MODELLING THE KINETICS OF BAINITE TRANSFORMATION IN STEELS

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Abstract

This work presents a new physically-based model describing the transformation of austenite into bainite. Thermodynamic criteria are used for the description of the nucleation and growth of bainite sub-units forming either at grain boundaries or autocatalytically on previous sub-units. The size of the sub-units is calculated for each alloy and temperature. The partitioning and the non-uniform redistribution of carbon is estimated as the transformation proceeds.

The transformation kinetics, as well as the incomplete reaction phenomenon, are correctly predicted. Furthermore, the influence of the austenite grain size on the bainite transformation rate is assessed even for austenite grains smaller than the length of unconstrained bainite sub-units. In this case, the observed enhanced nucleation rate is semi-empirically related to the austenite yield strength.

Introduction

Different mechanisms have been proposed for the bainite formation [1-5] but only a few quantitative models can predict the reaction kinetics. When considered to be a displacive transformation, the bainite reaction involves the repeated nucleation and growth of small sub-units of supersaturated bainitic ferrite, followed by the redistribution of carbon into the surrounding untransformed austenite [6]. Due to this carbon redistribution the bainite transformation may stop before the complete austenite transformation [6].

The effect of the austenite composition and grain size, the carbon redistribution, the entrapment of carbon-enriched austenite films between bainite sub-units and the role of newly formed bainite sub-units as potential nucleation sites (autocatalysis or sympathetic nucleation) are all issues that need to be considered in a model describing this reaction. Furthermore, the extreme case of very small austenite grains that constrain the growth of the bainite sub-units is particularly interesting, since it may involve the interaction of the stresses generated during the transformation with the transformation kinetics, and an early soft impingement. Hitherto, the bainite transformation in small grains has been hardly referred in the literature.

The purpose of the present study is to assess a model that addresses the above-mentioned issues and is able to predict the transformation kinetics of the bainite reaction and the final volume fractions of bainite, retained austenite and carbon-enriched austenite films for a wide range of steels.

Description of the model

Thermodynamic criteria for transformation

The criterion used for nucleation is described by Bhadeshia [6]. It infers that the magnitude of the maximum possible free energy change for nucleation, ΔG_m, needs to exceed the *universal nucleation function* G_N [6]. Once this criterion is fulfilled, the nucleus will grow into a sub-unit if the free energy change for diffusionless transformation from austenite to ferrite $\Delta G_{np}^{\gamma \to \alpha}$ becomes negative. Rigourously, this energetic term should be still negative once the stored energy term resulting from the transformation has been taken into account. The stored energy for bainite has been estimated to be as high as $400 \ \mathrm{J \cdot mol^{-1}}$ [6].

Since carbon partitioning and redistribution accompanies the progress of the bainite transformation, the thermodynamic parameters for nucleation and growth, ΔG_m and $\Delta G_{np}^{\gamma \to \alpha}$, will change continuously during the reaction, and the occurrence of the incomplete reaction phenomenon is not needed as an input parameter but results from the application of the thermodynamic criteria.

In the case of austenite grain boundary nucleation (*i.e.* primary nucleation) and growth, the average composition of the remaining untransformed austenite is used. However, in the case of autocatalytic nucleation, ΔG_m is calculated considering the equilibrium carbon composition of bainitic ferrite to account for the enhanced nucleation rate on a ferrite substrate [6].

Bainite sub-unit

Each bainite sub-unit is assumed to have a lenticular shape of maximum thickness α_b and diameter $\alpha_p \cdot \alpha_b$ [2]. The thickness of the bainite sub-units is estimated using a neural network model published by Singh and Bhadeshia [7].

The overall aspect ratio of the bainite sub-units, was characterised by Wang *et al.* as $\alpha_p = 40$ [8]. In the case of small austenite grains, the size of the forming sub-units is adjusted to the size of the austenite grain, while keeping their aspect ratio unchanged, to account for the fact that bainite can not grow across grain boundaries [6].

Kinetics

The kinetics of the bainite reaction can be described in terms of the nucleation and instantaneous growth of bainite sub-units. The reaction will proceed when both criteria for nucleation and growth are fulfilled simultaneously. Nucleation needs to be divided into primary and autocatalytic events.

The primary nucleation rate I_p is defined as

$$I_p = N_0 \cdot s_\gamma \cdot \nu \cdot E_p \tag{1}$$

where N_0 is the density of potential nucleation sites per unit surface; s_γ is the austenite grain surface available for nucleation; ν is an attempt frequency reflecting the thermal agitation of the atoms and E_p is a function that embodies the thermodynamic criteria for primary nucleation. The available austenite boundary area is determined from the original surface area of the austenite grain S_γ, and the volume fraction of remaining austenite v_γ as $s_\gamma = S_\gamma \cdot v_\gamma^{\frac{2}{3}}$. The attempt frequency is $\nu = \frac{k \cdot T}{\hbar}$ with k the Boltzmann constant, $\hbar$ the Planck constant and T the absolute temperature. The function E_p is defined as

$$E_p = \begin{cases} \tanh\left(-\frac{\Delta G_m - G_N}{RT}\right) & : & (\Delta G_m - G_N) < 0 \\ 0 & : & (\Delta G_m - G_N) \geq 0 \end{cases} \qquad (2)$$

where ΔG_m is the maximum possible energy for nucleation, G_N is the universal nucleation function, and R and T have their usual meanings. The function $\tanh(x)$ has been chosen since it allows a correct transition between regimes without any sharp transition.

Autocatalytic nucleation occurs on the surface of the already formed bainite sub-units. The number N_a of nucleation events triggered from each boundary nucleated sub-unit is obtained by,

$$N_a = \frac{2 \cdot D_\gamma}{\pi} \cdot \frac{1}{\alpha_b \alpha_p} \qquad (3)$$

where D_γ is the austenite grain diameter, and $\alpha_b \cdot \alpha_p$ the length of the bainite sub-unit.

The average number of sub-units that may nucleate from each bainite sub-unit tip, β_a, is one of the fitting parameters of the model.

The rate of activation of secondary nuclei per time interval is therefore calculated as,

$$I_a = I_p \cdot \beta_a \cdot N_a \cdot E_a \qquad (4)$$

where E_a is a function embodying the thermodynamic criteria for autocatalytic nucleation which is analogous to Eq. (2).

The amount of bainite formed during a time interval $d\tau$ is thus given by

$$dv_b^e = (I_p + I_a)E_g \cdot u_b \cdot d\tau \qquad (5)$$

where I_p and I_a are the primary and autocatalytic nucleation rates, respectively; u_b is the volume of one bainite sub-unit; and E_g is a function that embodies the thermodynamic growth criterion defined as

$$E_g = \begin{cases} \exp\left(-\frac{G_{np}^{\gamma \to \alpha}}{RT}\right) & : & \Delta G_{np}^{\gamma \to \alpha} < 0 \\ 1 & : & \Delta G_{np}^{\gamma \to \alpha} \geq 0 \end{cases} \qquad (6)$$

where $\Delta G_{np}^{\gamma \to \alpha}$ is the free energy change for diffusionless transformation from austenite to ferrite; R is the gas constant and T is the temperature.

A method based on Avrami's extended volume correction [9] has been used to account for nucleation site depletion and impingement of developing sub-units.

Carbon redistribution

As the bainite reaction happens at temperatures for which the mobility of carbon is low, the redistribution of carbon in austenite tends to be inhomogeneous. It has often been observed that films of carbon-enriched austenite become trapped between bainite sub-units [6]. The composition of these austenite films is close to the value given by the Ae_3' curve (i.e. the composition of the $(\alpha+\gamma)/\gamma$ phase boundary in paraequilibrium conditions [6]). The carbon-enriched austenite films act as carbon reservoirs, slowing the enrichment of the remaining austenite. The end of the bainite reaction is thus postponed.

The volume fraction of austenite trapped as thin films between sub-units depends on the volume fraction of bainite. The model presented here considers a volume fraction of enriched austenite v_h relative to the bainite volume fraction v_b as $v_h = P_h \cdot v_b$.

Transformation in small austenite grains

There are cases in which the length of the bainite sub-unit is potentially larger than the size of the austenite grain. As bainite cannot grow across grain boundaries, this issue will need to be incorporated in the model as described previously. The increased protagonism of the primary nucleation with respect to autocatalysis as the austenite grain diminishes is already described in the model. Only the build up of transformation stresses as bainite sub-units are forced to grow parallel to each other [10], needs to be included. It is well known that external and internal stresses affect the kinetics of many transformations, and particularly of the bainite reaction, by an enhancement of the nucleation rate [6, 11, 12]. The effect of the stresses generated during the transformation can therefore be described by including an additional term in the definition of the density of potential nucleation sites per unit surface N_0. This term takes the form of an enhanced activation rate, in which the activation energy is a function of the austenite yield strength, σ_y.

$$N_0 = N_s \exp\left(-\frac{B_s \cdot \sigma_y}{R \cdot T}\right) \tag{7}$$

where σ_y is the austenite yield strength; B_s is a function that describes the tensile state of the parent austenite; N_s is a potential nucleation site surface density and R and T have their usual meanings. As more work is still needed to characterise B_s and N_s thoroughly, they will be used as fitting parameters.

Fitting parameters

The present model uses the following fitting parameters. First, the surface density of potential nucleation sites N_0, which has been fitted to $N_0 = 2.0 \cdot 10^{-4}$ nuclei $\cdot$ m^{-2}. Second, the number of sub-units that, on average, can nucleate autocatalytically from each previously formed bainite sub-unit. This would be a complex function of grain size and geometry, and therefore it has been treated as a fitting parameter and its value adjusted to $\beta_a = 1.5$ as a realistic value. Third, the thickness of each one of the carbon-enriched austenite films trapped between bainite sheaves is a parameter difficult to evaluate. In the present model, it has been restricted to an upper boundary of 6% of the thickness of a bainite sub-unit. Finally, the nucleation rate in small austenite grains needs to be better understood. In the present model, it still needs to be described with two fitting parameters: $B_s = 4.0$, which is a function describing the stress state of the parent austenite and $N_s = 7.12 \cdot 10^4$ nuclei $\cdot$ m^{-2}, which is a potential nucleation site surface density enhanced by the internal stresses.

Validation of the model and Discussion

In order to assess the validity of the model, its predictions are compared with published experimental data of the bainite transformation kinetics. The austenite grain size and chemical composition of the investigated alloys are given in Table 1, and described elsewhere [10].

	Size /μm	/wt.%	C	Mn	Si	P	S	Al
Steel A	8, 50		0.58	1.66	1.35	0.006	0.02	0.03
Steel B	2		0.29	1.42	1.41	0.012	0.02	0.04

Table 1: Austenite grain size and chemical composition and of the investigated steels.

Figure 1 compares the predicted evolution of the bainite reaction with the experimental data for steel A with an austenite grain size of 8μm held at $360°$C. The model predicts correctly that the reaction first accelerates with the increasing volume fraction of bainite, and then decreases asymptotically up to the final bainite volume fraction described by the T_0' curve (incomplete reaction).
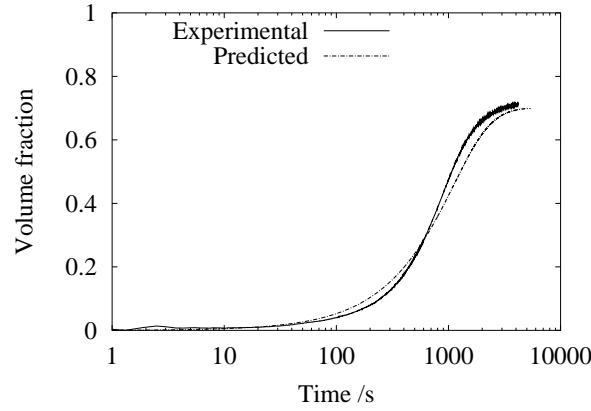

Figure 1: Experimental and predicted kinetics of isothermal bainite transformation at $360°$C for steel A with an austenite grain size of 8μm.

Figures 2 (a) to (c) present the experimental and predicted times for achieving bainite transformation levels of 30% and 60% and the maximum bainite volume fraction obtained when the incomplete reaction phenomenon occurs. The considered austenite grain sizes are 2, 8 and 50μm, and the temperatures of the isothermal heat treatments are 310, 360, 410 and $460°$C , respectively.
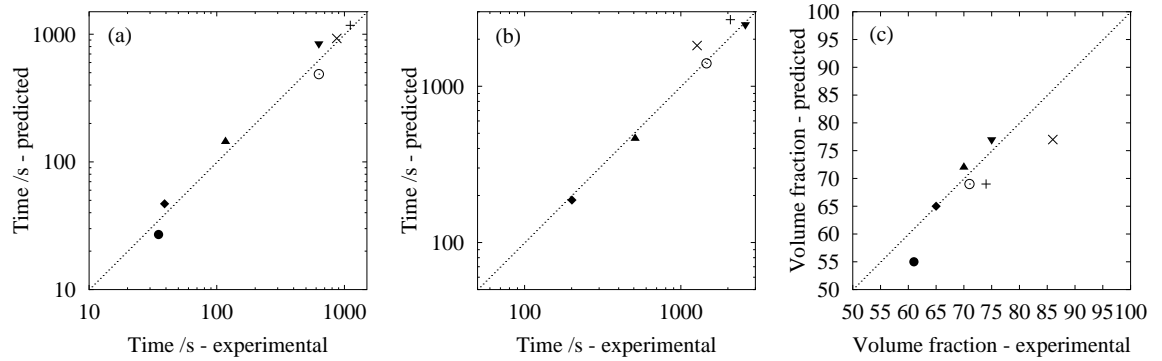

Figure 2: Predictions *vs.* experimental values of the time needed to reach (a) 30% of transformation, (b) 60% of transformation and (c) of maximum volume fraction of bainite. ▼ grain size 2μm at $310°$C; ▲ grain size 2μm at $360°$C; ♦ grain size 2μm at $410°$C; ● grain size 2μm at $460°$C; ⊙ grain size 8μm at $360°$C; × grain size 50μm at $310°$C; + grain size 50μm at $360°$C.

The prediction of the final volume fraction of bainite (incomplete reaction phenomenon), presents good agreement with experimental data. Only in the case of the transformation in a large grain at low temperature, where the carbon has low mobility, the model tends to underpredict the final volume fraction of bainite. On the other hand, the time for the several degrees of transformation is in all cases remarkably well predicted.

Conclusion

A model for the bainite reaction kinetics has been developed. This model takes into account the effects of the composition and austenite grain size, of the different nucleation sites, of the carbon partitioning and inhomogeneous redistribution, of the formation of carbon enriched austenite films between bainite sub-units and also of the varying dimensions of the forming bainite sub-units with temperature, austenite composition and yield strength. The model also takes into account the effect of the stress state resulting from transformation in the case of small austenite grains. As more work is still required, this effect is described using a semi-empirical equation function of the austenite yield strength. The model has been applied to published data and its predictions show remarkable agreement over a large interval of temperature and grain size.

Acknowledgements

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