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The role of carbon diffusion in ferrite on the kinetics of cooperative growth of pearlite: A multi-phase field study

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Abstract

Cooperative growth of pearlite is simulated for eutectoid steel using the multi-phase field method. The model considers diffusion of carbon not only in γ phase, but also in α phase. The lamellar spacing and growth velocity are estimated for different undercoolings and compared with experimental results from the literature and theoretical results from analytical models. The important finding of this work is that carbon diffusion in ferrite and growth of cementite from the ferrite increase the kinetics of the pearlitic transformation by a factor of four as compared to growth from austenite only, which is assumed by the classic Zener–Hillert model. This growth mode therefore must be considered to be the dominating growth mode and it explains at least some of the differences between experiment and theory, where diffusion in ferrite is excluded.

Keywords: Phase field models; Simulation; Pearlitic steels; Phase transformation kinetics; Microstructure

1. Introduction

The phase field method has proved to be a useful numerical tool to calculate the lamellar microstructure during eutectic solidification processes. In this paper, the method is applied to eutectoid transformation in the solid state. Analytical models of pearlite transformation and eutectic solidification are first reviewed and compared with each other.

Pearlite transformation is a well-known eutectoid transformation, where one parent phase decomposes into two solid phases simultaneously. It is similar to eutectic solidification, except for the phase state of the parent phase. The parent phase in the latter is liquid; in the former it is solid. Both transformations can lead to a lamellar microstructure. So far analytical models [1–3] have been suggested for the lamellar growth mode for either transformation. Three parameters are required to describe the formation of a lamellar structure, namely undercooling, lamellar spacing and growth velocity. Analytical models for both transformations differ in the thermal situation. While in the case of pearlitic growth the Zener–Hillert model [1,2] considers an isothermal situation, the Jackson–Hunt model [3] for eutectic solidification deals with directional solidification conditions. In the Zener–Hillert model, the growth velocity is free to adjust and undercooling is fixed. Jackson and Hunt applied the analytical solution from Ref. [2] to the growth conditions of eutectic growth in a temperature gradient, where the velocity is fixed by the growth condition and undercooling is free to adjust.

Concerning the velocity v of cooperative growth in pearlite transformation, Zener and Hillert derived the following equation as a function of lamellar spacing:

$$v = (2D_\gamma/f^\alpha f^{\mathrm{cm}})\{(C_{\mathrm{e}}^{\gamma/\alpha} - C_{\mathrm{e}}^{\gamma/\mathrm{cm}})/(C^{\mathrm{cm}/\gamma} - C^{\alpha/\gamma})\} \times (1/\lambda)(1 - \lambda_0/\lambda) \quad (1)$$

where D_γ, f^α and f^{cm} represent carbon diffusion coefficient in γ phase (cm^2/s), volume fraction of α phase and volume fraction of cementite, respectively. $C^{\alpha/\gamma}$ and $C^{\mathrm{cm}/\gamma}$ represent

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the carbon concentration in α phase and in cementite at the eutectoid transformation interface at a given undercooling, respectively. $C_e^{\gamma/\alpha}$ and $C_e^{\gamma/cm}$ represent the carbon concentration in γ phase in front of α phase and in front of cementite, respectively. The subscript e denotes equilibrium. λ_0 denotes the lamellar spacing where all energy is consumed for the formation of interfaces, i.e. $\lambda_0 = 2\sigma V_m/\Delta G$. Here σ, V_m and ΔG represent surface energy (J/m^2), molar volume (m^3/mol) and change of total free energy (J/mol), respectively. If a criterion is assumed that a system transforms at maximum velocity, Eq. (1) reduces to Eq. (2) under $\lambda = 2\lambda_0$:

$$v = (D_v/2f^{\alpha}f^{cm})\{(C_e^{\gamma/\alpha} - C_e^{\gamma/cm})/(C^{cm/\gamma} - C^{\alpha/\gamma})\}(1/\lambda) \quad (2)$$

The term $(C_e^{\gamma/\alpha} - C_e^{\gamma/cm})/(C^{cm/\gamma} - C^{\alpha/\gamma})$ is proportional to the reciprocal lamellar spacing. Consequently velocity is approximately proportional to $1/\lambda^2$.

If the deviation of the actual transformation temperature from the eutectoid temperature is small, ΔG is expressed approximately as $\Delta H \times \Delta T/T_E$, using the latent heat of pearlite transformation (ΔH) and the eutectoid temperature (T_E). The relationship between undercooling and lamellar spacing is given by Eq. (3) using $\lambda = 2\lambda_0$ and $\lambda_0 = 2\sigma V_m/\Delta G$:

$$\Delta T = 4\sigma T_E V_m/\Delta H(1/\lambda) \quad (3)$$

In the case of eutectic solidification, Jackson and Hunt [3] derived the following equation for lamellar growth:

$$\Delta T/m = Qv\lambda + a/\lambda \quad (4)$$

where m, Q and a are constants. If the criterion is assumed that a solid grows at minimum undercooling, which corresponds to the maximum growth criterion in pearlite transformation, Eq. (4) reduces to Eqs. (5) and (6):

$$\Delta T = 2ma(1/\lambda) \quad (5)$$

$$v = a/Q(1/\lambda^2) \quad (6)$$

Figs. 1 and 2 show the relationship between lamellar spacing and undercooling and between lamellar spacing and growth velocity. It is revealed that both pearlite transformation and eutectic solidification have similar relationships among the three parameters. Here two important things must be kept in mind. One is that these analytical models are based on the diffusion-controlled mode and the other is that they consider diffusion in the parent phase only.

Fig. 3 shows a schematic phase diagram of the Fe–C system related to the pearlite transformation. Here an undercooling of 50 K is supposed as an example. Dotted lines mean extrapolated lines of A_{e3}, A_{cm} and solubility line of α phase in γ phase. It is obvious that during isothermal transformation of pearlite with constant undercooling, there are concentration differences in both γ phase and α phase. These concentration differences create a driving force for diffusion in both phases as illustrated in Fig. 4. It is likely that diffusion in the α phase has a considerable influence on transformation behavior because the carbon diffusion coefficient in α phase is much larger than that in the γ phase. Therefore diffusion in both phases should be taken into consideration in order to simulate pearlite transformation. The importance of carbon diffusion in ferrite was first pointed out by Onsager in 1948 [4], and Fisher [5] calculated in 1959 a growth rate 7 times faster by this transformation path than by diffusion in austenite only. However, since the diffusion data used by Fisher were doubted [2] and in an experimental study by Mehl and Hagel [6] no evidence was found for a tapered form of the cementite behind the growth front, which should be characteristic for this transformation path, the possibility of the transformation path by cementite growth from ferrite was disregarded in further studies. As an alternative, grain boundary diffusion was proposed to explain the discrepancy between theory and experiment [7].

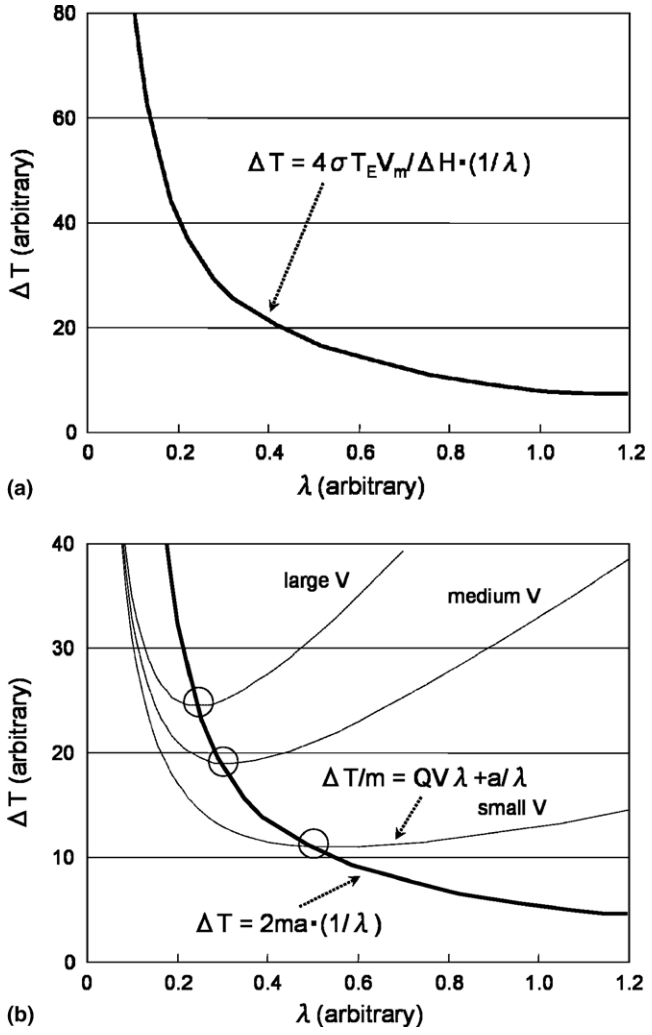

Fig. 1. Relationship between spacing and undercooling according to analytical models.

The purposes of this study are to investigate complex cooperative growth of pearlite transformation by a multi-phase field model and to clarify the influence of diffusion