Bainite transformation kinetics
Part 2 Non-uniform distribution of carbon

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The carbon concentration trapped in films of austenite between parallel platelets of bainite is often found to be much larger than that in the larger blocks of austenite between sheaves of bainite. The effect of this non-uniform distribution of carbon on the overall transformation kinetics of bainite is examined theoretically. It is found that the trapping of carbon in the films of austenite accelerates the bainite transformation. This effect increases with increasing film thickness and with decreasing average carbon concentration. *MST/1628*

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Introduction

Bainite in steels tends to grow in the form of clusters of small, parallel plates known as 'subunits', each of a limited size. All subunits within a particular sheaf have the same crystallographic orientation.[1,2] The individual plates within a sheaf, although interconnected in three dimensions, can be separated along most of their surfaces by thin films of untransformed austenite, especially in steels where carbide precipitation reactions are suppressed (it is these steels that are considered here).[1,2] This is in contrast to the large blocks of austenite that may remain untransformed as bainite sheaves growing in different directions impinge on each other. Figure 1 shows untransformed austenite regions of both types.

The maximum extent of the bainite reaction in steels is limited by the carbon that diffuses from the supersaturated bainitic ferrite plates into the untransformed austenite immediately after transformation. Such steels are of considerable technological importance from the point of view of ultrahigh strength alloys and welding alloys. The partitioned carbon enriches the austenite as reaction proceeds to such a degree that the driving force for transformation eventually reaches zero. The reaction then stops, although substantial amounts of untransformed austenite remain in the microstructure.

Bainite transformation kinetics have in the past been calculated assuming the carbon to be homogeneously distributed in the residual austenite, but there is now considerable evidence that this is not the case. The films of austenite between the ferrite plates are to a large extent isolated by the surrounding ferrite. They can achieve carbon concentration levels far in exess of those expected assuming a homogeneous distribution. Such 'trapping' of excess carbon in the isolated films would intuitively be expected to lead to a larger maximum volume fraction of ferrite, as the carbon concentration in the larger blocks of untransformed austenite will be correspondingly smaller at each stage of reaction. There is some experimental evidence for this. Continuous cooling experiments, in which the cooling rate is so low that there is a greater opportunity for partitioned carbon to homogenise, show that a higher degree of transformation is obtained when the carbon is inhomogeneously distributed.[3]

The purpose of this work is to examine theoretically the extent to which the trapping phenomenon influences both the kinetics and the maximum extent of transformation that can be achieved at any temperature, using the theory developed in Part 1[4] of this paper. The modifications and improvements made to the original kinetic theory are incorporated and extended here.

Accounting for trapping of carbon

The treatment of bainite kinetics as presented in Part 1[4] supposes the carbon that is rejected from the transformed bainitic ferrite to be homogeneously distributed in the untransformed austenite. In reality, some of the austenite is in the form of isolated films between the plates of ferrite. The carbon that diffuses into these films becomes trapped there, and should therefore change the way in which the reaction proceeds. A modification presented below takes account of the expected inhomogeneous distribution of carbon.

Some simplifying assumptions are necessary. It is assumed that one film of austenite is trapped for each subunit of bainite that grows. It is well established that the films trapped within sheaves are carbon enriched to concentrations that are in general much higher than would be expected from the T'_0 curve (explained in Part 1[4]). Therefore, it is assumed that the films are saturated with carbon. The composition of the austenite films is then given by the value of the Ae'_3 curve at the reaction temperature (this is the composition of austenite at the paraequilibrium $(\alpha+\gamma)/\gamma$ phase boundary). The paraequilibrium phase boundary is chosen because no substitutional alloying element partitioning occurs during bainite formation. With reference to a unit volume of austenite, a volume u is assigned to each bainitic subunit and a volume v_t to each film of trapped austenite.

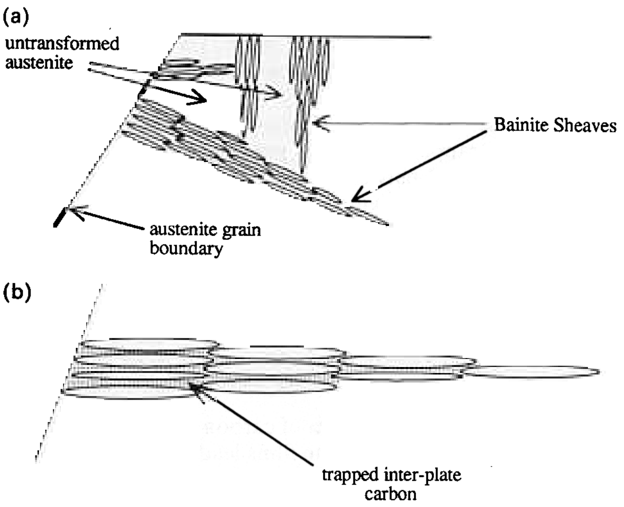
By a mass balance argument, the carbon content x_B of the untransformed blocky austenite after n plates of ferrite have formed in a unit volume of sample (i.e. when the volume fraction of ferrite is nu) is given by

$$x_B = \frac{\bar{x} - nu[x_\alpha + (v_t/u)x_{Ae'_3}]}{1 - nu[1 + (v_t/u)]} \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (1)$$

where $\bar{x}$ is the mean carbon content of the alloy, x_α is the carbon concentration of the ferrite, and $x_{Ae'_3}$ is the carbon content of the austenite saturated with carbon.

The reaction of austenite to ferrite will cease when the composition of the austenite has reached the T'_0 value.[2,3] This is the carbon concentration at which ferrite with a strain energy of 400 J mol^{-1} has the same free energy as austenite of the same composition, which therefore makes it the limiting austenite composition that can support transformation to bainite. By rearrangement of equation (1), a maximum allowable volume θ' can be calculated. This corresponds to the condition where the carbon concentration of the blocky austenite has reached the T'_0 value

$$\theta' = \frac{\bar{x} - x_{T'_0}}{[x_\alpha + (v_t/u)x_{Ae'_3}] - [1 - (v_t/u)x_{T'_0}]} \qquad (2)$$



a blocky regions of austenite between sheaves; *b* thin films of carbon enriched austenite between bainitic subunits

Location of untransformed austenite in bainitic microstructure

It is possible, however, for the austenite to become enriched in carbon to such an extent that the nucleation of ferrite by a displacive mechanism is impossible, before the carbon content of the austenite reaches $x_{\mathrm{T}_0'}$ (determined by the driving force for bainite growth). Under these conditions, if x_{N_0} represents the carbon content at which nucleation ceases, the maximum allowable extent of transformation is

$$\theta' = \frac{\bar{x} - x_{\mathrm{N}_0}}{[x_\alpha + (v_\mathrm{t}/u)x_{\mathrm{Ae}_3'}] - [1 - (v_\mathrm{t}/u)x_{\mathrm{N}_0}]} \quad . \quad . \quad . \quad . \quad (3)$$

Regardless of whether the termination of reaction occurs because the available driving force is insufficient for nucleation or for growth, it is convenient to express the mole fraction of ferrite in terms of a normalised volume fraction

$$\xi' = v/\theta' \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (4)$$

where, as demonstrated above, the actual volume fraction of ferrite $v = nu$.

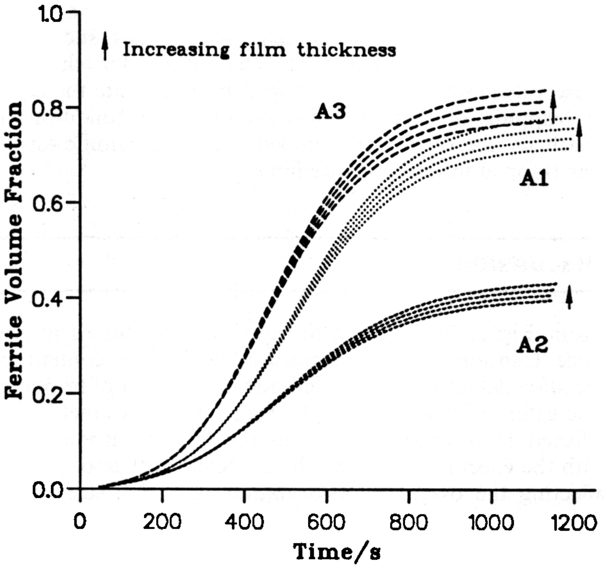
Computational details

The assumption that all films are of identical volume is of course an approximation. It is difficult to estimate the relative thickness of the plates and films meaningfully, as bainitic plates often touch along some of their surfaces. A series of hypothetical values is therefore used to represent the film thickness so that the sensitivity of the predicted transformation rate to the trapping effect can be investigated.

Calculations were performed for three hypothetical steels of different carbon and substitutional solute content (Table 1). As it is anticipated that carbon trapping will affect both the driving force and the allowable extent of reaction, it is of interest to perform calculations comparing reactions for two cases, i.e. alloys with different carbon levels but the same driving force and alloys with the same carbon content but different driving forces.

Table 1 Compositions of steels chosen for investigation of predicted effect of trapping of carbon in retained austenite films, wt-%

Steel	C	Si	Mn
A1	0·1		2·0
A2	0·2		1·87
A3	0·1		1·5



2 **Calculated effect of presence of trapped austenite films on bainite kinetics of three hypothetical steels (Table 1)**

Alloy A2 was chosen to have the same driving force as alloy A1 at 500°C so that special consideration could be given to the relative reaction rates at this temperature. Alloy A3 has the same carbon content in weight per cent as alloy A1, though the mole fraction of carbon will be slightly different for the two alloys. The important thermodynamic quantities for the three alloys at 500°C are given in Table 2. For all three alloys at this temperature, $x_{\mathrm{T}_0'}$ was found to be less than x_{N_0}. Termination of reaction will therefore be due to a failure of the thermodynamic criterion for growth in all three cases, and the maximum extent of transformation is calculated using $x_{\mathrm{T}_0'}$.

Note also that the maximum allowable fraction of ferrite for alloys A1 and A2 will be different at 500°C, as the carbon content is different. Carbon can also affect the reaction kinetics by altering the autocatalysis factor. It is therefore anticipated that the trapping phenomenon will affect the lower carbon alloy to a greater extent than the higher carbon alloys, as a greater fraction of the total carbon will be trapped in the thin film austenite.

Results

Figure 2 shows the calculated effect of the presence of trapped high carbon austenite films on the predicted reaction profiles of alloys A1, A2, and A3 at 500°C. For comparison, Table 2 gives the values of the important parameters from the bainite reaction kinetics theory for

Table 2 Comparison of parameters affecting predicted kinetics of bainite transformation at 500°C: values are independent of effect of trapping of carbon, and account for some differences in transformation rate shown in Fig. 2

Steel	ΔG^0_m, J mol^{-1}	β	$\bar{x}$, at. fraction	$x_{\mathrm{T}_0'}$, at. fraction	$x_{\mathrm{Ae}_3'}$, at. fraction
A1	−880	148·79	$4{\cdot}541 \times 10^{-3}$	$1{\cdot}396 \times 10^{-3}$	$5{\cdot}678 \times 10^{-3}$
A2	−880	125·12	$9{\cdot}050 \times 10^{-3}$	$1{\cdot}447 \times 10^{-3}$	$5{\cdot}194 \times 10^{-3}$
A3	−996	148·78	$4{\cdot}542 \times 10^{-3}$	$1{\cdot}673 \times 10^{-3}$	$6{\cdot}582 \times 10^{-3}$

these three steels at the reaction temperature. Four different film thicknesses are considered, with values such that $v_t/u = 0{\cdot}005$, $0{\cdot}01$, $0{\cdot}015$, $0{\cdot}02$. The reason for choosing these values was that it was hoped to investigate the effect of trapping of carbon while avoiding the condition in which *all* the carbon partitioned from the bainitic ferrite was trapped in the austenite films.

Discussion

From Fig. 2, for steels with equal driving forces at the same transformation temperature the carbon content of the alloy determines the magnitude of the effect of trapping. The extent of reaction and the transformation kinetics are affected to a greater degree in the lowest carbon alloy, with the effect of carbon on the autocatalysis factor greatly affecting the overall transformation rate. For steels with similar carbon contents but different driving forces, the effect of trapping on the extent of transformation is very similar. In these cases the different reaction kinetics are due mainly to the difference in driving force, as the effect of autocatalysis is the same in both alloys. Although the fraction of carbon trapped in the two steels is dependent on the respective Ae'_3 compositions, it appears that the magnitude of the effect is similar in both cases.

Intuition suggests that the presence of trapped films will have the largest effect on the extent of transformation and the kinetics of transformation for the low carbon alloy in the series being investigated. This is because, with the film composition set equal to the Ae'_3 composition, a larger fraction of the total carbon content of the alloy will be trapped.

The trend in the calculations is that the reaction is faster for the case of the larger film thickness, i.e. the larger the amount of carbon that is trapped, the faster the reaction proceeds. The limiting case is when the film thickness is related to the phase compositions by the expression

$$\frac{v_t}{u} = \frac{\bar{x} - x_\alpha}{x_{Ae'_3}}$$

as this represents the condition where all carbon partitioned by the ferrite ends up in the thin film austenite. Because there will be no enrichment of bulk untransformed austenite under this condition, reaction can proceed until all the bulk austenite is consumed. The resulting microstructure then consists solely of bainitic ferrite and thin film carbon enriched austenite.

Consideration of the effect of trapping on the maximum extent of the bainite reaction for the series of alloys shows that the magnitude of the increase in maximum volume fraction produced by the inhomogeneous distribution of carbon does not vary significantly with substitutional alloying element concentration. This is to be expected, because the effect of trapping is mainly dependent on the proportion of the total carbon that is trapped. The substitutional alloying element concentration can affect the T'_0 and N_0 compositions, but terms such as these are mainly dependent on driving force, so that their effect should be hidden when a comparison is made at constant driving force.

The higher carbon steels show less sensitivity to the presence of trapped carbon. A smaller fraction of the total carbon is trapped between the subunits in these cases. The maximum possible extent of transformation is also smaller. Consequently, the number of sheaves and the corresponding number of austenite films available for trapping is reduced.

Conclusions

The non-uniform distribution of carbon due to the trapping of carbon in isolated austenite films leads to an acceleration of transformation, and further to an increase in the limiting fraction of bainitic ferrite that can be obtained at any temperature. Steels of low carbon content are shown to be more sensitive to the trapping effect because a greater fraction of the total carbon can be accommodated in the films.

Carbide precipitation from austenite is most likely to occur from the film austenite, which is richer in carbon. The present model could in fact be used to estimate the effect of such carbide precipitation on transformation kinetics. The carbides, in effect, remove carbon from the austenite, in a way similar to that by which the films of austenite isolate excess carbon from the reacting bulky regions of austenite.

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