PAPER

Computational analysis of austenite film thickness and C-redistribution in carbide-free bainite

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Abstract

In this work, a methodology for the computational analysis of some essential microstructural features of a bainitic microstructure is developed. The focus lies in the accurate prediction of the ferritic subunit size, the thickness of the residual austenite films, their corresponding C-enrichment and the accompanying stabilization of the residual austenite. Basis of the approach is the T0-temperature concept in combination with the numerical simulation of C-diffusion profiles utilizing the cell diffusion module of the thermokinetic software package MatCalc. This methodology gives the opportunity to predict the C-distribution under consideration of consecutively forming subunits, which is necessary to estimate the C-content of austenite films. The simulations also take into account the effect of C trapping at the dislocations formed inside the ferritic platelets due to plastic deformation and its influence on the chemical potentials. Good agreement is achieved between measured and predicted retained austenite layer thickness and the C-enrichment of the layers accompanying the C redistribution process.

Introduction

Steels with a bainitic matrix have recently regained focus of steel-producing companies. Their special properties, on the one hand, and lean alloying concepts, on the other hand, which are in the region of low alloyed steel, make this material grade particularly interesting. However, bainite is probably the one steel microstructure where the discussion about the underlying phase transformation mechanisms, i.e., the nucleation and growth of the ferritic subunits and the lengthening and thickening of the bainitic sheaves, is still very controversial [1].

The variants of bainitic microstructures are manifold and they depend on the combination of chemical composition and temperature in a complex manner. Knowledge about the geometry of the bainitic ferrite platelets, the thickness of the retained austenite films and their C-content as well as possible Fe-carbide precipitation in either the ferritic platelet or the retained austenite are of great importance in the development of new steel grades and the choice of adequate heat treatment parameters.

Since cost saving is a major aspect for steel industry, the aspired bainitic microstructure should be achievable by an overall chemical composition, which corresponds to that of a low alloyed steel grade. These alloys provide good weldability, which is an important factor for further processing of bainitic steel products [2, 3]. In particular, the focus is on Transformation-Induced-Plasticity (TRIP)-aided steel. The TRIP-effect denotes the stress or strain-induced transformation of (residual) austenite to martensite and the accompanying plastic deformability.

TRIP steels achieve a superior combination of strength and formability [4, 5]. Their microstructure consists of bainitic ferrite platelets (subunits) with C-enriched, thin austenitic films in between. A conglomerate of these subunits with the same orientation is called a bainite sheaf. Eventually, a certain amount of residual (blocky) austenite is also present in these microstructures, which does not transform into bainite during austempering [6]. Figure 1 shows schematically the structure of the described microstructure. The enrichment of carbon is
generally higher in the film-like austenite due to its location between two bainitic ferrite platelets. Since the blocky austenite has a lower level of C-content and, therefore, less mechanical stabilization compared to the austenite films that are trapped between ferrite plates, it is more likely to transform to martensite at relatively small stresses or strains or during cooling to room temperature [7].

The brittle high-carbon martensite that forms at early stages of straining from blocky retained austenite can have negative effects on mechanical properties [8–10]. Films of retained austenite, which are more stable because of their higher carbon content and geometry, are potential microstructural features that improve toughness through the TRIP-effect [11–14]. Since the film-like retained austenite is a crucial part of the microstructure of many steels, which utilize the TRIP effect, it is important to understand the influence of temperature and composition on the properties of these features.

Chang and Bhadeshia [15] introduced a model that describes the thickness of austenite films based on the C diffusion profiles around the ferritic subunits. This approach was adopted by Li et al [16] and further improved by adding a second subunit. While these models already deliver important insights into the distribution of C within a bainitic microstructure, they do not take into account important factors, which affect the C diffusion in this complex environment. In these models, the C diffusion is described with an analytical approach that does not consider factors, such as, the influence of C concentration on C diffusivity. Additionally other mechanisms, which influence the diffusion of C, like dislocation density and trapping of C, can be considered with the approach of this work as will be shown in the following sections. Especially at low temperatures, the effect of C trapping can have a major impact on the resulting C distribution. A better understanding of the evolution of C distribution in bainitic microstructures can help to improve mean field models, which describe the overall transformation kinetics of bainite. Mean field models often assume that the diffusion of carbon from supersaturated subunits into the surrounding austenite happens instantaneous or only describe it based on simple analytical approximations [17–20]. It is shown in [21] that a mean field approach that describes the effect of C diffusion within the bainitic microstructure with an empirical relation improves its ability to predict the bainite transformation kinetics. The approach proposed in this work therefore aims, among other things, to provide insights into the C distribution during bainitic transformations, which can be used to identify possible improvements in mean-field models.

The present work introduces a versatile modeling and simulation concept for carbide-free bainite, which is produced via an isothermal heat treatment at the so-called austempering temperature. The target is to simulate the metallurgical processes involved in the formation of the bainitic microstructure utilizing the $T_0$-concept as suggested by Bhadeshia [22] with thermodynamic and kinetic data from CALPHAD-type databases [23, 24] as well as the diffusion module of the thermokinetic software package MatCalc [25], which is used for the numerical solution of the diffusional C-redistribution between ferritic subunits and residual austenite films accompanying the formation of the bainitic microstructure. Trapping of C atoms at dislocations inside the ferritic platelets is fully taken into account in the simulations on basis of the model developed recently by Svoboda et al [26–28] as well as utilized in the discussion of C-diffusion in the plastically deformed austenite surrounding the platelets.
Structure and thermodynamics of bainite

$T_0$-concept

The first step in the computational analysis of bainite formation is the estimation of the bainite start temperature during cooling from austenitization temperature. Although controversial hypotheses on the mechanism of bainite formation exist \cite{1}, the present authors assume that bainite formation is mostly a partitionless displacive transformation with the formation of a ferritic subunit in the first step, in accordance with the model suggested by Bhadeshia and Edmonds \cite{6}. Any diffusional redistribution of C-atoms between ferritic platelet and residual austenite occurs only in a subsequent step, after the platelet formation has completed. For a comprehensive description of this topic, reference is made to Bhadeshia \cite{22}.

For the description of bainite nucleation, the $T_0$-concept is adopted. $T_0$ denotes the particular temperature where the transformation parent and product phases, i.e., austenite and ferrite, have identical free energy at identical chemical composition. Consequently, any partitionless phase transformation can occur only below this characteristic temperature \cite{22}. Since the partitionless transformation from austenite to ferrite involves shear forces and a change in molar volume, a certain amount of mechanical energy must be expended to make the transformation commence. The corresponding amount of energy has been estimated to be in the order of 400 J mol$^{-1}$ in an Fe–Ni–Si–C steel \cite{29}. Depending on chemistry and the inherent strength of the parent austenite, this value can change and it is generally higher in higher strength alloys.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Calculated $T_0$, $T_0'$ (400 J mol$^{-1}$) and martensite start ($M_S$) temperatures. Composition is 1.5 wt% Si and 1.5% Mn, balance is Fe.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Comparison of $M_S$-temperatures calculated via the $T_0$-concept and empirical equations from literature (Composition: 1.5 wt% Si, 1.5 wt% Mn, balance Fe). Grain size for equation from Lee and Park, 2013, is chosen as 50 μm \cite{33–36}.}
\end{figure}
If this excess energy is taken into account in the \( T_0 \)-concept, the actual transformation start temperature becomes \( T_0' \). Figure 2 shows examples for calculated \( T_0 \) and \( T_0' \) curves for a steel with a classical TRIP-steel composition of 1.5 wt% of Si and Mn utilizing MatCalc with the corresponding thermodynamic and mobility databases [23].

In addition to predictions of the bainite start temperature, the \( T_0 \)-concept also allows for some estimation of the bainite transformation stop conditions. Under certain circumstances, the growing bainitic sheaves, which represent groups of subunits with intermediate austenite layers, lead to a C-enrichment of the remaining untransformed austenite. According to this concept, figure 1 shows that the \( T_0' \)-temperature decreases with increasing C-enrichment in the austenite and, eventually, the bainite reaction comes to a stop before all parent austenite has transformed. This effect is often referred to as the ‘incomplete reaction phenomenon’ [6, 30, 31].

In order to determine the stability of the residual austenite against a martensitic transformation during cooling to room temperature, it is important to have information also on the martensite start (\( M_S \)) temperature. Likewise the \( B_S \) temperature, which is given by the \( T_0' \) temperature, the value of \( M_S \) can also be estimated on basis of the \( T_0 \)-concept. The major difference between the bainite and martensite transformations is that the latter is an entirely athermal reaction, i.e., it is independent of the cooling rate and it involves higher driving forces to initiate the transformation. Typical values for martensite driving forces in low alloy steels are in the order of 1200 to 1700 J mol\(^{-1}\) [32]. In higher alloyed steels, the necessary driving forces to initiate the martensite transformation can exceed these values substantially, however.

In figure 3, \( M_S \)-temperatures are calculated via the \( T_0 \)-concept and compared to different empirical equations for \( M_S \)-temperatures from literature [33–36]. Accordingly, a C-content between 1.3 and 1.4 wt% stabilizes austenite down to room temperature. For the bainite transformation, this observation means that a minimum C level of approximately these values is necessary to stabilize the retained austenite films between the ferritic subunits.

**The numerical model**

In this section, the concepts of the numerical simulation strategy are outlined. According to Chang and Bhadeshia [15], the austenite film thickness is controlled by the diffusion field of C around a bainitic ferrite platelet into the surrounding residual austenite. This assumption has also been adopted by Li et al [16] to calculate the C-enrichment between two bainite subunits.

In this manner, the present model is based on the assumption of a displacive formation mechanism of the bainitic ferrite plates (=subunits), with subsequent partitioning of the excess C from bainitic ferrite into the
surrounding austenite as described by Bhadeshia [22]. According to this mechanism, C starts to diffuse out of the ferrite platelet, having a rather low solubility for C, into the austenite, having a comparably high C solubility. As a consequence, a C diffusion profile develops from the ferritic platelet into the residual austenite. Since C-diffusion is a thermally activated mechanism, this process takes time depending on the transformation temperature. The main feature of this concept is now that the austenite attached to the ferrite platelet develops a more or less steep concentration profile with the maximum being located at the ferrite/austenite interface (figure 4).

According to the $T_0'$-concept, newly formed parallel subunits, which originate from the same sheaf, can approach the initial subunit during transformation only so close until the C-concentration of the residual austenite reaches the value given by the $T_0'$-temperature. Once the displacive transformation has stopped, the retained austenite film between the original and the new ferritic platelet absorbs C also from the new platelet (figure 4). According to Chang and Bhadeshia [15] and Li et al [16], the following assumptions can be employed:

(i) C diffusion is only taken into account in the thickening direction of the bainitic subunits. Due to the significant lengthening of the bainite plates, other directions can be neglected.

(ii) Subunits parallel to the initial subunit form as soon as the initial subunit is decarburized. This implies that the time between subunit formation is equal or higher than the time needed for decarburization of the initial plate.

(iii) The adjacent subunit has the same size as the initial subunit.

(iv) The time needed for a subunit to grow to its final size is comparably fast and can be neglected, i.e. subunits reach their final size almost instantaneously.

(v) Precipitation of carbides in austenite and bainitic ferrite can be neglected (carbide-free bainite).

To apply the present model, the $T_0'$ curve is first calculated to obtain the C content up to which a bainite platelet can form. Figure 5 shows an example of a $T_0'$-curve for a 0.4C-1.5Si-1.5Mn (wt%) steel, where the critical carbon content at 400 °C is marked.

The diffusion calculation is performed in a planar 1D geometrical setup in the cell simulation module of MatCalc, which utilizes a finite differences scheme to calculate transient multi-component diffusion profiles. The evolution of carbon content in the individual cells after solving Fick’s law of diffusion implicitly is given by,

$$
\left[ 1 + \frac{D_{i+1} \Delta t}{(\Delta x)^2} + \frac{D_{i-1} \Delta t}{(\Delta x)^2} \right] c_{i+1}^{t+} - \frac{\Delta t}{(\Delta x)^2} \left[ D_{i+1} c_{i+1}^{t+} + D_{i-1} c_{i-1}^{t+} \right] = c_{i}^{t},
$$

where $c_i^t$ is the carbon content of cell $i$ at the time $t$, and $c_{i+1}^{t+}$ at the time $t + \Delta t$. $D_{i+1}$ is the mean diffusion coefficient of the cells $i$ and $i + 1$ and $D_{i-1}$ is the mean diffusion coefficient of the cells $i$ and $i - 1$. A system with N cells therefore is a linear equation system of N equations in N variables.

![Figure 5. Calculated $T_0'$-curve for a 0.4C-1.5Si-1.5Mn (wt%) steel. $T_A$ is the austempering temperature (400 C) and $C_{T0'}$ is the C-content up to which an adjacent bainite platelet can grow.](image-url)
Figure 6. Scheme of the simulation steps for the cell diffusion calculation. (a) $t_0$, initial state with nominal C-content, $C_0$, in all cells; (b) $t_1$, carbon profile after decarburization of the ferritic bainite platelet (=subunit), another bainite platelet is inserted into the simulation; (c) $t_2$, second bainite subunit has reached its equilibrium C-content; thickness of the austenite film $d_{\gamma}$, thickness of a bainite subunit $d_{\alpha}$, $C_0$ is the C-content of the ferritic subunits in equilibrium ($\sim 0.02$).
At phase boundaries, additionally a flux $J$ due to differences in chemical potential $\mu$ is considered. This flux is given by,

$$J = \frac{Dc \cdot \partial \mu}{R_g T \cdot dx},$$

with $D$ being the diffusion coefficient, $c$ the concentration, $x$ a 1D planar spatial coordinate and $R_g$ the gas constant. In discretized form, the flux $J_{i,i+1}$ for cell $i$ if a phase boundary exists between cell $i$ and $i+1$ is then calculated by,

$$J_{i,i+1} = -\frac{D_{i,i+1} \cdot c_{i,i+1} \cdot \mu_i - \mu_{i+1}}{R_g T \cdot |x_i - x_{i+1}|},$$

where $D_{i,i+1}$ and $c_{i,i+1}$ are the arithmetic mean values of diffusion and carbon concentration of the cells $i$ and $i+1$, $c_{i,i+1}$. The change of C concentration in cell $i$ is then calculated with

$$\Delta c_i = \frac{J_{i,i+1} \cdot A_{i,i+1}}{V_i} \Delta t,$$

with $A_{i,i+1}$ being the area between cells $i$ and $i+1$ and $V_i$ being the volume of cell $i$. In our 1D simulation, the factor $A_{i,i+1} / V_i$ can be reduced to a division by the thickness of the cell. The change in concentration is added to equation (1) on the right hand side if a cell is located next to a phase boundary, i.e. if a neighboring cell has a different matrix phase. The diffusion coefficients for each cell are taken from the diffusion database mentioned earlier [38]. More details and use cases with this approach can be found in [37] and [38]. The effect of dislocation density and other factors on the diffusion coefficients of C will be described in later sections of this work.

A main advantage of this numerical cell diffusion approach over analytic approximations is that the C diffusivity in each cell is evaluated as a function of the current chemical composition, the dislocation density and temperature. Different geometrical configurations with a number of bainitic subunits can be studied easily and, finally, each cell can perform a fully coupled precipitation kinetics calculation to evaluate the simultaneous long-range diffusion of C and precipitation kinetics of carbides inside the ferritic platelet. The latter is not carried out in the present analysis since it is assumed that the investigated alloys are carbide-free, however, it will be in the focus of follow-up future work.

In the simulation, initially, the FCC_A1 (austenite) phase with a chemical composition corresponding to the nominal composition of the investigated alloy is assigned to each cell ($t_0$). In the process of formation of a ferritic platelet, the status of the transforming cells is instantaneously switched to the BCC_A2 (ferrite) phase. The interface between the two phases is assumed to be mechanically arrested and it remains stationary throughout the further simulations. The assigned phase and its composition define the chemical potential and diffusional mobilities of elements within each cell and, thus, the multi-component diffusion kinetics in the course of the elemental redistribution process. Additional microstructural properties, such as, the dislocation density, are likewise assigned and impact the simulation results. The size of the one-dimensional diffusion simulation box is chosen as 500 nm, which corresponds to the necessary size for representation of an entire C-profile over several ferritic platelets and the remaining residual austenite.

When the simulation is started, a certain number of cells, corresponding to the half-thickness of a bainitic subunit, is switched from FCC to BCC on the left side of the simulation box. This choice is done due to symmetric boundary conditions on the left end. The simulation then runs until the ferrite platelet is depleted from C, but without equilibrating the carbon content of the austenite ($t_1$). At this moment, the simulation is interrupted, and the thickness of the austenite film is read from the C-profile plot at the critical C-content as shown in figure 6. The data in figure 6 are taken from an example simulation for a 0.4 C-1.5 Mn-1.5 Si wt% steel.

Starting with this cell, additional right-neighboring cells, representing the full thickness of a new bainitic subunit, are changed from FCC to BCC and the diffusion simulation continues. The simulation is again interrupted, when the new ferrite platelet is depleted from C ($t_2$). The C-content of the layer between the two ferrite platelets is taken as calculated C-concentration of retained austenite films of the corresponding alloy at a given temperature. The described simulation steps and an example of the corresponding C-concentration profile is given in figure 6. The temperature in this simulation is 400 C.

**Results**

**Austenite film thickness**

The capabilities of the present model to predict the thickness of austenite films is first challenged on experimental data from [15] and [39]. Chang and Bhadeshia [15] have used these data in order to show that the austenite film thickness depends on the diffusion of C out of the ferritic bainite plates into the surrounding austenite. For these alloys, a full set of experimental data consisting of composition, bainite plate thickness,
austenite film thickness and temperature are reported. Table 1 summarizes the composition of the investigated alloys. Composition, bainite plate thickness and temperature are used in the following as input parameters for the cell diffusion simulation, which delivers the austenite film thickness as a result.

Figure 7 compares the austenite film thicknesses as predicted by the present model and using the assumptions (i) to (v) made in the ‘Numerical model’ section with measured values from the aforementioned references. Interestingly, the measured film thickness is systematically larger than the calculated one. A comparable trend has been observed in the original analysis by Chang and Bhadeshia [15], where a similar modelling approach has been used. According to these authors, this underestimation of film thickness could

![Figure 7](image1.png)

**Figure 7.** Measured and calculated austenite film thickness assuming nucleation of successive subunits to commence as soon as the first platelet has become depleted from C. Experimental data from [15].

![Figure 8](image2.png)

**Figure 8.** Calculated evolution of C-concentration profiles in the vicinity of a subunit. The locations of the critical carbon content (horizontal dashed line), $d_i$, correspond to the simulation times, $t_i$. While the predicted film thickness increases from $t_0$ to $t_3$, it decreases afterwards and, eventually, reaches zero again after longer simulation times.

![Table 1](image3.png)

**Table 1.** Composition of reference alloys [wt%].

| Alloy | C  | Si | Mn | Cr | Ni |
|-------|----|----|----|----|----|
| A     | 0.27 | 1.98 | 2.18 | 1.9 | 0   |
| C     | 0.46 | 2.1  | 2.15 | 0   | 0   |
| E     | 0.1  | 1.77 | 2.12 | 0   | 2   |
| H     | 0.1  | 1.63 | 1.99 | 1.97| 0   |
stem from the assumption that successive parallel bainitic subunits form as soon as the existing platelets reach their equilibrium C-content. This assumption is, in its nature, intuition-based rather than founded on sound metallurgical basis and it is further investigated, next.

The present numerical simulations indicate that the depletion of a bainite subunit from C is a rather fast process, which is typically finished within the range of roughly 0.01 to 0.2 s, depending on temperature and thickness of the subunit. However, the time, which is required to progress the point of critical C content far enough into the remaining austenite to be in accordance with the experimental results for the austenite film thickness, is up to one order of magnitude longer. To analyze this observation in more detail, the diffusion simulations are run for extended times without the addition of a second bainite subunit to identify the point where the simulated film thickness is as close to the experimentally measured values as possible. Figure 8 illustrates the process of shift of the critical C-content with time and the resulting increase in austenite film thickness based on composition profiles of C for various isothermal holding times, exemplarily, for a 0.4C–1.5Si–1.5 Mn (wt%) steel.

In the beginning of the transformation, a sharp concentration peak for C is observed and the distance where the C-content corresponds to the calculated $T_0'$-temperature gradually moves into the parent austenite starting at the initial phase boundary. After a certain time, the peak of the C-distribution falls back below the critical C-content and a maximum possible film thickness exists for every alloy composition and temperature. To illustrate this behavior, the evolution of predicted film thickness for steels C and A, as determined by the $T_0'$-temperature, is exemplarily shown in Figure 9. For steel C, this distance moves into the parent austenite, reaches a maximum at roughly 70 nm at 430 C and then moves back to zero. Since the experimentally observed thickness is at around 50 nm, the ‘optimum’ time corresponding to this particular thickness can be read straightforwardly from the diagram. The same is performed for a temperature of 260 C, where the experimentally measured value is roughly 6 nm and the maximum calculated thickness is around 10 nm. For steel A, however, the predicted maximum thicknesses of roughly 6 nm and 28 nm never reach the experimentally ones of 11 nm and 40 nm, neither at 400 C nor at 300 C.

Figure 10 compares calculated austenite film thicknesses with literature data based on these ‘optimum’ times for the formation of the next parallel subunit ($t_{nu}$). Apparently, only for steel C, the calculations can match the experimental values exactly. For all other experimental data, the agreement can be made better but not perfect. One source for this discrepancy might be sought in the assumptions (i) to (v) defined earlier. Another source might be the possible enrichment of untransformed austenite regions that can become enriched in C. Consequently, bainite subunits that form in the beginning of the reaction can experience lower C-contents compared to subunits formed towards the later stages of the bainite transformation. The simulations, however, always refer to the initial C-content of the austenite. And, finally, another source might be present in simulation input parameters, which govern the evolution of C-profile in the residual austenite and, therefore, also the austenite film thickness. The most relevant parameter, in this context, is the diffusivity of C as a function of the microstructural state parameters stress, defect concentration (i.e. dislocation density) and C-content of the austenite. These factors are discussed in the following section.
Influence of elastic lattice stress on diffusivity

When a ferritic platelet forms, the molar volume of the new phase is larger than the molar volume of the surrounding parent austenite by roughly 1% [40]. Following the analysis of the deformation and stress state of a spherical inclusion in [41], a positive volumetric misfit between ferritic platelet and austenite matrix shall cause compressive stress in normal direction and tensile stress in tangential direction to the surface of the inclusion. In a first approximation, this observation should also hold for an ellipsoidal inclusion and a tensile stress field should prevail around a subunit normal to the C diffusion direction. This expansion of the austenite lattice leads to an enhancement of C diffusion in the normal of the subunit surface, which is quantified next.

In [42], the influence of the C-content on the diffusivity of C is analyzed and it is concluded that the effect of increasing diffusivity with increasing C content can be most accurately described with Asimow’s model [43]. This approach assumes that the faster C diffusion is induced by a lattice parameter expansion caused by interstitially dissolved C. To approximate the effect of stress on the diffusivity, in a rough estimation, it is assumed that the increase of the lattice parameter due to elastic stress has a comparable impact on the C-diffusivity as an increase of the lattice spacings due to dissolved C in the austenite matrix.

Due to the volumetric misfit, during transformation, both, the ferritic platelet and the surrounding austenite, are plastically deformed [44] and the amount of stress in the austenitic matrix corresponds roughly to its yield strength. This value, \( \sigma_y \), can be estimated by the empirical equation proposed by Eres-Castellanos et al [45] as

\[
\sigma_y = (52.3 + 47.0X_C + 31.3X_{Si} + 1.0X_{Mn} + 1.0X_{Cr} + 31.3X_{Mo} + 1.3X_{Ni} \\
+ 10.7X_V + 3.8X_{Al} + 16.8X_{Cu} + 15.2X_{Ti} + 53) \\
\times \left(1 + 0.001 \ln \left( \frac{\varepsilon}{0.001} \right) \right) \left(1 - \left( \frac{T_y}{1487 - 25} \right)^{0.658} \right)
\]

with \( X_i \) being the concentration of element \( i \) in at-%, \( \varepsilon \) the strain rate and \( T_y \) the temperature difference to room temperature (25 °C). The experimental data that was used to derive this empirical relation covers composition and temperature ranges of the reference steels that are investigated. Therefore, a reasonable approximation of the yield strength in the context of the presented approach should be possible. A comparison of calculated and experimental values for the yield strength of various steels at different temperatures and other empirical equations are extensively discussed by Eres-Castellanos et al in [45]. The strain rate is approximated with 1000 s \(^{-1} \) and the Youngs modulus is taken as the one used in the MatCalc simulations for the FCC_A1 phase with \( E = (193000 - 73.33 \cdot T) \cdot 10^6 \) and \( T \) inserted in °C. The resulting average expansion of the lattice \( \varepsilon_{lattice} \) can be calculated using Hooke’s law \( \sigma_y = E \varepsilon \) with roughly 0.13 to 0.16%.

The equation describing the lattice parameter of austenite depending on carbon concentration from Dyson and Holmes [46] is

\[
a_a = 3.5780 + 0.033w_C
\]

with \( a_a \) being the lattice parameter of austenite and \( w_C \) being the C-content in wt-%. According to equation (6), about 0.14 to 0.17 wt% of C are necessary for the same lattice expansion as calculated above. This carbon

![Figure 10. Comparison of measured and calculated austenite film thickness, with ‘optimized’ times for formation of the second bainitic subunit. Experimental data from [15].](image-url)
equivalent is used to evaluate the effect of stress on the diffusion of carbon. The dependence of diffusivity on carbon concentration is taken from Agren et al\textsuperscript{[47]}, who provided a corresponding equation as

\[
D_C = 4.53 \cdot 10^{-7} \left(1 + \chi (1 - \chi)^{1.8339.9} \right) \times \exp \left( -\left( \frac{1}{T} - 2.221 \cdot 10^{-4} \right)(17767 - 26436\chi) \right),
\]

with the composition variable \( \chi = X_C / (1 - X_C) \), where \( X_C \) is the mole fraction of carbon. According to the results of this approximation, the diffusivity of C in the austenite matrix is increased by a factor depending on temperature and composition. Figure 11 shows the factor by which the C diffusion is increased depending on temperature for the reference steels.

**Influence of dislocation density on diffusivity**

The plastic deformation of the austenite surrounding the ferritic subunit induces an increased dislocation density and, thus, increases the effective C diffusion kinetics through the mechanism of pipe diffusion. This effect is fully taken into account in the current simulations as \[48\]

\[
D_{eff} = D_0 \cdot (1 - \alpha_{disl}) + D_p \cdot \alpha_{disl}
\]

with the effective diffusion coefficient, \( D_{eff} \), \( D_0 \) being the diffusion coefficient in the undisturbed crystal, \( D_p \) being the diffusion coefficient along the dislocation core and \( \alpha_{disl} \) being the volume fraction of dislocation cores, which is calculated as,

\[
\alpha_{disl} = \pi R_{core}^2 \cdot \rho,
\]

with \( R_{core} \) being the radius of the dislocation core, which is assumed to be 0.5 nm, and \( \rho \) being the dislocation density. The equation describing the diffusion of C along a dislocation core is,

\[
D_p = D_0 \cdot \exp \left( \frac{Q_{DC}}{R_g T} \right),
\]

where \( Q_{DC} \) is 29.2 kJ mol\(^{-1}\) [48] and \( R_g \) is the universal Gas Constant.

Measurements from Cornide et al\textsuperscript{[49]} suggest that the dislocation density in austenite surrounding a ferritic subunit is similar to the dislocation density within the subunit. Therefore, it is reasonable to utilize data on the number of dislocations within the subunit to estimate, or at least give an upper boundary for, the amount in austenite. Takahashi and Bhadeshia\textsuperscript{[50]} propose an empirical equation for the upper limit of dislocations in bainite in the temperature range of 473–942 K as

\[
\log_{10} \rho_d = 9.28480 + \frac{6880.73}{T} - \frac{1780360}{T^2},
\]

with \( \rho_d \) being the dislocation density per m\(^2\) and \( T \) being the temperature in Kelvin. This equation is describing the experimental data, which was used to develop it quite well, but due to its mathematical structure it predicts a decrease in dislocation density below 245 °C without physical evidence for this effect according to the underlying experimental data. Therefore, an alternative equation is proposed in order to reproduce the same experimental data, but with monotonically decreasing behavior in the relevant temperature region. After fitting several
equation types to the experimental data by the method of least squares an equation with the structure of the probability density of a normal distribution was chosen. It achieved the best results, i.e. least mean square errors, while ensuring that there is no decrease of calculated dislocation density down to 0 °C. The resulting empirical equation is,

\[ \rho_d = 7 \cdot 10^{15} \cdot \frac{1}{0.28 \sqrt{2\pi}} \cdot e^{-\left(\frac{T_c}{280}\right)^2} \]  

(12)

with \( T_c \) being the temperature in °C. This equation is compared to the experimental data and equation (11) from \[50\] in figure 12.

**Impact of carbon diffusivity**

The time for the second ferritic subunit to form in order to obtain ‘optimum’ simulation results strongly depends on the diffusivity of C. Different aspects influencing C diffusion are discussed in the previous sections. The optimized times until the next subunit forms (\( t_{\text{rms}} \)), for different approaches for the effective C diffusion coefficient, are illustrated in figure 13. The approach designated as ‘low dislocation density’ assumes a fixed dislocation density of \( 10^{13} \) m\(^{-2}\) in austenite, which results in relatively low ‘excess’ C diffusivity and, therefore, longer times until the calculated film thickness is as close as possible to the experimentally obtained values. The points named ‘with lattice stress’ represent simulations, which take into account the effect of stress in the lattice,

**Figure 12.** Empirical equations (11) and (12) together with experimental data from \[50\].

**Figure 13.** Time until an adjacent bainite subunit forms in order to get best agreement between calculated and measured austenite film thicknesses; (a) linear y-scale; (b) log y-scale.
while still the fixed dislocation density of $10^{13} \text{ m}^{-2}$ is applied. ‘High dislocation density’ designates the simulations where the dislocation density in austenite is approximated by equation (12), resulting in the highest C-diffusivity. Exponential functions are fitted to the corresponding data points, which can be used as input parameters for further simulation studies with the present approach.

One implication of these empirical relations is that the nucleation/formation of an adjacent subunit needs more time at lower temperatures. This does not necessarily mean that the overall reaction kinetics become slower with decreasing temperature, but only that the thickening rate of single sheaves decreases with decreasing temperature. The phenomenon of longer times for the formation of the second subunit becomes less pronounced when effects that increase the carbon diffusivity are considered. Especially, the influence of dislocations decreases the increase in $t_{\text{nsu}}$ since the dislocation density increases with decreasing temperature.

For the following simulation studies, the ‘high dislocation density’ model is used, since there exists the aforementioned evidence of high dislocation densities in austenite around ferritic bainite subunits and a smaller increase in $t_{\text{nsu}}$ when compared to the other models. Since the effect of stress is much less pronounced than the effect of dislocation density, only the latter effect is considered. The function that is used in the following simulation studies for the time until the next ferrite plate forms is

$$t_{\text{nsu}} = 23 \exp^{-0.0144T},$$

with $T$ inserted in °C.

**General predictions of the model**

To derive general trends from the present model, an example composition of 1.5 Mn-1.5 Si (wt%) with varying C-concentrations is chosen because it represents a standard alloying concept for TRIP-assisted bainitic steels. To the knowledge of the authors, small changes in the composition of substitutional elements should not change the overall behavior to a decisive degree and the derived trends should, therefore, be valid for a broader selection of alloys, which undergo the bainite transformation as long as the formation of carbides in austenite is sufficiently suppressed.

The size of the bainitic ferrite plates is calculated by the formula given in [51]. It was originally developed by Parker [52], who empirically modelled the subunit thickness, $d_0$. Parker assessed the data of steels with C-contents between 0.095 and 0.5 wt% in a temperature range between 523 and 773 K and obtained

$$d_0 = 2 \cdot 10^{-7} \cdot \frac{T - 528}{150} [\text{m}].$$

Figure 14 illustrates the trends for thickness and C-content of austenite films for the aforementioned composition with 0.2 and 0.4 wt% of C as predicted by the present simulations. The film thickness increases with increasing temperature and C-content in the austenite matrix, whereas the C-concentration in the retained austenite varies only to a rather limited degree. According to the calculated and empirical martensite start temperatures in figure 3, the amount of C in the austenite films of both alloys is sufficient to stabilize them at room temperature against martensitic transformation.

Due to the lack of data available in literature, it is difficult to put the predicted trends of the present simulations into a quantitative context. Data from [53] show a C-content of ~1.8–2.2 wt% in austenite films for a 0.39 C - 4.09Ni - 2.05Si wt% alloy at a transformation temperature of 400 °C. For an initial C-content of 0.4 wt% the current model predicts C levels in the films of ~2.6 wt%. The simulation gives the C-content of films at the moment of their formation. It is possible that C diffuses out of the films and into the surrounding blocky austenite areas over time. This can happen, albeit slowly, because the austenite films can be connected to the blocky austenite on their narrow sides. Since in experimental setups the C-concentration in films is measured at a point where a lot of films already exist for some time, lower values are expected when compared to this kind of simulation.

**Austenite films at low temperatures**

At low bainite transformation temperatures, trapping of C-atoms at defects becomes an important effect, which needs to be accounted for in the diffusion simulation. For instance, in ‘nano-scale’ bainite, which forms at approximately 200 °C and below [54, 55], the strongly deformed ferrite platelets can bind substantial amount of C in stable solid solution at the dislocations. This C is unavailable for diffusion into and stabilization of the austenite films. The C-content of fresh martensite at 200 °C can be as high as 0.2 wt%, depending on the actual dislocation density [56], the trapping of C in bainitic ferrite is experimentally confirmed by x-ray and atom probe measurements [54, 57].

The effect of trapping is incorporated in the present simulations with the approach introduced by Svoboda et al [26–28]. The trapping enthalpy, $\Delta E$, and coordination number, $c$, are the main input parameters for this model. These are chosen as $\Delta E = 75000–20^0T$ [J mol$^{-1}$] and $c = A/T^2$, with the coefficient $A = 10^{6}$, as suggested by Mayer et al [58].
In [55], atom probe measurements of a bainitic microstructure consisting of ferritic bainite plates and austenite films, which formed at 200 °C, are reported. The bainite subunit thickness and location in the simulation is taken from the original source [55]. It is assumed that the thicker subunit formed first and the thinner one afterwards. Due to the smaller overall dimensions of the transformation observed experimentally, the size of the simulation box is defined with 140 nm. The dislocation density is taken as $3 \times 10^{15}$ m$^{-2}$, based on measurements in the range between 200 and 350 °C for this steel [59].

Figure 15 compares the measured and calculated carbon profiles over two ferrite platelets. The calculated thickness and carbon content of the austenite film between the bainitic ferrite plates is in good agreement with the APT measurements. The C content within the ferritic part of the microstructure seems to be slightly overestimated by the current trapping model, although some areas in the second subunit even exceed the carbon concentration as predicted by the model. The areas to the left of the initial subunit and to the right of the second

![Graph](image1.png)

**Figure 14.** Predicted austenite film thickness and C-concentration within the austenite films for 0.2 wt% and 0.4 wt% matrix carbon concentration, respectively.

![Graph](image2.png)

**Figure 15.** Simulation of bainite formation at 200 °C, with and without trapping taken into account. APT measurements from [55].

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one cannot be compared to the experimental results since the information about the surroundings, i.e., where is the next ferritic platelet is located, is missing in the simulation.

Bainite, which forms at temperatures as low as 200 °C, commonly occurs in the form of lower bainite, where carbide particles form within the bainitic ferrite subunits in competition with the C diffusion into the surrounding austenite [50]. According to Caballero and Bhadeshia [54], however, practically no carbides were found in similar steels although extensive TEM (transmission electron microscopy) investigations were performed. On the other hand, atom probe investigations from [59] reveal, that very small carbide particles may exist in the investigated steel. However, according to [59], the influence of carbide precipitates on the carbon distribution in the microstructure is extremely small. Therefore, neglecting them should have only a minor influence on the results of the simulations presented. It should be noted that for other compositions, carbide precipitation reactions could have a more pronounced effect and, therefore, should be considered in these cases. Corresponding modeling and simulation work is in process, however, will be reported elsewhere because carbide precipitation introduces additional complexity, which is exceeding the scope of the present manuscript.

Summary and conclusions

In the present work, a model for the simulation of austenite film thickness and carbon distribution in a bainitic microstructure is introduced. It is based on Chang and Bhadeshia’s [15] idea that the austenite film thickness depends on the carbon diffusion profile around the bainitic ferrite plates. The ability to describe the evolution of carbon concentration profiles in the presence of multiple subunits is one of the main features of our model. Consequently, this approach provides a more complete description of diffusion processes within bainite sheaves compared to simple analytical approaches because these often neglect important factors, such as, the influence of C concentration on C diffusivity. Furthermore, it is shown that the effects of stress and dislocation density on the diffusion of C can be considered with this method. Carbon trapping at dislocations, which plays an increasing role at decreasing transformation temperature, is accounted for by the presented model. Thus, carbon concentration profiles for bainitic microstructures that form at low temperatures (nanoscale bainite) can be consistently reproduced. Therefore, the presented model can be used to study trends in carbon concentration and size of retained austenite films for a broad variety of steels and over a wide range of temperatures.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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