Acta Materialia 123 (2017) 317–328

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Phase-field simulations of curvature-induced cascading of Widmanstätten-ferrite plates

Avisor Bhattacharya [a, b, *], Kumar Ankit [b, 1], Britta Nestler [a, b]

[a] Institute of Materials & Processes, Karlsruhe University of Applied Science, Moltkestr. 30, 76133, Karlsruhe, Germany
[b] Institute of Applied Materials, Karlsruhe Institute of Technology (KIT), Haid-und-Neu Str. 7, 76131 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 19 June 2016
Received in revised form
14 October 2016
Accepted 16 October 2016

Keywords:
Widmanstätten ferrite
Phase-field model
Diffusional transformation
Anisotropy
Steel

ABSTRACT

In the present study, we employ a multiphase-field model based on the grand chemical potential formulation to simulate the morphological evolution of secondary Widmanstätten ferrite (α') during isothermal γ (austenite) $\rightarrow\alpha$' transformation in binary Fe-C steels. We add the stored-energy to the free-energy data obtained from CALPHAD database to simulate realistic kinetics of α' plates in diffusion-controlled regime. By implementing an elliptic anisotropy in the interfacial energy, we study the influence of supersaturation on the growth kinetics and stable morphologies of the single plate and colonies while scrutinising the conformity of numerical simulations with theory. For the first time, we elucidate the curvature-driven mechanism by which, a cascade of parallel *offspring* plates evolve adjacent to the *parent* sideplate. The present phase-field simulations, while providing significant insights into the curvature-induced mechanism of evolution of α' colony, also close the gap with *in-situ* observations reported earlier.

1. Introduction

In steel manufacturing, a vast majority of desirable mechanical properties can be achieved by appropriately tailoring the processing conditions that control the volume fraction, size distribution and morphology of the resulting phases. In particular, the morphological transitions that accompany ferritic (α-bcc) growth from austenite (γ-fcc) is of particular interest because it is closely related to solid-state phase transformations occurring at lower temperature such as bainitic and martensitic transformations. The richness of this scientific problem as well as its technological importance is evidenced by an extensive literature compiled over the last decades ([11,26,59] and references therein).

Below A_3 (boundary of $\gamma/\gamma+\alpha$ phase-fields in the phase-diagram), austenite decomposes into various product-phases with distinct morphologies depending upon the processing conditions [12,17,31] and grain size [1,17,34]. The morphological transition from grain boundary allotriomorph ferrite to sideplates, commonly known as Widmanstätten ferrite have been the topic of numerous experimental and numerical studies. From an engineering perspective, such a transition is considered to be mostly detrimental to the ductility of steels [12,17,27,33]. Acicular morphologies, similar to Widmanstätten ferrite, are also observed in non-ferrous systems e.g. brass, Ag-Cd, Zr-Nb and Ti-based alloys. Widmanstätten ferrite either nucleates on grain-boundary (as primary) or from preexisting allotriomorphic ferrite as secondary sideplates. The two variants essentially differ in terms of their 3-D morphology; while primary possesses a wedge shape, the secondary can most appropriately be described as elongated wedges [15]. In 2-D, the secondary sideplates appear to be triangular in shape with very high ratio of length to width.

The electron microscopic observation has revealed that the formation of the Widmanstätten ferrite is accompanied by a tent shaped surface relief [32]. This observation has been attributed to martensite-like invariant-plain strain (IPS) [10,60]. According to Aaronson and his coworkers, the formation of ferrite sideplate takes place by diffusion-controlled ledge mechanism [2] and any involvement of IPS [3,32] is argued. The following investigation has revealed that the growth of Widmanstätten ferrite slows down considerably when austenite is deformed [52], which

* Corresponding author. Institute of Materials & Processes, Karlsruhe University of Applied Science, Moltkestr. 30, 76133, Karlsruhe, Germany.
E-mail address: Avisor.Bhattacharya@hs-karlsruhe.de (A. Bhattacharya).
[1] Present address: Materials Science & Engineering, Texas A&M University, College Station, TX 77843, United States.

http://dx.doi.org/10.1016/j.actamat.2016.10.035
1359-6454/

supports the philosophy of incumbent displacive mechanism over reconstructive growth. Despite large shear strain, the stored-energy in α' is comparatively less than that of bainite and martensite due to self-accommodating plates [60]. Detailed measurements have suggested that the stored-energy associated with α' is around 50 J/mole [7]. Townsend and Kirkaldy elucidate the formation of the secondary sideplate on the basis of Mullins-Sekerka morphological-instability theory [40,41,56]. Based on experiments, Aaronson correlated interplate-spacing with compositions of steel [1].

Phase-field modeling has played a pivotal role in the study of morphological evolution of Widmanstätten ferrite. Using anisotropic phase-field, diffusion controlled transformation of α' plates and colonies are simulated [36,63,64]. These simulations validate the theory of instability-growth [40,41,56]. Further progress has been made by incorporating strain-energy. The anisotropic growth of α' is explained by elastic deformation [21,51,65]. These models illustrate the mechanism of variant-selection in Ti alloys [48,51]. However, these works report parabolic thickening of α' sideplates [48,65]. But Aarsonson reports a large deviation in the kinetics of sideplate-thickening from parabolic growth. In fact, this deviation has led him to conclude that the coherent interface of broad face of the sideplate provides barrier to diffusional growth of ledges [32]. Phase-field modeling has made further advancement by visco-plastic coupling [20,22,57]. The main objective of these works is to support the theory of shear transformation. However, the kinetics of Widmanstätten plate simulated, is far below the experimental observations [22]. Additionally, it does not explain mechanical-stabilization and observed dislocation density in ferrites. These limitations are severe constraints on the general acceptability of these methods.

A widely accepted view is that α' plates sympathetically nucleate on allotriomorphic ferrite. This view is corroborated by findings from *in situ* laser confocal microscopy, orientation-mapping, three dimensional microscopy of steels [15,16,35,44,45]. Detailed microscopic studies have revealed the variation in cumulative misorientation from allotriomorph to plate-tip. These observations are attributed to sympathetic nucleation. However, the phase-field simulations on Widmanstätten ferrite, reported earlier while illustrating the Mullins-Sekerka-type evolution of plates and colony, do not recognise sympathetic nucleation as a plausible mechanism [36,63,64]. It is to be noted that once a plate starts to lengthen, the rejected carbon from the tip accumulates at the base of the plate (in front of allotriomorph), thereby inhibiting the propensity for any further sympathetic nucleation of α' [4]. In this context, none of the existing theories consistently explain the mechanism of colony formation. Further, our current understanding is inept to fully elucidate the mechanism by which new sideplates nucleate near the base of a progressively lengthening plate [15,16,44,45].

In the present work, we investigate the evolution of a single plate as well as colony of Widmanstätten ferrite with an arbitrarily perturbed allotriomorphic surface using a multicomponent multiphase-field model in Fe-C system. In Section 2.1 and 2.2, we briefly recount the phase-field model and a novel formulation for anisotropic interfacial energy respectively. In Section 2.3, we explain the approach for accounting the stored-energy of α' sideplate in the chemical free-energy density directly obtained from CALPHAD database followed by model validation. On the basis of phase-field simulations reported in Section 3, for the first time, we propose curvature-induced cascading mechanism of colony formation while highlighting the synergy between our numerical and previous experimental observations. Section 4 concludes the article.

2. Methods

2.1. The phase-field model

In the present study, we use CALPHAD coupled multiphase-field model based on grand-potential density formulation [19,42,46]. This model has already been used to simulate complex morphological evolution during solidification and solid-state transformation in multicomponent alloys [8,9,30,39,61]. The model formulation is based upon the construction of a grand-potential density functional Ω over the whole volume consisting of the homogeneous phases and the interfaces separating them. The evolution of phases is governed by the phenomenological minimization of Ω,

$$\Omega(T,\boldsymbol{\mu},\phi) = \int_V \left[\Psi(T,\boldsymbol{\mu},\phi) + \left(\varepsilon a(\phi,\nabla\phi) + \frac{1}{\varepsilon}w(\phi)\right)\right] dV, \tag{1}$$

where T is the temperature, $\boldsymbol{\mu}$ is the chemical potential vector comprising of $K-1$ independent chemical potentials, $\boldsymbol{\phi}$ is the phase-field vector containing the volume fractions of the N-phases and ε is the length scale related to the interface. $a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})$ and $w(\boldsymbol{\phi})$ represent the gradient and obstacle potential type energy density as e.g. formulated in Ref. [25], respectively and V represents the domain volume. The grand potential density $\Psi(T,\boldsymbol{\mu},\boldsymbol{\phi})$, which is the *Legendre transform* of the free energy density of the system $f(T,\boldsymbol{c},\boldsymbol{\phi})$ is written as an interpolation of individual grand potential densities

$$\begin{aligned}\Psi(T,\boldsymbol{\mu},\boldsymbol{\varphi}) &= \sum_{\alpha=1}^{N} \Psi_\alpha(T,\boldsymbol{\mu}) h_\alpha(\boldsymbol{\varphi}) \\ \Psi_\alpha(T,\boldsymbol{\mu}) &= f_\alpha(\boldsymbol{c}^\alpha(T,\boldsymbol{\mu}),T) - \sum_{i=1}^{K-1}\mu_i c_i^\alpha(T,\boldsymbol{\mu}),\end{aligned} \tag{2}$$

where $h_\alpha(\boldsymbol{\phi})$ is an interpolation function of the form $h_\alpha(\boldsymbol{\phi}) = \phi_\alpha^2(3-2\phi_\alpha)$. The evolution equation for the N phase-field variables are derived from the functional Ω according to a variational approach reading

$$\tau\varepsilon\frac{\partial\phi_\alpha}{\partial t} = \varepsilon\left(\nabla\cdot\frac{\partial a(\boldsymbol{\phi},\nabla\boldsymbol{\phi})}{\partial\nabla\phi_\alpha} - \frac{\partial a(\boldsymbol{\phi},\nabla\boldsymbol{\phi})}{\partial\phi_\alpha}\right) - \frac{1}{\varepsilon}\frac{\partial w(\boldsymbol{\phi})}{\partial\phi_\alpha} - \frac{\partial\Psi(T,\boldsymbol{\mu},\boldsymbol{\phi})}{\partial\phi_\alpha} - \Lambda, \tag{3}$$

where Λ is the Lagrange parameter to maintain the constraint $\sum_{\alpha=1}^{N}\phi_\alpha = 1$. τ is a relaxation constant. In the limit of infinite interface mobility, for the $\gamma \rightarrow \alpha$ transformation, τ is given by Ref. [19]:

$$\tau = \frac{\left(c_\alpha^{eq} - c_\gamma^{eq}\right)^2 (M+F)}{D_\gamma \frac{\partial c_\gamma}{\partial\mu}} \tag{4}$$

where c_α^{eq} and c_γ^{eq} are the equilibrium compositions in α and γ phases respectively. D_γ is the diffusivity in γ phase and μ is the chemical potential. M and F are constants, dependent on the interpolation functions. In the present work $M + F \approx 0.22$.

The concentration fields are obtained by a mass conservation equation for each of the $K-1$ independent concentration variables c_i. The evolution equation for the concentration fields results from the chemical-potentials μ_i by,