



A phase-field model for bainitic transformation



T.T. Arif, R.S. Qin*

Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, UK

ARTICLE INFO

Article history:

Received 6 January 2013

Received in revised form 16 March 2013

Accepted 18 April 2013

Keywords:

Displacive phase transitions

Phase-field model

Bainite transformation

Cubic crystal

Autocatalysis

ABSTRACT

A phase-field model for the computation of microstructure evolution for the bainite transformation has been developed. The model has a classical phase-field foundation, incorporates the phenomenological displacive transformation theory and the symmetric analysis of cubic crystals, and is able to reproduce realistic grain morphology and crystal orientation after adequate calibration. Using the free energy expression for the shape change of displacive transformations along with the free energy formula for the chemical free energy change of the two phases derived from established regular solution models, the current model is able to deal with autocatalysis.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

The phase-field (PF) method is used in the domain of materials science for simulating microstructure evolution on the mesoscale. The locations, sizes and shapes of the grains involved are represented by the PF variables. The evolution of the PF variables is then governed by a set of partial differential equations. They have nearly constant values within the grains but vary continuously over the interfaces between them. This means that the interface has a width and is not infinitesimally thin. Thus the method is said to have a diffuse-interface description. Unlike sharp interface methods, the diffuse-interface nature enables the computation of complex microstructures without explicitly tracking the interfaces. The method has been reviewed extensively, such as that in Refs. [1,2].

A PF model involves the formulation of a free energy functional of the PF variables and their gradients. - A form of the free energy functional includes the PF variable ϕ as a means of distinguishing coexisting phases along with the composition field C and temperature T as [3]

$$G = \int_V \left[g_0(\phi, C, T) + \frac{1}{2} \varepsilon_C^2 (\nabla C)^2 + \frac{1}{2} \varepsilon_\phi^2 (\nabla \phi)^2 \right] d\vec{r} \quad (1)$$

where ε_C and ε_ϕ are the gradient energy coefficients and $g_0(\phi, C, T)$ is the free energy density over the volume V . The governing equation for ϕ is derived from G in a thermodynamically consistent manner adhering to the second law of thermodynamics. Eq. (1) can be coupled with a thermodynamic database [4–7] and used for the simu-

lation of solidification [8], grain growth [9], solute drag [10] and many other processes. The method has thus gained momentum in microstructure formation and evolution. In solid state phase transformations there have been PF models that consider displacive transformations [11] and those that consider diffusive transformations [9,12].

Considered within the present work is a PF model able to utilise both diffusive and displacive mechanisms in its treatment of microstructure evolution. The microstructure focussed upon is bainite. Bainite is a microstructure resulting from the decomposition of austenite usually found to occur at a temperature between the pearlite reaction and the martensite start temperature (M_s). Initially detected as a unique microstructure in the early 1900s [13,14], interest in this multi-phase product of austenite grew once its benefits were realised. Bainitic steels boast improved strength without the expense of weldability and toughness and have applications in the railway, automotive industries and structural engineering [15–19]. The time-consuming process of producing bainitic steels prompted the desire to understand and formulate models for the kinetics and formation of bainite.

Following the kinetic model of Bhadeshia [20] the supersaturated ferrite sub-units form in austenite via a displacive mechanism. The ferrite sub-units form martensitically without the partitioning of alloying elements. Due to the higher temperatures when compared to martensite, the partitioning of the interstitial carbon from the supersaturated ferrite into the residual austenite follows soon after. Upon carbide precipitation in the austenite, the upper bainite microstructure forms. As the temperature is reduced, this diffusion process is slowed down which results in carbon precipitation within the bainitic ferrite giving lower bainite

* Corresponding author. Tel.: +44 207 5946803; fax: +44 207 5946757.

E-mail address: r.qin@imperial.ac.uk (R.S. Qin).

[21]. The transformation strains are accommodated plastically with the growth of the sub-unit limited by the dislocation debris [20,22–24]. The repeated nucleation and growth of these supersaturated bainitic ferrite sub-units gives the overall sheaf structure.

There have been efforts to model Bainitic phase transformation using a multiple order parameter phase-field model [25], in which both displacive transformation and carbon diffusion are considered. However, their work considers the entire sheaf as a single structure. This is opposed to the experimental fact that a sheaf consists of many individual sub-units. In the present work, a single order parameter phase-field model will be developed and the sub-units in bainite will be considered.

2. The phase-field model and the transformation theory

The governing equation for the phase-field order parameter, ϕ , derived from Eq. (1) using the second law of thermodynamics is given as [3,26]

$$\frac{\partial \phi}{\partial t} = M_{\phi} \left[\varepsilon^2 \nabla^2 \phi + \frac{1}{2\omega} \phi(1-\phi)(1-2\phi) - 30\phi^2(1-\phi)^2 (\mathbf{g}_{zB} - \mathbf{g}_{\gamma}) \right] \quad (2)$$

where $0 < \phi < 1$ is the interface between austenite and supersaturated ferrite with $\phi = 0$ representing the austenite and $\phi = 1$ the supersaturated ferrite. ε is the gradient energy coefficient and the coefficient ω is related to the kinetic barrier. \mathbf{g}_{zB} and \mathbf{g}_{γ} are the bulk free energies of the supersaturated ferrite and austenite, respectively. The parameters are related by the equations $\varepsilon^2 = 3\lambda\sigma/1.1$ and $\omega = \lambda/(26.4\sigma)$ [27], where σ and λ is the interface energy and half-thickness of the interface, respectively. $\mathbf{g}_{zB} - \mathbf{g}_{\gamma}$ is the driving force for microstructure evolution.

Bhadeshia expressed the strain energy of an ellipsoidal inclusion for the example of a martensitic grain as [28]

$$\mathbf{g}_{zB\gamma}^{\text{strain}} = \frac{a_1}{a_2} \mu \cdot m^2 = \frac{a_1}{a_2} \mu (s_x^2 + s_y^2 + \delta^2) \quad (3)$$

where m is the total deformation and is the sum of the shear strains along the x direction s_x and along the y direction s_y , and the uniaxial dilatation strain δ . a_1 and a_2 are the dimensions of the ellipsoid and μ is the shear modulus. In the current phase-field model, the supersaturated ferrite can be considered as an ellipsoidal inclusion. The orientation of the interface is represented by the gradient of the phase-field order parameter

$$\hat{n} = \frac{\nabla \phi}{|\nabla \phi|} = \frac{1}{|\nabla \phi|} \left(\frac{\partial \phi}{\partial x} \hat{x} + \frac{\partial \phi}{\partial y} \hat{y} + \frac{\partial \phi}{\partial z} \hat{z} \right) \quad (4)$$

Phase transformation takes place at the interface. For an interface with surface area δs and migration rate $\vec{v}(t)$, the volume of the new phase formed in the transformation within time duration δt is $\delta s \cdot \vec{v}(t) \cdot \hat{n} \delta t$. The dimension of the newly formed phase along the x direction is therefore represented as

$$\frac{\delta s \cdot |\vec{v}(t)| \cdot \delta t}{|\nabla \phi|} \cdot \frac{\partial \phi}{\partial x} \propto \frac{\partial \phi}{\partial x} \quad (5)$$

The growth of the new phase along different directions causes different amounts of strain. Therefore, one has $s_x \propto f_1 \frac{\partial \phi}{\partial x}$, $s_y \propto f_2 \frac{\partial \phi}{\partial y}$ and $\delta \propto f_3 \frac{\partial \phi}{\partial z}$. Eq. (3) is hence represented as

$$\mathbf{g}_{zB\gamma}^{\text{strain}} = f_1^2 \phi_x^2 + f_2^2 \phi_y^2 + f_3^2 \phi_z^2 \quad (6)$$

where $\phi_{x_i} = \partial \phi / \partial x_i$ is the rate of change of ϕ in the x_i direction. The change of chemical free energy only depends on the amount of new phase formed, and the free energy density difference between the new and parent phases.

The driving force is then

$$\begin{aligned} \mathbf{g}_{zB\gamma} &= \mathbf{g}_{zB} - \mathbf{g}_{\gamma} = (\mathbf{g}_{zB}^{\text{strain}} - \mathbf{g}_{\gamma}^{\text{strain}}) + (\mathbf{g}_{zB}^{\text{chem}} - \mathbf{g}_{\gamma}^{\text{chem}}) \\ &= (f_1^2 \phi_x^2 + f_2^2 \phi_y^2 + f_3^2 \phi_z^2) + \mathbf{g}_{zB\gamma}^{\text{chem}} \end{aligned} \quad (7)$$

The chemical free energy density difference can be obtained from a thermodynamic database and is usually isotropic [1,4], meaning $k_1 = k_2 = k_3 = k$ in the following equation:

$$\mathbf{g}_{zB\gamma}^{\text{chem}} = k_1 \phi_x^2 + k_2 \phi_y^2 + k_3 \phi_z^2 \quad (8)$$

It should be pointed out that f_i and k_i are unspecified coefficients so far and that the squares of the f_i can be omitted since the square of an unspecified constant remains an unspecified constant. Eq. (7) is therefore reduced to

$$\mathbf{g}_{zB\gamma} = (f_1 + k_1) \phi_x^2 + (f_2 + k_2) \phi_y^2 + (f_3 + k_3) \phi_z^2 \quad (9)$$

Given a transformation matrix from the growing crystal coordinate system to the parent crystal coordinate system with elements represented by H_{ij} , the final form of the driving force becomes for an isotropic chemical free energy ($k_1 = k_2 = k_3 = k$)

$$\mathbf{g}_{zB\gamma} = \sum_{i=1}^3 (f_i + k) (H_{i1} \phi_x + H_{i2} \phi_y + H_{i3} \phi_z)^2 \quad (10)$$

The phase transition from the parent phase to the new phase requires that $\mathbf{g}_{zB\gamma} < 0$. The f_i are specified as $f_1 = f_2$ and $f_3 = c_1 f_1$ according to the experimental observation of the morphology of the new phase. c_1 is a shape factor in the anisotropic driving force and related to the equilibrium aspect ratio of the bainite sub-unit. In displacive phase transformation, solute composition of the new phase is the same as that for the matrix due to its diffusionless nature. The volume change between the new phase and the parent phase is incorporated in the strain and the transformation matrix H_{ij} .

The width of the bainitic sub-units depend upon alloying elements. In particular, an increase in carbon concentration translates to a decrease in the aspect ratio of the sub-units [29]. This means that the shape factor $c_1 \equiv c_1(c)$ is a function of the carbon concentration c . Due to the shape change we must have that $c_1 f_1 + k \geq f_1 + k \forall c_1, k$. Since $k < 0$ we immediately have that $c_1 \geq 1$. c_1 is a monotonic decreasing function of c . Also at the equilibrium between bainitic ferrite and austenite (i.e. at T_0^* and c^*), we have zero driving force for bainite growth giving $c_1(c^*) f_1 + k(c^*) = f_1 + k(c^*) = 0$. Since $k(c^*) = -f_1$, we have that $f_1 + k(c^*) = 0$ holds. In order for $c_1(c^*) f_1 + k(c^*) = 0$ to be true we must have $c_1(c^*) = 1$.

Given a function $l(c)$ describing the aspect ratio of bainitic sub-units, we can impose the requirement that at a carbon composition $c_1(c) f_1 + k(c) = \beta(l(c))(f_1 + k(c))$ (11)

where β is a function relating the coefficient of the right hand side of Eq. (11) to the resulting aspect ratio. To clarify Eq. (11), $c_1(c)$ is the previously mentioned shape factor and $l(c)$ is the experimentally observed aspect ratio. However, observing Eq. (2) it is not obvious that the resulting aspect ratio of the bainite sub-units in the models output has a simple relation to $c_1(c)$. In other words, a shape factor of c_1 does not necessarily result in an aspect ratio of c_1 . Therefore, β is introduced to establish the connection between $c_1(c)$ and the resulting aspect ratio. For instance Fig. 1 shows that the evolution of the resulting aspect ratio given an input coefficient of 0.05 (i.e. $0.05(f_1 + k(c))$) tends to a limit (approximately 0.125). This would then mean that $\beta(0.125) = 0.05$.

Given reports that an aspect ratio of 0.025 is most frequently observed with 0.008 being the minimum, we require that $l(c^*) = 0.008$ and at the initial average composition of \bar{c} , $l(\bar{c}) = 0.025$. Then c_1 can be calculated as

$$c_1(c) = \frac{\beta(l(c))(f_1 + k(c)) - k(c)}{f_1} \quad (12)$$

Download English Version:

<https://daneshyari.com/en/article/7961800>

Download Persian Version:

<https://daneshyari.com/article/7961800>

[Daneshyari.com](https://daneshyari.com)