



# Phase-field modeling of cyclic phase transformations in low-carbon steels



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## ARTICLE INFO

### Article history:

Received 7 December 2014  
Received in revised form 14 January 2015  
Accepted 17 January 2015  
Available online 10 February 2015

### Keywords:

Cyclic phase transformation  
Phase-field modeling  
Low-carbon steels  
Gibbs energy dissipation  
Solute drag

## ABSTRACT

A phase-field model has been developed to describe microstructure evolution during cyclic phase transformations for two low-carbon steels (Fe–0.1 wt%C, Fe–0.1 wt%C–0.5 wt%Mn). The austenite–ferrite transformations are assumed to occur under negligible-partition conditions for Mn and only long-range diffusion of carbon is considered. A Gibbs-energy dissipation model has been integrated with the phase-field model to describe the stagnant stages during cyclic phase transformations in the ternary alloy. Experimental results, e.g. the stagnant stages and the cyclic phase transformation kinetics, have been successfully replicated with 2D phase-field simulations.

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## 1. Introduction

The mechanism of the austenite formation and decomposition in the intercritical region is of great interest due to its practical importance in steel design and production, and it has been investigated with a number of experimental approaches, e.g. conventional isothermal or continuous heating/cooling experiments [1,2] and decarburization experiments [3], and modeling techniques, e.g. one-dimensional sharp-interface models [2,4,5] and multi-dimensional mesoscale models [6–10].

Chen et al. [11,12] proposed a cyclic partial phase transformation approach, in which the complex nucleation process can be avoided, to study the austenite-to-ferrite transformation and its reverse transformation in Fe–C–Mn alloys. The approach employs a cyclic heat treatment in the intercritical region where partial austenite-to-ferrite and ferrite-to-austenite transformations take place alternatively. For cyclic partial transformations, a special feature has been observed, i.e. a particular temperature range during both heating and cooling where the change in phase fractions remains negligible. Such temperature ranges are termed “stagnant stages”. In order to explain this special feature, one-dimensional sharp-interface models (Local-Equilibrium model (LE) [13–15] and Para-equilibrium model (PE) [16,17]) were used to simulate the cyclic phase transformations in the Fe–C–Mn alloys [12]. It

was found that the LE model considering redistribution of substitutional elements can replicate the stagnant stages quite well, whereas the PE model predicts no stagnant stages. Thus it was concluded that the stagnant stage is due to the redistribution of substitutional alloying elements near the interface. The LE model, albeit powerful, is limited to 1D simulation so far, due to high computational cost, since fine meshes are required to resolve the diffusion length of substitutional elements.

In contrast, Gamsjäger et al. proposed a one-dimensional mixed-mode model to investigate the stagnant stages in cyclic phase transformations [18]. In the mixed-mode model, the substitutional elements were assumed to be immobile in their sublattice and effective austenite/ferrite interface mobilities were used to account for the effect of solutes on cyclic phase transformations. In order to obtain a good description of the transformation kinetics, the austenite/ferrite interface mobility was assumed to not obey an Arrhenius relationship, i.e. the activation energy of mobility was taken as a linear function of temperature. This assumption leads to a great variation of the austenite/ferrite interface mobility with temperature such that a small mobility at the stagnant stages is obtained to mimic the sluggish interface migration. Further, the fitted mobility values are different for the austenite-to-ferrite transformation and the reverse ferrite-to-austenite transformation.

The effective-mobility approach used by Gamsjäger et al. [18] has been widely employed in the past and integrated with mesoscale models, e.g. phase-field models [8,9,19]. This approach has been applied successfully in simulating the austenite-to-ferrite transformation during continuous cooling [8,19,20]. In selected

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cases, however, the effective mobility was found to depend unreasonably on cooling rate which was attributed to potential segregation of alloying elements at migrating interfaces [21,22]. Two theories have been developed to model the effects of solute segregation on slowing down phase transformations: (i) solute drag theory [23,24]; (ii) Gibbs-energy dissipation theory [25]. In the solute drag theory, a drag pressure is assumed to be exerted on a migrating interface by segregated solute atoms. In the Gibbs-energy dissipation theory, it is proposed that solute diffusion inside a migrating interface (trans-interface diffusion) leads to dissipation of Gibbs energy [25]. Hillert found these two theories were actually equivalent, i.e. the solute drag pressure is equal to the dissipated Gibbs-energy [26]. To be consistent, the term “Gibbs-energy dissipation” will be used in the present work. Based on these two theories, several models have been developed to investigate the effects of alloying elements on phase transformation in steels. By making suitable assumptions for the solute-interface binding energy and the trans-interface diffusivity they have been successfully applied to describing the austenite-to-ferrite transformation [2,4,5,22]. In all these models, solute diffusion is assumed to occur inside the interface only but not in the bulk. These models have yet to be used to describe cyclic phase transformations.

The present paper is devoted to developing a two-dimensional phase-field model capable of accounting for microstructural morphologies and describing quantitatively the experimentally measured transformation kinetics during cyclic heat treatments of low-carbon steels. In particular, Gibbs-energy dissipation by trans-interface diffusion of solutes is taken into account in the phase-field model. The model is applied to two low-carbon steels (Fe–0.1 wt%C, Fe–0.1 wt%C–0.5 wt%Mn) and validated with experimental observations.

## 2. Method

### 2.1. Phase-field model

A single-phase-field model [27] is used in this work:

$$\frac{d\phi}{dt} = m_{\alpha\gamma} \left\{ \sigma_{\alpha\gamma} \left[ \nabla^2 \phi + \frac{\pi^2}{\eta^2} \left( \phi - \frac{1}{2} \right) \right] + \frac{\pi}{\eta} \sqrt{\phi(1-\phi)} \Delta G_{\alpha\rightarrow\gamma} \right\} \quad (1)$$

where  $\alpha$  denotes ferrite,  $\gamma$  denotes austenite, the phase-field variable  $\phi$  represents the local fraction of austenite,  $\eta$  is the interface thickness,  $m_{\alpha\gamma}$  is the ferrite/austenite interface mobility,  $\sigma_{\alpha\gamma}$  is the interface energy and  $\Delta G_{\alpha\rightarrow\gamma}$  is the driving pressure. The mobilities are assumed to obey an Arrhenius relationship, i.e.

$$m_{\alpha\gamma} = m_{\alpha\gamma}^0 \exp \left( -\frac{Q_{\alpha\gamma}}{RT} \right) \quad (2)$$

where  $m_{\alpha\gamma}^0$  is the pre-factor,  $Q_{\alpha\gamma}$  is the activation energy,  $T$  is the temperature and  $R$  is the ideal gas constant.

The driving pressure in the phase-field model is a function of both temperature and carbon concentrations for austenite–ferrite transformations in low-carbon steels. Long-range diffusion of carbon is considered and coupled to the phase-field model. Thus, the model is of mixed-mode character [28], i.e. both long-range diffusion of carbon and interface reaction are taken into account. The carbon diffusion equation is given by:

$$\frac{\partial C}{\partial t} = \nabla(D_{\alpha}(1-\phi)\nabla C_{\alpha} + D_{\gamma}\phi\nabla C_{\gamma}) \quad (3)$$

where  $D_{\alpha}$  and  $D_{\gamma}$  are the carbon diffusivities in ferrite and austenite,  $C$  is the local carbon concentration which, in the interface region, is the sum of the carbon concentrations ( $C_{\alpha}$  and  $C_{\gamma}$ ) in both phases weighted with the phase-field parameter:

$$C = (1-\phi)C_{\alpha} + \phi C_{\gamma} \quad (4)$$

The redistribution of carbon between austenite and ferrite within the interface is approximated by [29]:

$$C_{\alpha} - C_{\alpha}^* = \frac{k_{\alpha\gamma}}{k_{\gamma\alpha}} (C_{\gamma} - C_{\gamma}^*) \quad (5)$$

where  $C_{\alpha}^*$  and  $C_{\gamma}^*$  are the equilibrium carbon concentrations,  $k_{\alpha\gamma}$  and  $k_{\gamma\alpha}$  are the slopes of equilibrium carbon-concentration lines on a linearized phase diagram [29]. For the Fe–C–Mn system, the equilibrium carbon concentration is determined based on para-equilibrium.

### 2.2. Driving pressure for austenite–ferrite transformation

The chemical driving pressure for the ferrite-to-austenite transformation ( $\alpha \rightarrow \gamma$ ) is described by:

$$\Delta G_{\alpha\rightarrow\gamma}^t = \chi_{\alpha\rightarrow\gamma} (C_{\gamma} - C_{\gamma}^*) \quad (6)$$

where  $\chi_{\alpha\rightarrow\gamma}$  is a positive constant that is calculated with Thermo-calc® (TCFE7 database). The chemical driving pressure for the reverse austenite-to-ferrite transformation ( $\gamma \rightarrow \alpha$ ) is given by  $\Delta G_{\gamma\rightarrow\alpha}^t = -\Delta G_{\alpha\rightarrow\gamma}^t$ .

For the Fe–C–Mn alloy, a part of the chemical driving pressure on an austenite/ferrite interface (Eq. (6)) is dissipated by the trans-interface diffusion of Mn, such that the driving pressure for interface migration in the phase-field equation (Eq. (1)) is:

$$\Delta G_{\alpha\rightarrow\gamma} = \Delta C_{\alpha\rightarrow\gamma}^t - \Delta G^{dis} \quad (7)$$

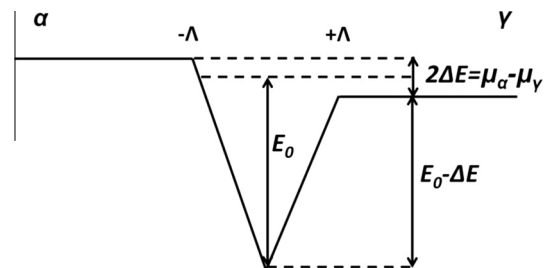
where the dissipated Gibbs-energy ( $\Delta G^{dis}$ ) is given by [24,30]:

$$\Delta G^{dis} = \int_{-A}^{+A} (x_{Mn}^0 - x_{Mn}(y)) \frac{dE(y)}{dy} dy \quad (8)$$

Here  $2A$  is the physical interface thickness that is distinct from the numerical interface thickness  $\eta$  in the phase-field model,  $x_{Mn}^0$  is the molar fraction of Mn in the bulk,  $x_{Mn}$  is the molar fraction of Mn across the interface and  $E(y)$  is the interaction potential of solute Mn with the austenite/ferrite interface. A wedge-shaped profile is assumed for the Mn-interface interaction potential [24], as shown in Fig. 1, where  $E_0$  is the Mn-interface binding energy and  $2\Delta E$  is the potential difference between ferrite and austenite which is calculated with Thermo-calc®. It is noted that the Mn-interface interaction potential will become a linear interpolation between the chemical potentials in ferrite and austenite, if the binding energy ( $E_0$ ) is zero.

The concentration profile ( $x_{Mn}(y)$ ) of the substitutional element (Mn) across an interface moving with a velocity of  $V$  is given by [24]:

$$D_{int}^{Mn} \frac{\partial x_{Mn}(y)}{\partial y} + \frac{D_{int}^{Mn} x_{Mn}(y)}{RT} \frac{\partial E(y)}{\partial y} + V(x_{Mn}(y) - x_{Mn}^0) = 0 \quad (9)$$



**Fig. 1.** Schematic of the chemical potential of Mn inside the austenite/ferrite interface with a nonzero binding energy ( $A$  is half of the interface;  $E_0$  is binding energy;  $\mu_{\alpha}$  and  $\mu_{\gamma}$  are chemical potentials of Mn in ferrite and austenite respectively).

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