

Regular article

Bainite formation kinetics in steels and the dynamic nature of the autocatalytic nucleation process



Ashwath M. Ravi*, Jilt Sietsma, Maria J. Santofimia

Dept. of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, Delft 2628 CD, The Netherlands

ARTICLE INFO

Article history:

Received 27 February 2017

Received in revised form 2 June 2017

Accepted 29 June 2017

Available online xxxx

Keywords:

Bainite

Kinetics

Nucleation

Isothermal heat treatments

ABSTRACT

Over the years, a quantitative theory to explain bainite formation kinetics has been proposed based on the nucleation kinetics of bainitic sub-units. Although the theory shows acceptable correlation with experimental results, it is observed that the kinetic models show a certain degree of discrepancy with actual kinetics. It is identified that these mainly arise due to the inadequate estimation of autocatalytic nucleation, especially as a function of progress of bainite formation. With the help of this observation, the kinetic model is modified and a better insight into the process of autocatalytic nucleation, essential in bainite formation, is obtained.

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Among the wide variety of products formed by the decomposition of austenite in steels, formation of bainite is one of the least understood phenomena [1–8]. According to the displacive theory of bainite formation, the rate of bainite formation, df/dt , is proposed as

$$df/dt = (1 - f)(1 + \lambda f)\kappa_f \quad (1)$$

where f is the bainite fraction, λ is the autocatalytic parameter and κ_f is the rate parameter which accounts for the thermally activated nature of the bainite nucleation process [9–15]. This equation was derived based on the displacive mechanism of bainite formation [9,13]. Bainite formation in steels begins with nucleation of bainitic ferrite at austenite grain boundaries. Subsequently, nucleation continues further through autocatalytic nucleation of bainitic ferrite at the newly created bainitic ferrite/austenite interfaces [16]. The difference in nucleation rate of bainite formed by autocatalysis compared to the nucleation rate of bainite due to grain-boundary nucleation is accounted for by the term λf in Eq. (1) [9–13]. Most studies applying Eq. (1) treat λ as an empirical dimensionless fitting constant [13]. The values obtained for λ are however not satisfactorily analysed in the literature [6]. Recently, the present authors [15] proposed that λ is determined by the difference in activation energy for bainite nucleation at austenite grain boundaries and bainite

nucleation at bainite/austenite interfaces (autocatalytic nucleation) and can be expressed as

$$\lambda = \exp\left(\frac{\Delta Q^*}{kT}\right) \quad (2)$$

where ΔQ^* is the difference ($Q_G^* - Q_A^*$) in the activation energy for grain-boundary nucleation (Q_G^*) and autocatalytic nucleation (Q_A^*), k is Boltzmann's constant and T is the bainite formation temperature.

Studies claim that nucleation based models using the functional form described in Eq. (1) accurately predict the bainite formation kinetics in steels [9,11–13,15]. However, a close examination of the published results suggests that these models still show a certain degree of miscalculation of kinetics [10–12,14]. Santofimia et al. [13] evaluated the applicability of several kinetic models which are based on the displacive theory of bainite formation. They also observed that the models imprecisely estimate the nucleation rate and called for a better treatment of autocatalytic nucleation [13]. Although these discrepancies are rarely investigated in detail, they have been attributed to improper estimation of final volume fraction of bainite or to unaccounted carbide precipitation [13]. This implies that these discrepancies are generally considered to be due to the improper estimation of the degree of carbon enrichment of austenite, since the carbon content in austenite determines final volume fraction of bainite [10,14] and the degree of carbide precipitation during bainite formation [11].

In the current work, it is shown that an adequate estimation of carbon enrichment alone is not sufficient to accurately simulate the

* Corresponding author.

E-mail addresses: A.M.Ravi@tudelft.nl (A.M. Ravi), J.Sietsma@tudelft.nl (J. Sietsma), M.J.SantofimiaNavarro@tudelft.nl (M.J. Santofimia).

Table 1
Chemical compositions of steels used for study (values in wt%).

Steel	C	Mn	Si	Mo	Al	Reference
S1	0.2	3	–	–	–	Current work
S2	0.2	3.51	1.52	0.25	0.04	[17]

rate of bainite formation. A strong argument for this is presented here. A fundamental change in the assumptions for autocatalytic nucleation, especially as a function of increasing bainite fraction, is required to adequately estimate bainite formation kinetics. Based on these new assumptions, the bainite kinetics is simulated and compared with experimental results.

The compositions of the steels used for the present work are given in Table 1. Studies in the current work have been carried out using kinetic data obtained from isothermal bainite formation experiments on Steel S1. The bainite formation experiments were carried out in a Bähr DIL805A/D dilatometer. Specimens were first austenized at 1273 K and then isothermally held at 653 K. The bainite fraction formed as a function of time was determined based on the dilatometer data obtained. Results obtained from these studies were further validated using the kinetic data published in the literature on Steel S2 (isothermal treatment at 603 K for 1 h after austenization at 1173 K) [17].

Fig. 1 (a) gives the experimentally obtained bainite fraction, f vs time for both steels, while Fig. 1 (b) gives the rate of bainite formation, df/dt , as bainite formation progresses. Fig. 1 (c) and (d) shows experimentally obtained $(df/dt)_v$ as a function of f in Steel S1 and Steel S2 respectively, where $(df/dt)_v$ is the rate of bainite formation per unit volume of untransformed austenite (volume fraction available for bainite formation). It is given as

$$(df/dt)_v = (df/dt)/(1-f). \quad (3)$$

$(df/dt)_v$ is an important parameter in understanding the bainite formation kinetics. The overall rate of bainite nucleation in steels mainly depends number of grain-boundary nucleation sites available and the potency of these nucleation sites to form bainitic ferrite sub-units. It should be noted that the rate of autocatalytic nucleation also depends on the rate at which grain-boundary nucleation occurs, since grain-boundary nucleation is a prerequisite for creating bainite/austenite interfaces and subsequent autocatalytic nucleation. The potency of grain-boundary nucleation sites to transform into bainitic sub-units and facilitate autocatalytic nucleation is influenced by rate governing parameters such as bainite formation temperature and carbon concentration in austenite [12,13,18,19]. $(df/dt)_v$ gives a measure of this potency. Physically, it represents the rate at

which grain-boundary nucleation sites can contribute to the overall nucleation rate. Numerically, $(df/dt)_v$ can be determined using experimentally obtained (df/dt) data and the corresponding bainite fraction, f .

The displacive theory of bainite formation suggests that the rate of bainite formation is determined by the nucleation of bainitic sub-units. Thus from Fig. 1 (c) and (d), the rate at which bainite nucleation occurs within the available austenite can be interpreted. It can be seen from these figures that the rate of austenite transformation into bainite constantly changes as bainite formation progresses.

One of the well documented reasons for such a change in the austenite transformation rate is due to the possible carbon enrichment of austenite during bainite formation [20]. Since $(df/dt)_v$ is a measure of the rate of austenite to bainite transformation, the effect of carbon enrichment on the rate of bainite formation can be understood by interpreting its effect on $(df/dt)_v$. Using Eqs. (1) and (3), $(df/dt)_v$ can be given as

$$(df/dt)_v = (1 + \lambda f)\kappa_f. \quad (4)$$

With the help of Eq. (4) and the kinetic model proposed by the authors [15], a physically based interpretation of $(df/dt)_v$ can be derived since the carbon enrichment of residual austenite during bainite formation is well accounted for in the proposed model. The underlying principles used in Ref. [15] for calculation of bainite formation kinetics are similar to other published models [12,13,18,19] that use displacive theory of bainite formation. In Ref. [15], the effect of carbon enrichment on the rate of bainite formation is calculated using a fitting constant, X_b . X_b accounts for the carbon which does not participate in the carbon enrichment of austenite. Using the approach given in Ref. [15], κ_f in Eq. (1) can be given as

$$\kappa_f \propto (T_h - T)(T'_0 - T) \exp\left(-\frac{Q_G^*}{kT}\right) \quad (5)$$

where T_h and T'_0 are the critical temperatures which define the thermodynamic conditions for bainite formation [3]. The factor $(T_h - T)$ signifies the driving force available for bainite nucleation, while the factor $(T'_0 - T)$ signifies the driving force available for bainite growth [3]. T_h , T'_0 and Q_G^* are all functions of carbon concentration of austenite [3,15,20] and can be expressed in terms of f and X_b [15]. Studies suggest that T_h and T'_0 decrease linearly and Q_G^* increases linearly with increasing carbon enrichment of austenite [15].

In order to understand the effect of carbon enrichment of austenite on the rate of bainite formation, $(df/dt)_v$ was calculated assuming varying degrees of the carbon enrichment (by numerically varying the value of X_b) using Eqs. (2), (4), and (5). In Eq. (5), the proportionality constant is a material dependent parameter and is calculated according to Ref. [15] (for Steel S1 = $1.92 \text{ s}^{-1} \text{ K}^{-2}$). According to the

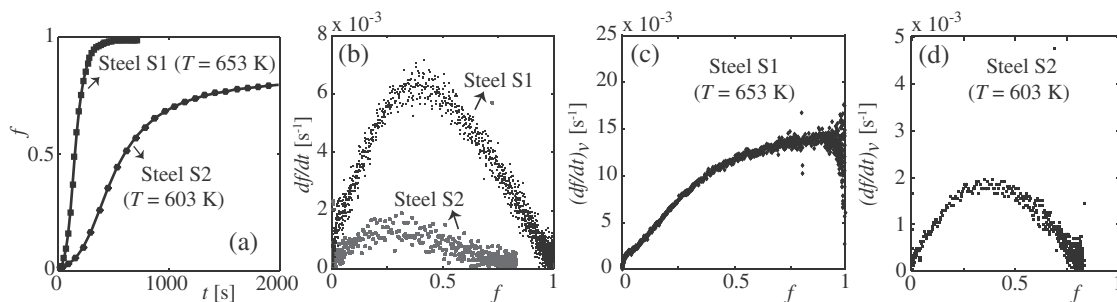


Fig. 1. (a) Comparison of experimentally obtained kinetics (Steel S1 at $T = 653 \text{ K}$, Steel S2 at $T = 603 \text{ K}$). (b) Experimentally obtained df/dt vs f , (c, d) Experimentally obtained $(df/dt)_v$ vs f .

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