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Theoretical and numerical study of lamellar eutectoid growth influenced by volume diffusion

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Abstract

We investigate the lamellar growth of pearlite at the expense of austenite during the eutectoid transformation in steel. To begin with, we extend the Jackson–Hunt-type calculation (previously used to analyze eutectic transformation) to eutectoid transformation by accounting for diffusion in all the phases. Our principal finding is that the growth rates in the presence of diffusion in all the phases are different compared to the case when diffusion in growing phases is absent. The difference in the dynamics is described by a factor 'ρ' which comprises the ratio of the diffusivities of the bulk and the growing phases, along with the ratios of the slopes of the phase coexistence lines. Thereafter, we perform phase-field simulations, the results of which are in agreement with analytical predictions. The phase-field simulations also reveal that diffusion in austenite as well as ferrite leads to the formation of tapered cementite along with an overall increase in the transformation kinetics as compared to diffusion in austenite (only). Finally, it is worth noting that the aim of present work is not to consider the pearlitic transformation in totality; rather it is to isolate and thereby investigate the influence of diffusivity in the growing phases on the front velocity.

Keywords: Pearlite; Phase-field method; Coupled-growth; Jackson–Hunt analysis

1. Introduction

The mechanism of eutectoid transformation in steel has been a topic of theoretical as well as experimental investigation since the inception of steel as a structural material. The eutectoid transformation involves the formation of a pearlite colony which appears as alternate lamellae of ferrite and cementite phases and grow as a common front with the austenite. Cementite is the carbon-rich phase whereas the carbon solubility in ferrite is relatively low [1–3].

The two principal mechanisms of eutectoid reaction, i.e. the austenite to pearlite phase transformation, cited in the literature are volume diffusion and grain boundary diffusion. The former suggests the volume diffusion of carbon ahead of the phase interface, while the latter emphasizes the role of grain boundary diffusion as the rate-controlling step. The pioneering work of Zener [4], Hillert [5] and Tiller [6] on pearlite formation explains the relation between the lamellar spacing and undercooling during the phase transformation. In spite of making a generous effort to explain the phenomenology of pearlitic transformation, the classical Zener–Hillert model show large deviations from the experimentally measured lamellar growth velocities. The model assumes no diffusion in the ferrite phase whilst considering diffusion in austenite phase (only). This would be a reasonable assumption in the case of eutectic solidification problem, where the diffusivity in solid is lower than the diffusivity in liquid (bulk phase) by a factor of 1000. However, in a solid-state phase transformation such as the eutectoid reaction, the diffusivity in austenite (bulk phase)

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is comparable to the ferrite. Thus, it is reasonable to expect some disagreement of experimental velocities with corresponding values derived from the Zener–Hillert co-operative growth model.

Jackson and Hunt [7] adapt the Zener–Hillert model to investigate directional solidification in eutectics with a constant velocity of the growth front, which broadly falls in the same class of moving-boundary problem as the eutectoid transformation. Recently, Nakajima et al. [8] use the multiphase-field method to simulate co-operative pearlite growth by accounting for diffusion in the ferrite as well as the austenite phase. They predict a successive process of diffusion in ferrite and growth of cementite from the ferrite, resulting in an increase in the kinetics of pearlitic transformation by a factor of 4 as compared to growth from austenite alone. The simulated cementite lamella is found to be tapered and exhibits a conical morphology. This is interpreted as an effect of diffusion in ferrite. Steinbach and Plapp [9] claim an overlap of phase-field results with Hillert's model in the absence of diffusion in ferrite. Further, they couple a stress-driven diffusion field to the phase field and study the effect of transformation strains. However, Pandit and Bhadeshia [10] argue that pearlite forms by reconstructive transformation, in which case transformation strains should not be significant. They also emphasize the need to consider both the mechanisms, volume as well as interfacial diffusion simultaneously to achieve an overlap with experimental findings.

In the present article, we extend our previous work on Jackson–Hunt (JH) analysis of ternary eutectic alloys [11] to study the eutectoid transformation. The main question which we address is: can a JH type analysis (previously done for eutectics) be extended to predict lamellar growth velocities of pearlite by accounting for diffusion in austenite as well as ferrite? In order to answer this question, we first extend the JH analysis for eutectics by accounting for diffusion in austenite as well as ferrite. We analyze the case of stable lamellar coupled growth and derive the expressions for lamellar growth velocity as a function of undercooling and lamellar spacing. This is followed by comparison of the analytical prediction with the numerical results of a thermodynamically consistent phase-field model.

The remainder of this article is organized as follows. In Section 2 we derive an expression for lamellar growth velocity as a function of undercooling and spacing in pearlite using a JH-type analysis. In Section 3 the quantitative phase-field model used to simulate pearlite growth is outlined. In Section 4, we describe the thermodynamic data-fitting procedure to approximate the variation of the grand-potential of the respective phases as a function of chemical potential. In Section 5 we derive the relation between the simulation parameters and corresponding quantities in the sharp interface limit. In Section 6 we compare the lamellar growth velocity obtained from phase-field simulations to the analytical expressions for the velocity, derived in Section 2. Section 7 concludes the article.

2. Theoretical analysis of coupled growth

We consider the diffusion of the components A and B ahead of the planar eutectoid front. In order to calculate the concentration fields ahead of the growth front in question, we make the following Fourier series expansion for c_A and c_B:

$$c_X^{\gamma} = \sum_{n=-\infty}^{\infty} X_n e^{ik_n x - q_n z} + \left(c_X^{\infty}\right)_{\gamma}, \quad X = A, B \tag{1}$$

where γ is the austenite phase. In the respective growing phases (α and β) the concentration fields can be respectively written as:

$$c_X^{v} = \sum_{n=-\infty}^{\infty} X_n e^{ik_n x + q_n z} + \left(c_X^{\infty}\right)_{v}, \quad X = A, B \;\; v = \alpha, \beta. \tag{2}$$

An elaborate description of the terms involved in the above expression and derivation from a stationary diffusion equation has been described in detail in the previous work on eutectic growth [11]. In the field under consideration, the growth front is assumed to be at $z = 0$. Further, $z > 0$ depicts austenite phase where exponential profiles for the concentrations of components A and B exist. For $z < 0$, the composition profile in pearlite (for ferrite and cementite phases) has similar exponential profiles. Therefore, to account for the symmetry across the interface, we change the sign of the exponent $e^{-q_n z}$ to $e^{q_n z}$ when treating the concentration profiles in ferrite and cementite phases ($\forall \; z < 0$).

In the JH analysis for the calculation of diffusion field in liquid and solid, Stefan's condition at the $v - \gamma$ interface, which expresses mass conservation upon phase transformation, reads as:

$$D^{v} \partial_n c_X^{v}|_{z=0} - D^{\gamma} \partial_n c_X^{\gamma}|_{z=0} = v_n \Delta c_X^{v}, \quad v = \alpha, \beta \tag{3}$$

where $\partial_n c_X^{v}$ denotes the partial derivative of c_X^{v} in the direction normal to the interface. The quantity v_n is the normal velocity of the interface (positive for a growing front) and $\Delta c_X^{v} = c_X^{\gamma} - c_X^{v}$. D^{γ} and D^{v} are chemical diffusion coefficients for bulk and growing phases, respectively. To use the Stefan condition, we take the derivative of c_X^{v} with respect to the z coordinate:

$$\partial_z c_X^{v}|_{z=0} = \sum_{n=-\infty}^{\infty} q_n X_n e^{ik_n x} \quad v = \alpha, \beta \tag{4}$$

for the growing phases, and:

$$\partial_z c_X^{\gamma}|_{z=0} = \sum_{n=-\infty}^{\infty} - q_n X_n e^{ik_n x}, \tag{5}$$

for the austenite phase. Integration across one lamella period (lamellar spacing) λ gives:

$$q_n X_n^{\alpha} D^{\alpha} \eta_{\alpha} \lambda + q_n X_n^{\beta} D^{\beta} \eta_{\beta} \lambda + q_n X_n^{\gamma} D^{\gamma} \lambda = \sum_{j=0}^{M-1} \int_{x_j \lambda}^{x_{j+1} \lambda} v_n \Delta c_X^{vj} e^{-ik_n x} dx. \tag{6}$$