorph ferrite and the morphology is in good agreement with metallographic observations. However, the simulation based on the Loginova model always predicts faster kinetics of Widmanstätten ferrite formation than experimental results. For quantitative computations, Kim et al. [30] proposed the "KKS model" with a thin interface thickness which could enlarge the simulation domain to a large dimension. Although the interface thickness should be smaller than the characteristic length of the solute diffusion field as well as the radius of interface curvature, this restriction in the KKS model can be less severe than that in the Loginova model [31]. The KKS model has been applied to provide quantitative insight into the dendrite formation in solidification [32]. To the best of our knowledge, however, there are no related reports about whether this model could be used to quantitatively predict the formation of Widmanstätten ferrite in steels.

In the present study, we used Loginova and KKS models to simulate the growth of Widmanstätten ferrite from allotriomorph ferrite with perturbed interface during isothermal austenite–ferrite transformation. We first studied the effects of the interface thickness, amplitude of anisotropy and interfacial energy on the growth of Widmanstätten ferrite group. Then the influences of the degree of undercooling and supersaturation on the transformation kinetics, spacing between plates and microstructure evolution of Widmanstätten ferrite group were investigated.

2. Phase-field model and numerical method

For the formation of Widmanstätten ferrite in binary Fe–C alloys the phase-field model has been detailed by Loginova et al. [28] and Yamanaka et al. [29]. In the case of the KKS model, the phase-field equation for a dilute alloy is given by Ref. [30] as follows, in which $\phi = 1$ and $\phi = 0$ for the austenite and ferrite phase, respectively, and varies continuously from 1 to 0 across the interface

$$\frac{\partial\phi}{\partial t} = M_\phi\left[\varepsilon^2\nabla^2\phi - \frac{\partial}{\partial x}\left(\varepsilon\varepsilon'_\theta\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial y}\left(\varepsilon\varepsilon'_\theta\frac{\partial\phi}{\partial x}\right)\right] + M_\phi\left[p'(\phi)\left(g_m^\gamma(u_c,T) - g_m^\alpha(u_c,T) - \left(u_c^\gamma - u_c^\alpha\right)g_m^\gamma(u_c,T)\right) - g'(\phi)W\right] \quad (1)$$

In this model, any point within the interface region is assumed to be a mixture of two phases with the same chemical potential instead of the same composition in the Loginova model. If the relationship between the phase-field mobility M_ϕ and the real interface mobility M_p is adopted properly, then the dynamics of the interface with a vanishing interfacial thickness can be correctly described by the KKS model with a thin, but finite interface thickness. By assuming a planar γ/α interface moving at a velocity in one-dimensional system, Huang et al. [33] obtained a new relationship as follows:

$$M_\phi = M_p\frac{\sigma}{\varepsilon^2} \quad (2)$$

where $M_p = 0.035\exp\left(\frac{-17{,}700}{T}\right)$, ε is related to the interface energy σ and the interface thickness δ, W (=$6\beta\sigma/\delta$) is the energy barrier height of the double-well potential, β (=2.94) depends on the definition of the interface thickness [30]. $g(\phi) = \phi^2(1-\phi)^2$ is the double-well potential function, $p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$ is a monotonously changing function. $g_m^\alpha(u_c,T)$ and $g_m^\gamma(u_c,T)$ are the molar Gibbs energy density of ferrite and austenite, respectively. In the case of Widmanstätten ferrite the coherent broad sides should have a low interfacial energy while the more or less incoherent tip would have a high interfacial energy. The interfacial energy dependence on phase boundary orientation is highly anisotropic, and thus the gradient energy coefficient ε can be expressed as [29]

$$\varepsilon = \sqrt{\frac{3\sigma\delta}{\beta}}\times\begin{cases}1+\xi\cos k(\theta-\theta_0), & 2\pi i/k+\theta_m \leqslant \theta-\theta_0 \leqslant 2\pi(i+1)/k-\theta_m\\ \frac{1+\xi\cos k(\theta_m)}{\cos\theta_m}\cos(\theta-\theta_0), & 2\pi i/k-\theta_m \leqslant \theta-\theta_0 \leqslant 2\pi i/k+\theta_m\end{cases} \quad (3)$$

In the above expression ξ is the amplitude of the anisotropy, k is the mode number of the anisotropy, $\theta = \arctan(\phi_y/\phi_x)$ is introduced as the angle between the interface normal and the x axis, θ_0 is the preferred growth orientation, θ_m is the first missing orientation and i denotes integers from 0 to $k-1$. In Eq. (1) the solute concentration u_c is obtained from the solute conservation equation

$$\frac{\partial u_C}{\partial t} = \nabla[D(C,\phi)\nabla u_C] + \nabla\left[D(C,\phi)p'(\phi)\left(u_c^\gamma - u_c^\alpha\right)\nabla\phi\right] \quad (4)$$

where u_c is defined from normal mole fraction of C, the diffusion coefficient of the interface is $D = \left(D_C^\gamma\right)^{1-p(\phi)}\left(D_C^\alpha\right)^{p(\phi)}$, and D_C^α, D_C^γ are the diffusional coefficient in α and γ, respectively.

The governing equations, i.e. Eqs. (1) and (4), are transformed into dimensionless form. Length and time are scaled with a reference length $l = 0.9\delta_0$ and the diffusion time $l^2/(RTM_C^\alpha)$, respectively. The C++ code is implemented to solve the non-dimensionalized equations using adaptive finite element method based upon the AFEPack package (R. Li and W.B. Liu, http://dsec.pku.edu.cn/~rli/). The vanished flux boundary condition is adopted. The simulation domain size is 1.0 μm × 1.0 μm. The initial state of the system is homogeneous austenite, except for a thin layer of ferrite on the bottom of the domain. The initial composition of C in ferrite $u_C^{\alpha 0}$ at a given temperature is the equilibrium value (obtained from Ref. [34]), whereas initial $u_C^{\gamma 0}$ and temperature vary in different simulation cases. The mode number of anisotropy k is considered to be 2. The initial interface morphology is disturbed by a combination of sinusoidal curves. We have thus used the following function presented in Ref. [29].

$$h(x) = h_0 + \sum_{i=1}^{3} a_i\sin\left(\frac{2\pi N_i}{B}x + \phi_i\right) \quad (5)$$

where θ_0 is the growth direction, and h_0 is the height of the initial interface. The following parameters are used: $\theta_0 = 7\pi/18$, $h_0 = 2.8l$,

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