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A 2D analysis of the competition between the equiaxed ferritic and the bainitic morphology based on a Gibbs Energy Balance approach

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ABSTRACT

Upon austenite decomposition, either of two ferritic morphologies may result depending on the steel composition and the transformation temperature, i.e. equiaxed (i.e. quasi spherical) or plate-like ferrite. A 2-D model based on the Gibbs Energy Balance (GEB) model and the Zener–Hillert equation is presented to explain the conditions leading to either morphology. To this aim the kinetics of isotropic growth and plate-lengthening, plate-thickening are modeled with appropriate assumptions regarding the interface conditions respectively. The competition between the two morphologies is determined by the fastest minimization of the total Gibbs energy of the system during transformation. The model is first applied to a ternary alloy containing an austenite forming element (Fe-0.23C-1.86Mn) and the predicted morphology competition is in good agreement with experimental observations. In the refined model, the effect of nucleation on the growth of a plate is rationalized. For the plate-like bainitic transformation, a new concept of 'single plate-thickening stasis' is proposed, in addition to the commonly discussed 'global stasis of the bainitic transformation', i.e. the incomplete bainitic transformation. A general model of the global transformation kinetics bridging the single plate stasis and the global stasis is depicted. Finally, without changing any of the model assumptions or transition conditions the model is applied to a ternary alloy containing a ferrite forming element (Fe-0.375C-1.48Si) The predicted morphology competition is fully in line with the experimental observations for samples subjected to isothermal decomposition at different temperatures.

1. Introduction

Ferrite and bainite are the two primary microstructural constituents in advanced automotive steels and are essential in determining the mechanical properties [1]. While they both have the same crystal structure, their morphologies are rather different. Many terms are used to describe these morphological differences such as polygonal ferrite, allotrimorphic ferrite, widmanstätten ferrite, bainitic ferrite, granular bainite etc. It is well known that the morphology depends on both the transformation temperature and the chemical composition. For a steel with a fixed composition, allotrimorphic ferrite tends to grow into an equiaxed (i.e. quasi spherical) shape at higher temperatures, while the bainitic plate-like morphology is usually observed for transformations at lower temperatures [2–5]. For example, for an Fe-0.23C-1.86Mn alloy ferrite grows into an equiaxed shape at 650 °C, but into a plate-like morphology at 600 °C and 500 °C [5]. On the other hand, for the same heat treatment condition, the morphology of the decomposition product will also be affected by the chemical composition [6,7]. Various modeling attempts have been made to quantify the growth kinetics for different morphologies. For the growth of a spherical reaction product, Zener established an analytical solution based on the diffusional theory [8], which has been proven to be particularly suitable for the high temperature transformation in describing the parabolic development of the grain radius over time. For plate shaped precipitates, Fang et al. proposed a ledgewise growth model [9]. According to this model, the rate of new ledge formation in combination with the movement of ledge riser strongly influences the final ferrite morphology. Purdy and Brechet suggested an alternative approach to model the bainite growth

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based on solute drag theory and ledge mechanism [10], but their model does not allow a direct comparison between model prediction and experimental observations. Moreover, due to the preference of crystallography orientation and the anisotropy, the lengthening and thickening kinetics of the plate-like product can be very different. Various models have been proposed for the lengthening kinetics [11–14] and their results have been compared to experimental observations obtained via in-situ experiments [15,16]. Enomoto gave an excellent overview of the observations and made detailed comparisons between the various approaches [17]. Nevertheless, very little effort can be found in literature on capturing the kinetics of the thickening behavior and its impact on total transformations kinetics, either from an experimental point of view or from a modeling perspective. Chang and Bhadeshia [18] only measured the thickness of bainitic ferrite plate in the final transformation product but did not link it to the transformation kinetics. On the modeling side, earlier attempts have been restricted to solving diffusion equations for different morphologies [19]. However, a purely diffusional approach based on Fick's law seems to be insufficient to capture the physical factor behind the different morphologies.

Apart from the models mentioned above, solute drag theory also plays an important role in studying the ferrite and bainite transformations. The solute drag theory, firstly established by Lücke and Detert [20] for the recrystallization process, focuses on the speed of migration of interface by considering the retarding force exerted by solute atoms segregated to the phase (grain) boundaries. Later, the theory was extended and very successfully applied in explaining how solute drag force influences the kinetics of phase transformation [21–28]. Nevertheless, most of those solute-drag related studies concentrated on the high temperature decomposition, i.e., pro-eutectoid allotrimorphic ferrite and polygonal ferrite, while leaving Widmanstätten ferrite and bainitic ferrite unresolved. Chen et al. [29] made a step further to explain bainitic stasis (incomplete transformation) phenomenon based on the solute drag approach. In his work, the stasis is caused by enrichment of carbon in the austenite, which decreases the chemical driving force, while at the same time substitutional elements enrichment at the moving interface takes place. Once the remaining austenite volume fraction drops below a critical point, a sudden kinetic transition would occur, i.e. from a high velocity to the one several orders of magnitude slower. Thus, transformation seems to 'stop' while the austenite has not yet fully decomposed. The current models related to solute drag effects are essentially 1-D planar interface models which only describe the isotropic growth but not the common occurring plate-like morphology.

In the present study, the kinetics of plate-lengthening, plate-thickening and isotropic growth are modeled by imposing appropriate interface conditions and interface migration mechanisms, i.e. either the Gibbs Energy Balance (GEB) model or the Zener–Hillert equation. The competition between the different morphologies is analyzed by examining the rate of the energy minimization as a function of the growth and the transition conditions compared to experimental observations. The morphology evolution and competition as function of the transformation temperature is investigated, both for a ternary alloy containing an austenite forming element (Fe–C–Mn) and a ternary alloy containing a ferrite forming element (Fe–C–Si).

2. Model description

To simplify the model and to capture the underlying physical principle behind the two ferrite morphologies, the different ferritic and bainitic microstructures are classified into only two categories according to their principal morphological characteristics, i.e. an equiaxed (quasi spherical) shape or a plate-like morphology. The first group stands for polygonal or allotrimorphic ferrite, while the second category includes widmanstätten ferrite and bainitic ferrite. It should be mentioned that this work focuses on a 2-D geometry which can be extended to a 3-D geometry at a later stage. The 2-D plate-like morphology in the plane of observation could in the 3-D reality be a needle-like or disc-like shape. A recent experimental 3-D reconstruction of ferrite plates formed at 570 °C and 600 °C indicated that the out of plane third dimension lies between the other two dimensions [30], which allows us to simplify it to a 2-D simulation. Hence, a 2-D geometry is accurate enough to present the concept of the morphology competition. A schematic illustration of the morphologies considered is shown in Fig. 1. For plate-like growth, the lengthening and thickening of a single plate, also called 'edgewise growth' and 'sidewise growth', proceed with two different rates and hence the aspect ratio changes continuously. For the isotropic growth, the interface moves without an orientation preference, resulting in a half spherical shape. Nucleation of ferrite is assumed to take place on the austenite grain boundaries, as the nucleus would benefit from the internal energy at the grain boundary in overcoming the energy barrier. In this paper, the three growth rates are named 'plate-lengthening rate', 'plate-thickening rate' and 'isotropic rate' respectively.

2.1. Calculation of lengthening rate with Zener-Hillert equation

Plate lengthening rate is treated by the modified Zener–Hillert equation, which is described in detail in Ref. [11]:

$$v_{len} = \frac{D_c}{8^* \rho_c} \frac{\Omega_0}{1 - \Omega_0} \tag{1}$$

$$\rho_c = \frac{\sigma^* V_m}{RT\left(x_c^{\gamma/\alpha} - x_c^0\right)} \tag{2}$$

$$\Omega_0 = \frac{x_c^{\gamma/\alpha} - x_c^0}{x_c^{\gamma/\alpha} - x_c^{\alpha/\gamma}} \tag{3}$$

Where v_{len} is the lengthening rate of single plate; ρ_c is the critical radius of the circular cylinder tip; σ is the interfacial energy between austenite and ferrite; V_m is the molar volume of austenite; R is the ideal gas constant; T is the absolute temperature; Ω_0 is the supersaturation of Carbon; x_c^0 is the mole fraction of bulk Carbon concentration; $x_c^{\gamma/\alpha}$ and $x_c^{\alpha/\gamma}$ are equilibrium mole fraction of Carbon in austenite and ferrite, respectively, according to thermodynamic equilibrium calculation performed by *ThermoCalc* from TCFE6 database [31] and D_c is the diffusivity of Carbon in austenite as obtained from Mob2 database [32];

2.2. Calculation of plate thickening rate and isotropic growth rate

2.2.1. Dissipation of Gibbs energy

The Gibbs energy dissipation in a moving interface consists of two parts: the dissipation due to substitutional solute trapped in the interface and that due to the interface friction itself:

The solute enrichment at the moving interface can be modeled by allocating a potential well to the interface which attracts solute atoms to the ferrite/austenite boundaries and hence Gibbs energy is consumed by pulling these atoms forward together with interface migration. Various potential well functions have been proposed including homogeneous [33,34], truncated wedge [21], parabolic [35] and triangular [36,37]. In the present work a triangular potential well is employed. The drag force is determined by the extent