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A mixed-mode model for the ferrite-to-austenite transformation in a ferrite/pearlite microstructure

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Abstract—A concise semi-analytical mixed-mode model is proposed to describe the ferrite-to-austenite transformation kinetics. The initial microstructure for the model consists of a ferrite matrix with supersaturated austenite grains. The carbon supersaturation of austenite grains resulted from the rapid dissolution of pearlite colonies present in the initial microstructure. A similar approach to the one used for describing the ferrite growth kinetics (Bos and Sietsma, 2007) was used, employing a sharp interface between the phases. In comparison to ferrite growth, the carbon concentration profile of the growing austenite contains an additional parameter, which is the carbon concentration at the centre of the grain. This extra parameter is accounted for by assuming a parabolic carbon profile in the austenite. A comparison with a numerical solution of the differential equations shows that the developed semi-analytical mixed-mode model gives a good description of the ferrite-to-austenite transformation, significantly more accurate over the entire course of the transformation than the classical interface-controlled and diffusion-controlled models. Significant deviations from the numerical solution, as a result of the parabolic approximation, are limited to the initial stage of the transformation.
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1. Introduction

In the past years, there has been a significant increase in the use of high strength Dual-Phase (DP) steels in the automotive industry. The favourable combination of strength and formability of DP steels makes these materials suitable for the construction of several parts of the car body. The microstructure of cold-rolled and annealed DP steels, consisting of a dispersion of hard martensite in a soft ferrite matrix, is typically obtained by annealing in the intercritical temperature range to produce an austenite-ferrite microstructure, followed by quenching to room temperature to transform austenite to martensite. Since the properties of DP steels markedly depend on the fraction, distribution and carbon content of the martensite phase, the understanding of the mechanism of austenite formation during heating and holding at the intercritical temperature is of primary importance. Despite this fact, the kinetics of austenite formation during heating has not been studied in such detail as the austenite-to-ferrite transformation on cooling. The explanations for this are several: first, the austenite formed during heating is transformed back to different product phases during cooling and therefore direct observation of the austenite formed on heating is very difficult; second, the austenite formation occurs very rapidly as the temperature increases and consequently conventional techniques, like dilatometry and metallography, usually employed to study the transformation on cooling, are less adequate for studying the austenite formation. Another aspect makes the study of the austenite formation kinetics on heating difficult: the distribution and morphology of phases present in the starting microstructure affect the process of austenite formation, which then must be studied starting from different initial microstructures, whereas the ferrite formation usually occurs from homogenous austenite. This increases the number of required experiments.

For similar reasons physically based models for the austenitisation formation are relatively underdeveloped. From experiments it is known that during intercritical annealing of steel having an initial ferrite plus pearlite microstructure the austenite formation occurs in two steps: the pearlite transforms to carbon-supersaturated austenite and subsequently ferrite transforms to austenite. The first step is controlled by the carbon diffusion within the pearlite regions. Since the diffusion distances involved are short, it is much more rapid than the second step. Therefore most models in the literature restrict the analysis of the austenitisation process to the ferrite-to-austenite transformation, starting from a microstructure of carbon-supersaturated austenite grains in a ferrite matrix [1–4]. In the literature, the ferrite-to-austenite transformation is often modelled assuming that the carbon diffusion in austenite controls the rate of transformation and the lattice transformation is

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such a fast process that the carbon fractions in ferrite and austenite at the interface are equal to the equilibrium fractions [5–6]. The transformation is therefore diffusion controlled. In the more general case of finite interface mobility, carbon fractions at the interface differ from the equilibrium values and the transformation has a mixed-mode character, which means that it is controlled by both carbon diffusivity and interface mobility.

While the mixed-mode character of the austenite dissolution on cooling was extensively analysed in the literature, e.g. [7–13], few studies can be found on the mixed-mode character of austenite formation on heating [14–15]. In terms of modelling the phase transformation, phase-field modelling (e.g. [16–18]) does take the mixed-mode character into account in a diffuse-interface approach, but the method is too computationally intensive to allow 3D microstructural simulations. A more efficient modelling approach is therefore needed, similar to the concise analytical model that has been formulated recently to describe the austenite-to-ferrite transformation [19]. The model in Ref. [19] simply considers the conservation of carbon at the interface and the dependence of the driving force on the deviation from equilibrium to derive the carbon fraction in austenite at the interface, the width of carbon profile within the austenite and the interface velocity. The comparison with a fully numerical solution of the differential equations describing the carbon flux through the moving interface has shown that this analytical model is able to quite accurately describe the mixed-mode character of the austenite-to-ferrite transformation [19].

In the present paper the ferrite-to-austenite transformation during holding at an intercritical temperature is modelled by using a mixed-mode semi-analytical model similar to that formulated for the austenite-to-ferrite transformation in Ref. [19]. The results of the model and its limitations are discussed. A comparison with numerical solutions of the equations involving the movement of the interface and carbon diffusion is also presented. The obtained results are compared with those obtained for diffusion-controlled kinetics and interface-controlled kinetics.

2. Theory

In this work the ferrite-to-austenite phase transformation is assumed to occur with the partitioning of a single element as it happens in binary alloys or in ternary alloys in which one of the elements has a negligible diffusivity with respect to the effective interface motion. This is the case of the Fe–C–Mn system, in which the transformation can be assumed to take place without Mn partitioning since the Mn diffusion is a slow process compared to the motion of the interface as a consequence of the large difference in diffusivity of Mn and C in both austenite and ferrite: the transformation is said to occur under para-equilibrium conditions. This section will present a physical model of the interface motion of a sharp austenite/ferrite interface during the austenite-to-ferrite phase transformation under mixed-mode conditions, governed by carbon partitioning and diffusion and the interface mobility. This approach leads to analytic expressions for the interface motion and the carbon fractions at the interface and within the austenite.

2.1. Semi-analytical model

A ferritic matrix of dimension L is assumed as the initial microstructure, in which an austenite grain of width $2{\cdot}s_0$ is present, produced from the rapid transformation of a pearlite colony at a temperature T above A_1, when austenite becomes thermodynamically stable. If z is the distance from the centre of the austenite grain, the carbon mole fraction $x_C(t,z)$ at $t = 0$ is given by

$$x_C(0,z) = x_C^p \; for|z| < s_0 \text{ and } x_C(0,z) = x_C^{\alpha eq} \; for|z| > s_0 \tag{1}$$

where x_C^p is the average pearlite carbon mole fraction and $x_C^{\alpha eq}$ is the equilibrium carbon mole fraction in ferrite at T (Fig. 1). The origin of the z-axis is in the centre of the grain. Because of the symmetry in this system, in the remainder we will consider only $z > 0$.

The model focusses on hypo-eutectoid systems, for which the equilibrium carbon mole fraction in austenite (γ) in equilibrium with ferrite, $x_C^{\gamma eq}$, is lower than x_C^p at intercritical temperatures. Therefore the austenite/ferrite interface experiences a driving force, ΔG, to move into the ferrite phase. This driving force ΔG depends on the carbon mole fraction at the interface in the austenite, x_C^i, which develops during the phase transformation. In the present approach ΔG is assumed to be proportional to the deviation of the carbon fraction at the interface from the equilibrium fraction in austenite, that is

$$\Delta G = \chi(x_C^i - x_C^{\gamma eq}), \tag{2}$$

with x_C^i the carbon mole fraction in austenite at the interface position s, $x_C(t,s) = x_C^i$.

Although it has been shown [20–21] that the chemical potential of interstitial elements should always be equal at the interface of a sharp interface model here it is assumed that ferrite forms at the equilibrium carbon fraction, also when the interface carbon fraction in austenite is different from the equilibrium value. The differences in the ferrite carbon fractions caused by this simplification are negligibly small.

The interface velocity v is proportional to this driving force, i.e.

$$v = M\Delta G \tag{3}$$

with M the interface mobility.

For finite carbon diffusivity, a carbon gradient is established within the austenite. In line with the analytical description of the austenite-to-ferrite transformation [9][19], the carbon-fraction profile in austenite ($z < s$) is assumed to be exponential in z (see Fig. 1) and given by

$$\begin{aligned} x_C(t,z) &= x_C^h + (x_C^i - x_C^h)\frac{\exp(z/z_0) + \exp(-z/z_0) - 2}{\exp(s/z_0) + \exp(-s/z_0) - 2} \\ &= x_C^h + (x_C^i - x_C^h)\frac{\cosh(z/z_0) - 1}{\cosh(s/z_0) - 1} \end{aligned} \tag{4}$$

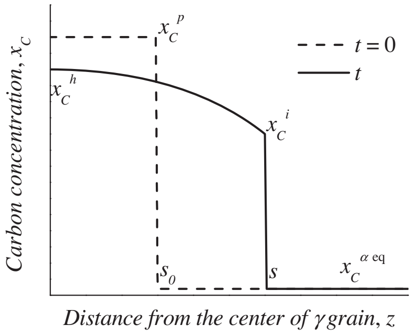

Fig. 1. Carbon mole fraction in austenite ($z < s$) and in ferrite ($z > s$); the initial carbon mole fraction is given by the dashed line, the fraction at a certain stage during the transformation by the solid line.

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