



Full length article

Displacive and elastic driving forces in the bainitic transformation: A multiphase-field study with experimentally observed chemically heterogeneous austenite

Thea Kannenberg^{a,b}, Bowen Zou^c, Wenwen Song^c, Daniel Schneider^{a,b,d,*}

^a Karlsruhe University of Applied Sciences, Institute of Digital Materials Science (IDM), Moltkestr. 30, Karlsruhe, 76133, Germany

^b Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-MMS), Straße am Forum 7, Karlsruhe, 76131, Germany

^c University of Kassel, Institute of Materials Engineering (IfW), Department of Granularity of Structural Information in Materials Engineering (GWS), Mönchebergstr. 7, Kassel, 34125, Germany

^d Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT-MSS), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany

ARTICLE INFO

Keywords:

Bainitic transformation
Displacive theory
Manganese heterogeneity
Flash austenitization
Multiphase-field method
Atom probe tomography

ABSTRACT

The bainitic transformation in steels is a complex process involving phase transformations, carbon redistribution, elastic interactions, and other coupled thermodynamic effects, making its prediction a long-standing challenge in computational materials science. Grounded in the displacive and diffusionless theory of bainitic sub-unit growth, a multiphase-field approach is adopted to study the bainitic transformation. Electron backscatter diffraction maps the overall phase distribution, while combined correlative scanning transmission electron microscopy, transmission Kikuchi diffraction, and energy-dispersive X-ray spectroscopy reveal strong manganese gradients in the final microstructure. Atom-probe tomography quantifies these manganese heterogeneities to define input parameters for the simulations to isolate the effect of chemical heterogeneity on bainitic transformation behavior. The transformation is modeled as a sequence of diffusionless growth events of supersaturated sub-units followed by carbon rejection. Displacive driving forces are formulated using CALPHAD data, while elastic driving forces are derived from balance equations on singular surfaces and the Hadamard jump conditions. Simulations of sheaf formation through successive sub-unit addition show that heterogeneous manganese enrichment can locally reduce the driving force, leading to earlier growth arrest. Additionally, a pure shear transformation strain is compared with a shear-dominated transformation strain that includes a dilatational strain component. Following sub-unit growth, carbon partitioning is described within a chemo-mechanically fully coupled phase-field model using a carbon-constrained equilibrium, and its effect on the driving forces is assessed via a combined chemo-mechanical growth criterion. By linking experimentally observed chemical heterogeneities and phase-field simulations, this work advances towards a more consistent description of bainitic transformation under chemically heterogeneous conditions.

1. Introduction

Motivation. A primary factor contributing to the preeminence of steels is the vast multitude of microstructures and the resulting properties that can be produced through solid-state transformation and processing, cf., e.g., [1]. A deep understanding of the underlying microstructural processes is necessitated to ultimately control the microstructure properties. Nanostructured carbide-free bainitic steels have been proven to become a promising steel grade with an extraordinary balance of strength, ductility, and toughness, cf., e.g., [2–4]. They have considerable potential, e.g., in the field of transportation (e.g., railway components [5]) and in bearing applications, cf., e.g., [6]. Consequently, the

investigation of the bainitic transformation is of significant scientific interest and essential for the predictive design and development of next-generation high-performance steels.

Growth mechanism of bainite. There has been an extensive debate over decades on the growth mechanism of bainite. The opposing views were that the growth mechanism is either *diffusion-controlled*, cf., e.g., [7,8], or *displacive and diffusionless*, cf., e.g., [9]. An overview on the debate is given, e.g., in [10,11]. A prominent proponent of the displacive theory is Bhadeshia, cf., e.g., [12–14]. This theory proposes that bainite

* Corresponding author at: Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-MMS), Straße am Forum 7, Karlsruhe, 76131, Germany.
E-mail addresses: thea.kannenberg@kit.edu (T. Kannenberg), bowen.zou@uni-kassel.de (B. Zou), song@uni-kassel.de (W. Song), daniel.schneider@kit.edu (D. Schneider).

<https://doi.org/10.1016/j.mtla.2026.102906>

Received 17 July 2026; Accepted 20 September 2026

Available online 1 October 2026

2589-1529/© 2026 The Authors. Published by Elsevier Inc. on behalf of Acta Materialia Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Open access funding enabled and organized by Projekt DEAL.

forms by diffusionless growth of supersaturated sub-units and subsequent rejection of carbon (C). According to [15], there is growing acknowledgment within the community that the bainite transformation is displacive. Correspondingly, the studies in this work consider a displacive and diffusionless growth of supersaturated bainitic sub-units followed by C rejection.

Simulation studies on bainite with phase-field methods. The phase-field model provides a computationally efficient framework for modeling phase transformations and the associated evolution of interfaces without explicit interface tracking [16–20]. Despite its broad applicability, comparatively few phase-field studies have addressed bainitic phase transformations, owing to the complexity of the transformation mechanisms involved. Arif and Qin [21,22] presented one of the first papers on the subject, accounting for the displacive nature of the transformation, but considering mechanical driving forces only in a phenomenological manner. Toloui and Militzer [23] proposed a model for the transformation of austenite into ferrite and carbide-free upper bainite assuming diffusional growth. The needle-shaped growth of the bainite has been studied by means of anisotropic mobility and interfacial energy. Similarly, Song et al. [24] achieve a faceted growth in a diffusional framework by considering an anisotropic mobility and interfacial energy. Düsing and Mahnken [25] presented an approach for the simulation of lower bainite including diffusion, but without considering any kind of stress and strain. In subsequent works, they extended this generalized stress and microforce-based framework to a coupled multiphase-diffusion-mechanics formulation to study the displacive growth of bainite [26,27]. In mechanically coupled models, mechanical driving forces inherently contribute to the evolution of the microstructure. Consequently, artificial anisotropy in the mobility or interfacial energy is not necessary to obtain needle-like morphologies of the sub-units, cf., e.g., [28]. In this manner, Hüter et al. [29] compare a stress-coupled approach to a study with anisotropic mobility and interface energy. Schoof et al. [30] focus on the autocatalytic growth and elastic interaction of sub-units and did not consider C partitioning. Salama et al. [31] consider the simultaneous evolution of sub-units and diffusion, noting the lack of a clear separation of time scales between mechanical deformation and diffusion. A preliminary investigation of a combined chemo-mechanical criterion with a single bainitic sub-unit has been presented in [32, ch. 6], which provides a conceptual basis for the present work.

Impact of chemical heterogeneity on bainite transformation. Experimental studies of nanostructured bainitic steels have established that the characteristic scale of bainitic ferrite depends strongly on the transformation temperature and on the evolving state of the prior austenite [33–35]. Low-temperature isothermal transformation can produce an intimate mixture of slender bainitic-ferrite plates and C-enriched retained austenite, while changes in austenite stability, transformation driving force and kinetics influence the resulting plate thickness [33,34,36]. Beyond these variables, experiments on chemically segregated bainitic steels show that local variations in substitutional-solute content, such as chromium (Cr) and manganese (Mn), produce heterogeneous transformation kinetics and bainitic microstructures with different phase fractions and morphologies [37,38]. Dilatometry investigations have demonstrated that an elevated Mn content is associated with a reduced bainite fraction and the bainite transformation kinetics are found to be strongly depend on the Mn content, due to the corresponding drop in the displacive driving force, cf., e.g., [39,40]. In addition to an elevated Mn content, the presence of competing transformations, such as pearlite formation, has been shown to exert an influence on the transformation kinetics [41]. Recent studies have introduced or retained Mn heterogeneity to modify bainitic transformation kinetics and refine bainitic-ferrite and retained-austenite microstructures [42–44]. These observations motivate the Mn chemical heterogeneity concept adopted here, in which an Mn-enriched region is treated as a localized variation in austenite stability and transformation driving force. At the

same time, flash austenitization offers a route to preserve and exploit such Mn heterogeneity rather than homogenize them [45–47]. In the present work, atom probe tomography (APT) provides information on the local chemical composition range and width scale of an Mn chemical gradient, which is used as a basis for representation in the phase-field simulation to isolate its effect on bainitic sub-unit growth and arrest.

Objective. Motivated by experimentally observed Mn gradients, the objective of this work is to investigate the interplay of elastic and displacive driving forces during the bainitic transformation. Specifically, the impact of Mn heterogeneities on bainitic transformation and the impact of C diffusion on the displacive driving force is investigated. To this end, the purely elastic criterion presented in [30] is extended to encompass displacive driving forces. This extension facilitates the analysis of their evolution, in particular the analysis of the decrease in displacive driving force associated with chemical gradients and C partitioning from bainite to austenite. Experimentally, electron backscatter diffraction (EBSD) provides an overview of the final phase distribution, and correlative scanning transmission electron microscopy, transmission Kikuchi diffraction, and energy-dispersive X-ray spectroscopy (STEM-TKD-EDS) relate the morphology and phase distribution of a plate-like bainitic ferrite grain to local Mn gradients. APT then characterizes Mn heterogeneity in both initial and final conditions after the complete heat-treatment cycle. The measured Mn concentration ranges provide a basis for constructing an experimentally informed Mn field for the simulations. In addition, the effect of a dilatational contribution in the transformation eigenstrains is discussed to clarify their role in the elastic part of the growth criterion.

Originality. A combined chemo-mechanical approach has been demonstrated to be essential for investigating the displacive transformation of bainite and the subsequent C partitioning. A combined framework for the prediction of elastic and displacive driving forces is proposed. Through a combination of simulations and experimental observations, it is indicated that chemical heterogeneities facilitate the development of a finer-grained microstructure. APT measurements provide not only evidence of Mn chemical boundaries and gradients, but also offer input features for the phase-field simulations. STEM-TKD-EDS-identified chemical gradients, APT-based chemical input, and phase-field simulations collectively indicate that Mn chemical heterogeneities can promote finer body-centered cubic (bcc) grains by locally reducing the displacive driving force and arresting bainitic sub-unit growth.

Notation. In the present work, a direct tensor notation is adopted: scalars, vectors, 2nd-order, and 4th-order tensors are denoted by a , $\mathbf{a}$, $\mathbf{A}$, and $\mathbb{A}$, respectively. A linear mapping of a vector $\mathbf{b}$ by a 2nd-order tensor $\mathbf{A}$ is written as $\mathbf{A}\mathbf{b}$ and the mapping of a 2nd-order tensor by a 4th-order tensor reads $\mathbb{A}[\mathbf{B}]$. Compositions are written as $\mathbf{A}\mathbf{B}$ and $\mathbb{A}\mathbb{B}$, and scalar products read $\mathbf{a} \cdot \mathbf{b}$, $\mathbf{A} \cdot \mathbf{B}$, and $\mathbb{A} \cdot \mathbb{B}$. A dyadic product is written as $\mathbf{a} \otimes \mathbf{b}$. The material time derivative of a field a is $\dot{a}$, and the gradient of a scalar is ∇a . In the phase-field context, a jump of a quantity ψ across a diffuse interface representing a material singular surface is defined as $\{\psi\}^{\alpha\beta} = \psi^\alpha - \psi^\beta$.

Outline. This paper is organized as follows: The simulation method is outlined in Section 2 and the experimental methods and the material are presented in Section 3. The link between both methods is presented in Section 4. Results are presented and discussed in Section 5. Finally, this work is concluded in Section 6.

2. Simulation method

2.1. Model formulation

Remark. The simulations are divided into two parts: the growth of bainitic sub-units and the C partitioning, each described within a phase-field framework using tailored formulations appropriate to the underlying physical processes.

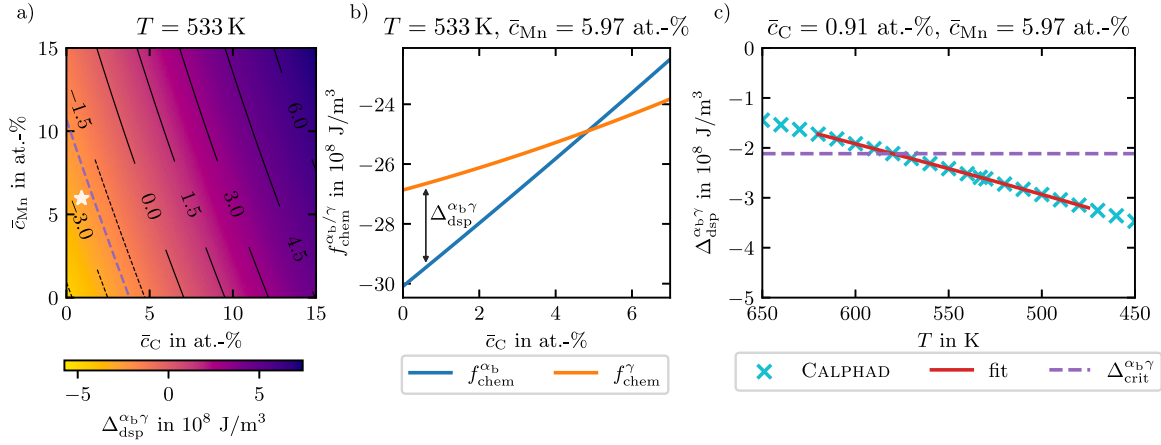


Fig. 1. The driving force heat map for diffusionless growth of a ternary Fe-Mn-C system at $T = 533$ K is illustrated in (a), where the composition of the investigated alloy is marked by a white star. The displacive driving force $\Delta_{\text{dsp}}^{\alpha_b, \gamma}$ for a fixed Mn content with variable C content is given as the difference in chemical free energy densities (b). For a constant composition, the magnitude of the driving force in diffusionless growth increases with increased undercooling (c).

Sub-unit growth. The growth of bainitic sub-units is modeled using an isothermal and diffusionless multiphase-field framework. The system is described by a Ginzburg–Landau-type [48] free energy functional, given by

$$F[\phi, \bar{c}, u] = \int_V f_{\text{intf}}(\phi, \nabla \phi) + \bar{f}_{\text{chem}}(\phi, \bar{c}) + \bar{f}_{\text{el}}(\phi, \bar{c}, \text{grad}(u)) dv. \quad (1)$$

It is composed of an interfacial f_{intf} , chemical $\bar{f}_{\text{chem}}$, and mechanical $\bar{f}_{\text{el}}$ contribution, and depends on the N -tuple of order parameters $\phi = \{\phi_1, \dots, \phi_N\}$, the tuple of concentrations $\bar{c} = \{\bar{c}_C, \bar{c}_{\text{Mn}}\}$, and the displacement field u . The interface contribution is expressed as a sum of the multi-obstacle potential energy density

$$f_{\text{pot}} = \frac{16}{\epsilon \pi^2} \sum_{\beta=2}^N \sum_{\alpha=1}^{\beta-1} \gamma_{\alpha\beta} \phi_{\alpha} \phi_{\beta}, \quad (2)$$

cf., e.g., [49], and the gradient energy density

$$f_{\text{grad}} = -\epsilon \sum_{\beta=2}^N \sum_{\alpha=1}^{\beta-1} \gamma_{\alpha\beta} \nabla \phi_{\alpha} \cdot \nabla \phi_{\beta}, \quad (3)$$

cf., e.g., [50], which depends on the tuple of order parameter gradients $\nabla \phi = \{\nabla \phi_1, \dots, \nabla \phi_N\}$. Together, the gradient energy density and the multi-obstacle potential, i.e., the interfacial energy density $f_{\text{intf}} = f_{\text{pot}} + f_{\text{grad}}$, ensure stable diffuse interfaces. The multi-obstacle potential is defined to be ∞ if ϕ lies outside of the Gibbs simplex $\mathcal{G} = \{\phi : \sum_{\alpha=1}^N \phi_{\alpha} = 1, \phi_{\alpha} \geq 0\}$, cf., e.g., [49]. The interfacial energy $\gamma_{\alpha\beta}$ is modeled isotropic. With the chosen interfacial energy density, the interface parameter ϵ relates to the equilibrium interface width through $l_{\text{eq}} = \epsilon \pi^2 / 4$. The chemical free energy density $\bar{f}_{\text{chem}}$ is obtained through the interpolation of the phase-specific chemical free energy densities f_{chem}^{α} as

$$\bar{f}_{\text{chem}} = \sum_{\alpha=1}^N \phi_{\alpha} f_{\text{chem}}^{\alpha}. \quad (4)$$

In a small strain framework, the infinitesimal strain tensor $\bar{\epsilon}$, given by interpolation of the phase-specific strains ϵ^{α} , relates to the displacement field u with $\bar{\epsilon} = \sum_{\alpha=1}^N \phi_{\alpha} \epsilon^{\alpha} = \text{sym}(\text{grad}(u))$. The elastic energy density $\bar{f}_{\text{el}}$ is given by linear interpolation of the phase-specific elastic energy densities f_{el}^{α} , i.e.,

$$\bar{f}_{\text{el}} = \sum_{\alpha=1}^N \phi_{\alpha} f_{\text{el}}^{\alpha} = \sum_{\alpha=1}^N \phi_{\alpha} \frac{1}{2} (\epsilon^{\alpha} - \bar{\epsilon}^{\alpha}) \cdot (\mathbb{C}^{\alpha} [\epsilon^{\alpha} - \bar{\epsilon}^{\alpha}]), \quad (5)$$

with the phase-specific stiffness tensors $\mathbb{C}^{\alpha}$. Moreover, the phase-specific eigenstrains $\bar{\epsilon}^{\alpha}$ are additively composed of the transformation eigenstrains $\bar{\epsilon}_{\text{trafo}}^{\alpha}$ and the concentration-dependent eigenstrains

$\bar{\epsilon}_c^{\alpha} = (c_C^{\alpha} - c_{\text{ref},C}^{\alpha}) \bar{\epsilon}_{\text{ref},C}^{\alpha}$, where $\bar{\epsilon}_{\text{ref},C}^{\alpha}$ and $c_{\text{ref},C}^{\alpha}$ denote the C reference eigenstrain tensor and concentration, respectively. The substitution of Mn for Fe introduces negligible lattice distortion due to the nearly identical atomic radii of Mn and Fe and is therefore neglected. Moreover, during the initial sub-unit growth, $c_C^{\alpha} = c_{\text{ref},C}^{\alpha}$ everywhere. Consequently, in this step, the concentration-dependent eigenstrains do not contribute to phase evolution. The phase evolution is modeled as the superposition of pairwise interactions of $\bar{N}$ locally present phases as

$$\dot{\phi}_{\alpha} = -\frac{1}{\epsilon} \sum_{\beta=1, \beta \neq \alpha}^{\bar{N}} M_{\alpha\beta} \left(\frac{1}{\bar{N}} \left(\frac{\delta f_{\text{intf}}}{\delta \phi_{\alpha}} - \frac{\delta f_{\text{intf}}}{\delta \phi_{\beta}} + \Delta_{\text{stab}}^{\alpha\beta} \right) + \frac{4(\phi_{\alpha} + \phi_{\beta}) \sqrt{\phi_{\alpha} \phi_{\beta}}}{\pi} \Delta_{\text{bulk}}^{\alpha\beta} \right), \quad (6)$$

cf., e.g., [17,51]. To improve numerical stability, an additional stabilization term $\Delta_{\text{stab}}^{\alpha\beta}$ is introduced into the evolution equation, details in Appendix A. This term has no energetic contribution to the equilibrium state and is for numerical purposes only, cf., e.g., [52]. In Eq. (6), the variational derivative

$$\frac{\delta}{\delta \phi_{\alpha}} = \frac{\partial}{\partial \phi_{\alpha}} - \text{div} \left(\frac{\delta}{\delta \nabla \phi_{\alpha}} \right), \quad (7)$$

cf., e.g., [53, Eq. (13.63)], is employed. The bulk driving force is given as $\Delta_{\text{bulk}}^{\alpha\beta} = \Delta_{\text{dsp}}^{\alpha\beta} + \Delta_{\text{mech}}^{\alpha\beta}$. The displacive driving force $\Delta_{\text{dsp}}^{\alpha\beta}$ is derived as

$$\Delta_{\text{dsp}}^{\alpha\beta} = \left(\frac{\delta}{\delta \phi_{\alpha}} - \frac{\delta}{\delta \phi_{\beta}} \right) \bar{f}_{\text{chem}} = \{f_{\text{chem}}\}^{\alpha\beta}. \quad (8)$$

In the context of diffusionless growth, the driving force corresponding to chemical fields is not derived by the common tangent construction. It is defined as the difference in chemical free energy, which is represented by a vertical line in a plot of chemical free energies, as illustrated in Fig. 1(b). Consequently, the chemical free energy densities, as introduced in Eq. (4), are modeled as a function of $\bar{c}$, i.e., $f_{\text{chem}}^{\alpha} = f_{\text{chem}}^{\alpha}(\bar{c})$, and $\bar{c} = c^{\alpha} \forall \alpha$. The transformation from austenite to bainite is thermodynamically favorable only below the critical temperature T_0 , where the chemical energy of bainite is below that of austenite with an identical composition. This critical temperature further decreases when accounting for stored energy due to shape deformation, cf., e.g., [15]. The mechanical driving force $\Delta_{\text{mech}}^{\alpha\beta}$ is analogously derived as

$$\Delta_{\text{mech}}^{\alpha\beta} = \left(\frac{\delta}{\delta \phi_{\alpha}} - \frac{\delta}{\delta \phi_{\beta}} \right) \bar{f}_{\text{el}} = \{f_{\text{el}}\}^{\alpha\beta} - \bar{\sigma} \cdot \{\epsilon\}^{\alpha\beta}, \quad (9)$$

where the Cauchy stress $\bar{\sigma}$ is given by interpolation of the phase-specific stresses σ^{α} , i.e., $\bar{\sigma} = \sum_{\alpha=1}^N \phi_{\alpha} \sigma^{\alpha}$. Here, a jump condition approach [54–57] is employed, i.e., the Hadamard jump conditions and the balance

equations at singular surfaces are fulfilled at each point within the diffuse interface. The phase evolution is solved under mechanical equilibrium, i.e., the quasi-static linear momentum balance without body forces

$$\text{div}(\tilde{\sigma}) = 0 \quad (10)$$

is solved for the displacement u .

Carbon partitioning. The simulation of C partitioning following growth is performed using a chemo-mechanically fully coupled phase-field model that accounts for stress-driven diffusion and diffusion-induced stresses [58]. Since Mn diffusion is negligible on the timescale of C partitioning, cf., e.g., [15], a binary Fe-C model is employed for this simulation step. During C partitioning the phasefield is assumed to remain constant, such that chemo-mechanically driven diffusion solely governs the evolution of the system. Equilibrium is approached by enforcing equal chemo-mechanical diffusion potentials μ_C , i.e., $\mu_C = \mu_{\text{chem},C}^{\alpha} + \mu_{\text{el},C}^{\alpha} \forall \alpha$, which can be interpreted geometrically as the parallel tangent construction. The chemical and mechanical diffusion potentials are defined as $\mu_{\text{chem},C}^{\alpha} = \partial f_{\text{chem}}^{\alpha} / \partial c_C^{\alpha}$ and $\mu_{\text{el},C}^{\alpha} = \partial f_{\text{el}}^{\alpha} / \partial c_C^{\alpha}$, respectively, cf. [58, Eqs. (16)–(17)]. In contrast to the model for diffusionless growth, the chemical free energy densities during C partitioning are formulated as functions of the phase-specific concentrations c_C^{α} , i.e., $f_{\text{chem}}^{\alpha} = f_{\text{chem}}^{\alpha}(c_C^{\alpha})$. The concentrations c_C^{α} generally differ from the concentration $\bar{c}_C$, i.e., $\bar{c}_C \neq c_C^{\alpha}$. Instead, c_C^{α} depends on the order parameters ϕ , the concentration $\bar{c}_C$, and the displacement field u , and is obtained as part of the chemo-mechanically fully coupled solution procedure. Locally, in addition to the momentum balance at singular surfaces $\{\sigma\}^{\alpha\beta} n^{\alpha\beta} = 0$, and equal chemo-mechanical diffusion potentials, the condition $\bar{c}_C = \sum_{\alpha=1}^N \phi_{\alpha} c_C^{\alpha}$ is ensured. The concentration evolution equation reads

$$\dot{\bar{c}}_C = \text{div} \left(\sum_{\alpha=1}^N \left(\phi_{\alpha} D_C^{\alpha} \left(\frac{\partial \mu_{\text{chem},C}^{\alpha}}{\partial c_C^{\alpha}} + \frac{\partial \mu_{\text{el},C}^{\alpha}}{\partial c_C^{\alpha}} \right)^{-1} \right) \nabla \mu_C \right), \quad (11)$$

cf., e.g., [58, Eq. (41)], where the phase-specific diffusion constants are denoted by D_C^{α} . Furthermore, during the simulation of C partitioning, concentration-dependent eigenstrains $\tilde{\epsilon}_C^{\alpha} = \tilde{\epsilon}_{\text{ref},C}^{\alpha}(c_C^{\alpha} - c_{\text{ref},C}^{\alpha})$ are non-zero and contribute to the evolution. For a more detailed model description and validation, the reader is referred to [58,59], and for a multicomponent formulation to [60].

Growth criterion. The growth of a bainitic sub-unit α_b in the austenite γ is driven by the displacive driving force $\Delta_{\text{dsp}}^{\alpha_b\gamma}$. The displacive driving force must be sufficiently large, i.e., a sufficient undercooling is required, to overcome two contributions: the elastic contribution $\Delta_{\text{mech}}^{\alpha_b\gamma}$, that is introduced by transformation strains in the growing bainite and elastic heterogeneity between the phases, and the surface (capillary) contribution $\Delta_{\text{cap}}^{\alpha_b\gamma}$ associated with the formation of a new austenite-bainite interface. This is expressed as

$$\Delta_{\text{dsp}}^{\alpha_b\gamma} < -(\Delta_{\text{cap}}^{\alpha_b\gamma} + \Delta_{\text{mech}}^{\alpha_b\gamma}). \quad (12)$$

The sign corresponds to Eqs. (6)–(9), i.e., if $\Delta_{\text{dsp}}^{\alpha_b\gamma} + \Delta_{\text{cap}}^{\alpha_b\gamma} + \Delta_{\text{mech}}^{\alpha_b\gamma} < 0$, the transformation is thermodynamically favorable and sub-unit growth is possible. As discussed, e.g., by Schoof et al. [30], the interaction between preceding sub-units and new sub-units can be quantified by the elastic interaction $W_{\text{int}}^{\alpha_b}$, defined as

$$W_{\text{int}}^{\alpha_b} = -\tilde{\sigma} \cdot \tilde{\epsilon}^{\alpha_b}, \quad (13)$$

cf., e.g., [30, Eq. (33)], which promotes or impedes the growth of a secondary sub-unit depending on the local stress field. This contribution is contained in the last term in Eq. (9). For the analysis and visualization of the simulation results, an effective displacive driving force

$$\Delta_{\text{eff}}^{\alpha_b\gamma} = \Delta_{\text{dsp}}^{\alpha_b\gamma} + W_{\text{int}}^{\alpha_b} \quad (14)$$

is defined which combines the displacive driving force $\Delta_{\text{dsp}}^{\alpha_b\gamma}$ with the elastic interaction contribution $W_{\text{int}}^{\alpha_b}$. This decomposition reflects that

$W_{\text{int}}^{\alpha_b}$ can either enhance or reduce the driving contribution, whereas the capillary term $\Delta_{\text{cap}}^{\alpha_b\gamma}$ and the remaining elastic contribution oppose transformation. Consequently, $\Delta_{\text{eff}}^{\alpha_b\gamma}$ represents the portion of the driving force that can actively promote sub-unit growth. The thermodynamic growth criterion remains Eq. (12), where $W_{\text{int}}^{\alpha_b}$ is contained within $\Delta_{\text{mech}}^{\alpha_b\gamma}$.

2.2. Simulation setup

Parameters. The simulation parameters are summarized in Table 1. The designed composition of the alloy for material preparation is reported in Table 2. The experimentally measured composition shows small deviations from these target values, as expected from processing tolerances. The displacive driving force, introduced in Eq. (8), is derived by employing the CALPHAD database TCFe7 of Thermo-Calc [64], utilizing a ternary Fe-Mn-C approximation. The contributions of Si, Cr, Mo, and Nb are treated as constant throughout the system, in accordance with the designed composition detailed in Table 2. The chemical free energy densities f_{chem}^{α} are fitted as parabolic functions at various temperatures. For homogeneous distributions of C and Mn with designed composition, a temperature-dependent fit of the displacive driving force $\Delta_{\text{dsp}}^{\alpha_b\gamma}(T, \bar{c}_C = 0.91 \text{ at.-%}, \bar{c}_{\text{Mn}} = 5.97 \text{ at.-%})$ is derived. In simulations involving chemical heterogeneities (C or Mn), the displacive driving force is evaluated at the simulation temperature $T = 533 \text{ K}$ based on the local C and Mn composition expressed as $\Delta_{\text{dsp}}^{\alpha_b\gamma}(T = 533 \text{ K}, \bar{c}_C, \bar{c}_{\text{Mn}})$. The parameters for both cases are reported in Table 1. The resulting displacive driving force $\Delta_{\text{dsp}}^{\alpha_b\gamma}$ for diffusionless growth is visualized in Fig. 1. A critical temperature is defined, where a single sub-unit grows under the given conditions.

Transformation strain. In this work, bainitic sub-units within a sheaf are assumed to belong to a single variant, cf., e.g., [14]. The transformation strain is dominated by shear components, however, minor dilatation contributions are also present and included in this investigation, in contrast to the study in [30]. In [12, p. 47], the shear strain parallel to the habit plane is reported as $s = 0.22$ and the dilatation normal to the habit plane as $\zeta = 0.03$. The orientation of the nuclei are chosen in such a way, that the normal to the habit plane is parallel to the e_y -axis. The transformation strain tensor of a bainitic sub-unit $\tilde{\epsilon}_{\text{trafo}}^{\alpha_b}$ is visualized in terms of the elastic anisotropy in Fig. 2(a) (see also Appendix B) and the elastic interaction $W_{\text{int}}^{\alpha_b}$, as introduced in Eq. (13), is compared to a strain tensor without dilatation strains as used in [30] in Fig. 2(b) and (c). It should be noted that plastic accommodation is not explicitly accounted for in the present formulation. The strain values are reduced by a prefactor to circumvent unphysical high stress levels, thereby accounting for plastic accommodation in an approximate manner, rather than modeling it explicitly, cf., e.g., [29]. However, the accumulation of plastic strains at the tip of a sub-unit is essential to capture the arrest of sub-unit growth [12,68]. In the present model, this effect is instead approximated by introducing a threshold value for the phase fraction of the growing sub-unit. Once this threshold is reached, further growth is inhibited.

Constrained-carbon-equilibrium criterion. During the C partitioning following growth, a constrained-carbon-equilibrium (CCE) criterion is utilized to account for volume fractions of austenite and ferrite that are far away from the ortho-equilibrium. The CCE criterion originates from quenched and partitioned steels and is described by the following key aspects, cf., e.g., [69,70]:

- C diffusion is complete when the chemical potential of C in both austenite μ_C^{γ} and bainite $\mu_C^{\alpha_b}$ is equal.
- The number of substitutional (here iron) atoms must be conserved in each phase (i.e., absence of substitutional movement).
- Partitioning occurs at an immobile interface (i.e., fixed volume fractions during partitioning).

Table 1
Simulation parameters.

Description	Symbol	Unit	Austenite γ	Bainite α_b	Reference
Young's modulus	E	MPa	$204000 - 91.0\bar{T}^*$	$212000 - 52.7\bar{T}^*$	[61]
Poisson's ratio	ν	–	$0.223 + 0.00025\bar{T}^*$	$0.344 + 0.00010\bar{T}^*$	[61]
Transformation strain	$\bar{\epsilon}_{\text{trafo}}$	–	–	$0.0072e_y \otimes e_y$ $+ 0.099(e_x \otimes e_y + e_y \otimes e_x)$	based on [12]
Reference strain	$\bar{\epsilon}_c$	–	$0.214214I$	–	
Reference concentration	c_{ref}	at.-%	0.91	–	
Diffusivity C	D_C	$\text{m}^2 \text{s}^{-1}$	5.708×10^{-19}	1.162×10^{-14}	[62,63]
Fitting parameters for C partitioning	A	J mol^{-1}	180 146 505.30	38 779 833 333.04	**
	B	J mol^{-1}	–3 041 154.78	265 195.13	**
	C	J mol^{-1}	–5843.50	–21 061.529 838	**
Displacive driving force	$\Delta_{\text{dsp}}^{\alpha_b/\gamma}(T)$	J m^{-3}	$-4.04 \times 10^2 T^2 + 1.46 \times 10^6 T - 9.22 \times 10^8$		[64]
	$\Delta_{\text{dsp}}^{\alpha_b/\gamma}(\bar{c}_C, \bar{c}_{\text{Mn}})$	J m^{-3}	$-(48059.51\bar{c}_C^2 + 14140.98\bar{c}_{\text{Mn}}^2 + 27694.00\bar{c}_C\bar{c}_{\text{Mn}} - 50500.38\bar{c}_C$ $-18751.10\bar{c}_{\text{Mn}} + 3323.36)/V_m$		[64]
Molar volume	V_m	$\text{m}^3 \text{mol}^{-1}$	7×10^{-6}		[65]
Interfacial energy	$\gamma_{\alpha_b/\gamma}$	J m^{-2}	0.2		[66]
Mobility phase-field	$M_{\alpha_b/\gamma}$	$\text{m}^4 \text{J}^{-1} \text{s}^{-1}$	stability criterion		[30]
Temperature	T	K	533		
Spacial discretization	Δx	nm	1.5		
Interface parameter	ϵ	Δx	$8/(\pi^2/4)$		

* $\bar{T}$ denotes the temperature in °C.

** Parameters are fitted assuming a CCE criterion based on the Thermo-Calc [64] TCFe7 CALPHAD database.

Table 2
Designed and measured chemical composition of the investigated bainitic steel in wt.-% and at.-%.

	unit	C	Si	Mn	Cr	Mo	Nb	P	S	N	Fe
designed	wt.-%	0.2	1.5	6.0	1.0	0.3	0.05	–	–	–	bal.
	at.-%	0.91	2.92	5.97	1.05	0.17	0.03	–	–	–	bal.
measured	wt.-%	0.21	1.56	5.92	1.07	0.33	0.052	0.004	0.004	0.005	bal.
	at.-%	0.95	3.03	5.88	1.12	0.19	0.03	0.007	0.007	0.019	bal.

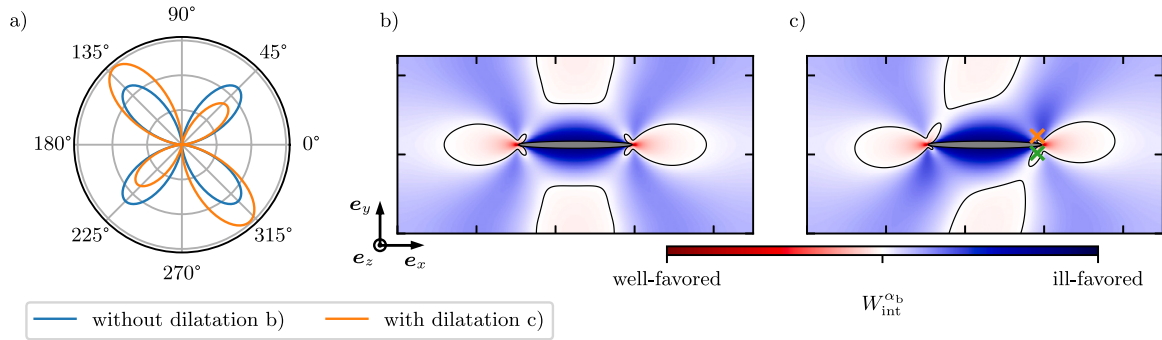


Fig. 2. The anisotropy in the elastic energy introduced by the transformation strain $\bar{\epsilon}_{\text{trafo}}^{\alpha_b}$ is visualized in (a) as polar plots of an orientation-dependent elastic energy function [67] (see Appendix B for more details). The orientation of the bainitic nuclei is such that the normal to the habit plane is parallel to the e_y -axis. The dilatation contribution introduces an asymmetry with respect to the habit plane. In (b), the elastic favorability map of pure-shear transformation strain is illustrated, cf. [30, Fig. 2]. The zero isoline marks the boundary between regions where the elastic interaction $W_{\text{int}}^{\alpha_b}$ either promotes or opposes the displacive driving force, cf. Eq. (14). The map corresponding to the shear-dominated transformation strain, including dilatation components, is displayed in (c). It has been observed that while a secondary sub-unit exhibits growth at the green cross, its growth is impeded at the orange cross.

The CCE criterion is expressed through the following formulae:

$$\mu_C^{\alpha_b}(c_{\text{CCE}}^{\alpha_b}) = \mu_C^{\gamma}(c_{\text{CCE}}^{\gamma}) \quad (15)$$

$$\xi_{\text{CCE}}^{\gamma}(1 - c_{\text{CCE}}^{\gamma}) = \xi_0^{\gamma}(1 - c_{\text{tot,C}}) \quad (16)$$

$$c_{\text{tot}} = \xi_{\text{CCE}}^{\alpha_b} c_{\text{CCE}}^{\alpha_b} + \xi_{\text{CCE}}^{\gamma} c_{\text{CCE}}^{\gamma} \quad (17)$$

$$\xi_{\text{CCE}}^{\alpha_b} + \xi_{\text{CCE}}^{\gamma} = 1, \quad (18)$$

cf., e.g., [69]. The C content in bainite and austenite after partitioning are denoted by $c_{\text{CCE}}^{\alpha_b}$ and c_{CCE}^{γ} , the respective phase fractions as $\xi_{\text{CCE}}^{\alpha_b}$ and $\xi_{\text{CCE}}^{\gamma}$, respectively. The average C content of the alloy is referred to as $c_{\text{tot,C}}$. The discrepancy between the austenite phase fraction before and after partitioning, denoted by ξ_0^{γ} and $\xi_{\text{CCE}}^{\gamma}$, respectively, appears to be inconsistent with the assumption of an immobile interface. However, this discrepancy can be attributed to the negligible change in phase fractions due extensive C diffusion, cf., e.g., [71]. Eq. (15) ensures an

equilibrium C diffusion potential. This is written as

$$c_{\text{CCE}}^{\gamma} = c_{\text{CCE}}^{\alpha_b} \left(\exp \frac{76789 - 43.8T - (169105 - 120.4T)c_{\text{CCE}}^{\gamma}}{RT} \right), \quad (19)$$

cf., e.g., [69, Eq. (2)], where R and T denote the universal gas constant and the temperature, respectively. Eq. (16) ensures the matter balance of iron (no iron is transferred across interface during partitioning), Eq. (17) guarantees the total C matter balance, and Eq. (18) establishes the phase-fraction relationship. This work does not consider a sublattice structure, thus, the CCE criterion, cf. Eqs. (16)–(19), is used primarily to establish the endpoints of the diffusion process. Accordingly, the numerical approach adopted in this work to manipulate chemical free energy parabolas focuses on enforcing the CCE parameters, while ensuring consistency with the CALPHAD-based description of chemical free energy densities [71] and a common tangent at the CCE endpoints.

The phase-specific chemical energy densities are written as parabolic functions $f_{\text{chem}}^a(c_C^a) = (A^a(c_C^a)^2 + B^a c_C^a + C^a)/V_m$. The molar volume V_m is considered phase-independent. The employed parameters during C partitioning are reported in Table 1.

Simulation domain and boundary conditions. The simulation studies on one and two sub-units are performed on a $1500\Delta x \times 749\Delta x$ grid. Simulation studies on sheaves are performed on a $4000\Delta x \times 800\Delta x$ grid. The spatial discretization of $\Delta x = 1.5\text{ nm}$ ensures sufficient resolution of nano-scale concentration gradients while each cell contains several atoms. The C concentration field is interpreted as a coarse-grained ensemble average rather than literal atomic count. So the local value reflects an average atomic occupancy rather than a literal count of individual atoms. In all simulations, periodic boundary conditions are employed for the concentration fluxes, order parameters, and the displacement field.

Remarks. The nucleation of bainitic sub-units is not part of this study. New bainitic sub-units are added manually to the simulation domain. For the simulation of rapid displacive growth, a dimensionless time step Δt is employed. The phase-field mobility is defined accordingly to ensure a numerically stable temporal evolution [30,52]. In contrast, C partitioning is treated with a dimensional time step $\Delta t = 10\text{ }\mu\text{s}$. All simulations are performed using the in-house software Pace3D [72].

3. Material and experimental methods

Material. The investigated alloy was a laboratory processed medium-Mn bainitic steel with a nominal composition of Fe-6Mn-1.5Si-1Cr-0.3Mo-0.05Nb-0.2C in wt.-%, cf. Table 2. The steel was produced by vacuum induction melting, homogenized at 1250°C for 5 h, hot forged between 1200°C and 900°C , hot rolled to 2 mm and subsequently cold rolled to a final thickness of 1.5 mm without interpass annealing. Specimens were cut from the cold rolled sheets with the long direction parallel to the rolling direction. The chemical composition was measured by pulse discrimination analysis optical emission spectrometry and is listed in Table 2.

Heat treatment design. All specimens first underwent an austenite reversion treatment (ART) at 700°C for 10 min in a salt bath, followed by air cooling to room temperature. This condition is denoted as ART710, where “710” refers to 700°C and 10 min. The ART710 treatment was selected to obtain a submicrometre ferrite/austenite microstructure and introduce local Mn chemical boundaries near ferrite/austenite interfaces through short-range Mn redistribution before subsequent flash austenitization [45,73]. For the 710-F260 condition, ART710 specimens were heated to 900°C at 100 K s^{-1} without isothermal holding at the peak temperature, cooled to 260°C at 50 K s^{-1} , held for 2 h, and finally quenched to room temperature. This cycle was selected to limit high-temperature exposure before isothermal bainitization and to examine local Mn heterogeneity within the final microstructure. The flash austenitization and bainitization cycle were performed using a DIL 805 A/D dilatometer (TA Instruments) [45]. The specimens used for the thermal cycling had dimensions of $10\times 4\times 1.5\text{ mm}^3$. They were induction-heated while held between quartz push rods. Temperature was monitored and controlled using a thermocouple spot-welded to the specimen surface. The chamber was evacuated and backfilled with Ar to limit oxidation.

Experimental characterization procedure. The characterization strategy proceeds from an EBSD overview of the final 710-F260 microstructure to correlative STEM-TKD-EDS analysis of local morphology, phase distribution, and Mn gradients. APT complements these measurements with nanoscale chemical information from the initial ART710 condition and the final 710-F260 condition. The correlative measurements relate the three signals within the same lamella region, whereas APT characterizes independently sampled local volumes.

Electron backscatter diffraction. EBSD was used to characterize the overall bcc/face-centered cubic (fcc) phase distribution and the characteristic size of bcc domains in the 710-F260 condition after final quenching. Specimens were mechanically ground, polished and finally electropolished using A2 electrolyte at 40 V. EBSD measurements were performed using a Helios 5 Hydra plasma focused ion beam scanning electron microscope (PFIB-SEM) equipped with a CMOS based EBSD detector from Oxford Instruments. Data were acquired at 20 kV, a probe current of 13 nA, a working distance of 10 mm and a step size of $0.04\text{ }\mu\text{m}$. EBSD data were acquired using AZtec and analyzed using AZtecCrystal. The phase maps were used to determine the fcc and bcc area fractions. Grains were reconstructed using a high angle grain boundary threshold of 15° . The characteristic bcc-domain size was expressed as the area-weighted mean fitted ellipse major diameter, $\bar{L}_A = \sum_j A_j L_j / \sum_j A_j$, where A_j and L_j are the area and fitted ellipse major diameter of bcc domain j , respectively.

Correlative STEM-TKD-EDS characterization. Correlative scanning transmission electron microscopy (STEM), transmission Kikuchi diffraction (TKD), and energy-dispersive X-ray spectroscopy (EDS) were performed on the 710-F260 condition to relate local microstructural morphology and phase distribution to Mn gradients within the same region of the lamella. Electron-transparent lamella were prepared in the Helios 5 Hydra Plasma FIB-SEM and thinned to approximately 80–150 nm. The correlative measurements were performed in the same instrument, using a thin region of the lamella shown in Fig. S1 of the Supplementary Material. STEM bright-field images were acquired at 30 kV and 50 pA, with a working distance of 4.65 mm, to resolve the local morphology. TKD maps of the selected STEM region were acquired at 30 kV and 3.2 nA, with a working distance of 5 mm and a step size of 10 nm. The lamella was mounted on a Cu grid within a 52° pre-tilted holder, corresponding to a specimen pretilt of -38° . A stage tilt of 38° compensated this pretilt, resulting in an effective specimen tilt of approximately 0° , with the lamella normal approximately parallel to the incident electron beam. The TKD phase maps provided bcc/fcc phase identification and were interpreted together with STEM morphology to support the assignment of the selected bainitic ferrite region. Prior-austenite grain boundaries (PAGBs) were annotated based on microstructural morphology, with reference to the prior-austenite grain reconstruction results presented in Fig. S2 of the Supplementary Material. Three EDS line scans were acquired across the selected grain and its surroundings at 20 kV and 1.6 nA, with a working distance of 4.65 mm, using 10 passes and a bin-size setting of 2. The line-scan positions and directions shown in Fig. 3(d) link the local Mn concentration profiles to the microstructural features identified by STEM and TKD. Mn concentrations are reported in wt.-%. Raw profiles are shown together with trend curves using adjacent-averaging smoothing with a 15-point window to aid visualization of the local Mn concentration trends. TKD and EDS data acquisition was performed using AZtec, and TKD post-processing was conducted using AZtecCrystal.

Atom probe tomography. To complement the EDS measurements with nanoscale chemical information, APT was performed on the ART710 and 710-F260 conditions to characterize the initial Mn chemical boundary and the local Mn chemical gradient after the complete heat-treatment cycle, respectively (Fig. 4). Needle-shaped specimens were prepared using an FEI Helios Nanolab 660 dual-beam FIB-SEM system. For the ART710 condition, site-specific preparation targeted a region containing an fcc/bcc phase boundary. For 710-F260, specimens were extracted from the vicinity of presumed PAGBs. A wedge shaped lamella was lifted out, mounted on a Si coupon and sharpened by annular milling, followed by a final low voltage cleaning step at 5 kV to reduce FIB induced surface damage. APT measurements were carried out using a CAMECA LEAP 5000 XR system in voltage-pulsing mode at a base temperature of 60 K. The pulse frequency was 200 kHz, the pulse fraction was 20 %, and the detection rate was 0.5 %. Three dimensional (3D) reconstructions and local composition analyses

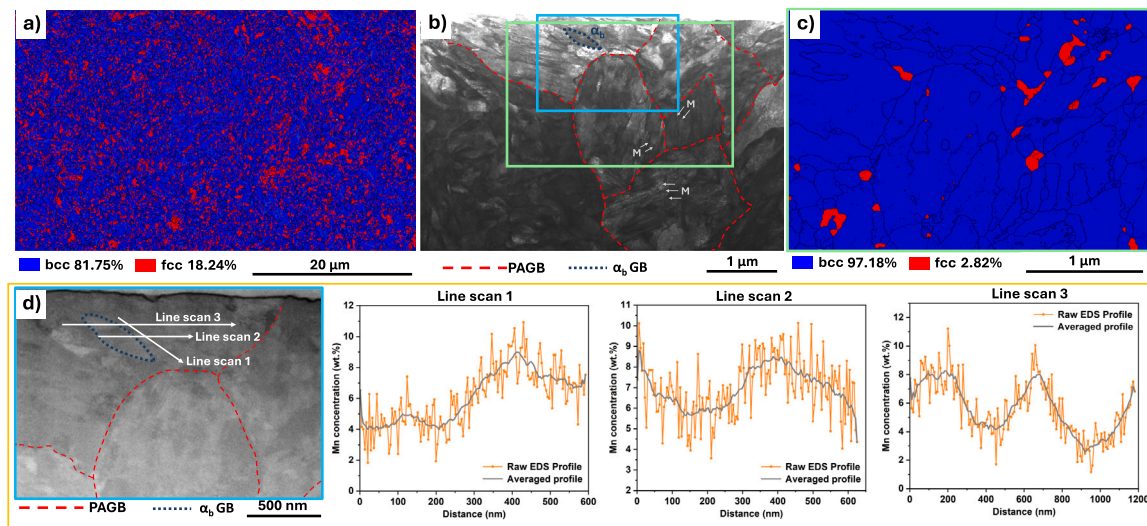


Fig. 3. EBSD overview and correlative STEM-TKD-EDS characterization of the 710-F260 condition after final quenching. In (a), the EBSD phase map shows the bcc (blue) and fcc (red) phase distributions. In (b), the STEM image shows the local microstructure, with inferred prior-austenite grain boundaries marked by red dashed lines, a selected bainitic ferrite grain (α_b) outlined by blue dotted lines, and martensite marked M. In (c), the TKD phase map corresponds to the green rectangle in (b), using the same phase colors as in (a). In (d), a magnified FSD enhanced image (corresponding to the blue rectangle in (b)) and three EDS line profiles show the spatial relationship between the selected bainitic ferrite grain and local Mn gradients. White arrows indicate the line-scan positions and directions; orange and gray curves represent the raw and averaged Mn concentration profiles, respectively.

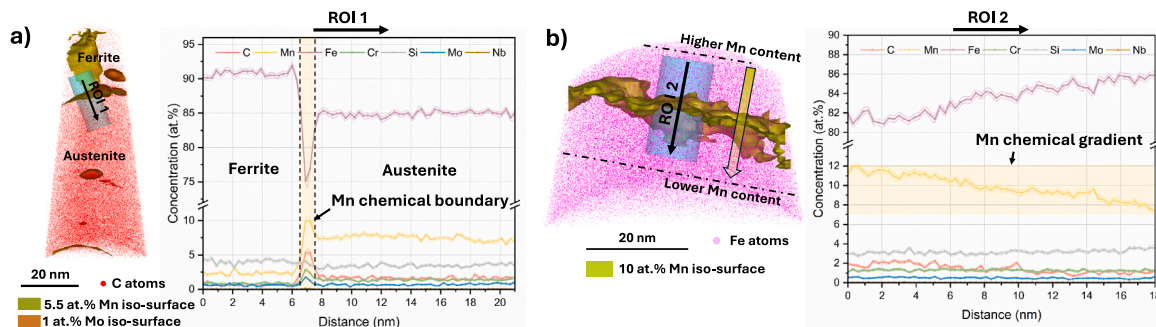


Fig. 4. APT characterization of Mn heterogeneity in the ART710 and 710-F260 conditions. In (a), the ART710 reconstruction shows C atoms (red), a 5.5 at.-% Mn iso-concentration surface delineating the ferrite/austenite interfacial region, and 1 at.-% Mo iso-concentration surfaces marking Mo-enriched particles. The 1D concentration profiles extracted along the marked region of interest (ROI 1) show elemental partitioning and a localized Mn-enriched layer on the austenite side adjacent to the interface. In (b), the 710-F260 condition was analyzed after flash austenitization, isothermal holding at 260 °C for 2 h, and final quenching. Fe atoms (pink) are shown together with a 10 at.-% Mn iso-concentration surface. The concentration profiles extracted along ROI 2 show an overall decrease in Mn content from approximately 12 to 7.5 at.-% over the sampled distance, demonstrating local Mn heterogeneity in the final heat-treated state. Black arrows within the ROIs indicate the profiling directions. The vertical dashed lines and yellow shading in (a) highlight the localized Mn-enriched chemical boundary, whereas the yellow shading in (b) highlights the Mn concentration gradient.

were performed using AP Suite 6.3. One-dimensional (1D) elemental concentration profiles were extracted along the selected regions of interest (ROI) shown in Fig. 4 to quantify local compositional variations. The measured Mn concentration ranges informed the prescribed chemical heterogeneity in the simulations, as described in Section 4.

4. Linking experiment and simulation

Conceptual framework. The present work links multiphase-field simulations and experimental observations to advance towards a consistent description of the bainitic transformation under chemically heterogeneous conditions. The goal is to establish an enhanced understanding of the role of chemical heterogeneities in the formation of a bainitic microstructure. The experimental sequence starts with an EBSD overview, proceeds to correlative STEM-TKD-EDS analysis of the local morphology, phase distribution, and Mn gradients, and concludes with APT characterization of independently sampled local chemical distributions. STEM-TKD-EDS measurements provide evidence of strong Mn

gradients in the final microstructure, yet their role in the bainitic transformation remains difficult to resolve from characterization alone. The objective of this work is therefore to investigate the impact of such chemical heterogeneities on the bainitic transformation, and to do so through a combined experiment-simulation strategy. Informed by experimental results, simulations allow to isolate the effect of chemical heterogeneity from the superimposed contributions of the overall processing route. This complementary strategy allows experimentally observed trends to be interpreted within a physically grounded modeling framework.

Chemical heterogeneities. Experimentally, APT is used to quantify the Mn heterogeneity in the microstructure. The initial Mn chemical boundary in ART710 and the final-state Mn gradient in 710-F260 provide experimentally measured concentration ranges for constructing the Mn field for the simulations. In this way, the role of chemical heterogeneities in the local growth criterion for bainitic sub-units can be analyzed in a controlled model setting. It is worth to note that the EDS profiles supply the local microstructural context, while APT provides

nanoscale chemical information from separate sampled volumes. The two techniques did not measure the same Mn gradient. The interpretation of the final-state Mn heterogeneity inherited from the ART state is discussed in Section 5.3. The corresponding simulations are formulated as a controlled comparison between two chemical scenarios: a chemically homogeneous austenite matrix and an austenite matrix containing an APT-informed Mn chemical heterogeneity. The prescribed local Mn content enters the CALPHAD-based chemical free energy density and allows the displacive driving force $\Delta_{\text{dsp}}^{\alpha\beta}$ to be evaluated as a function of the local C and Mn content. Overall, the experiment-simulation link in this work consists of three steps: Correlative STEM-TKD-EDS first reveals strong Mn gradients in the final microstructure and the spatial relationship between a selected bainitic ferrite grain and Mn gradients, motivating the subsequent investigation. APT then characterizes local Mn heterogeneity at the nanoscale in the initial and final conditions, providing the Mn chemical heterogeneity information that is used in the simulations. Finally, the phase-field simulations isolate how this chemical heterogeneity influences bainitic sub-unit and sheaf growth.

5. Results and discussion

5.1. Experimental results

EBS and correlative STEM-TKD-EDS characterization. Fig. 3(a) shows the EBSD phase map of 710-F260 after final quenching. The mapped area contains 81.75 % bcc and 18.24 % fcc, with retained austenite distributed between the predominantly elongated bcc regions. The area-weighted mean fitted ellipse major diameter of the bcc domains is $1.63 \pm 1.09 \mu\text{m}$. This value describes the final bcc-domain morphology rather than the thickness or growth length of individual bainitic ferrite plates.

Correlative STEM-TKD-EDS measurements were performed in a thin region of the lamella shown in Fig. S1 of the Supplementary Material. The bright-field (BF) STEM image in Fig. 3(b) resolves the local lath and plate morphologies, while the TKD map in Fig. 3(c), corresponding to the green rectangle, identifies the bcc and fcc regions. The local TKD area fractions of 97.18 % bcc and 2.82 % fcc describe this selected thin-foil region and are not treated as representative bulk phase fractions. The relatively low fcc fraction may also partly reflect preparation-induced transformation of metastable retained austenite during PFIB milling [74]. The red dashed lines mark PAGBs inferred from the morphology observed in the BF-STEM image, with reference to the prior-austenite reconstruction in Fig. S2 of the Supplementary Material.

The bcc/fcc phase indexing used in EBSD and TKD does not distinguish bainitic ferrite from pre-existing ferrite or quenched martensite indexed as bcc. Consequently, assigning the entire EBSD-indexed bcc area fraction to bainitic ferrite would overestimate the bainitic ferrite fraction. Interpreted together, the STEM morphology and TKD phase distribution support a mixed microstructure containing bainitic ferrite, martensite, and retained austenite. Within the thin region (Fig. 3(b)), the elongated bcc feature outlined in blue has a plate-like shape with tapered ends and is assigned to bainitic ferrite (α_b), in contrast to the surrounding lath arrangements identified morphologically as martensite (marked M). Its projected length is approximately $0.6 \mu\text{m}$, with an apparent maximum width of approximately $0.15 \mu\text{m}$. These dimensions characterize only the selected feature in the observed section.

Our previous study reported a submicrometre fcc/bcc microstructure in the initial ART710 condition [45]. In contrast, the inferred prior-austenite grains observed in 710-F260 extend over at least several micrometres, indicating that the initially submicrometre austenite grains grew to the scale of several micrometres during the flash austenitization and bainitization cycle. The selected plate-like feature, identified as a bainitic ferrite grain, is substantially smaller than its parent grain, and its tapered end lies within the parent grain rather than coinciding with the nearest annotated PAGB in the observed section. This spatial relationship provides a typical local microstructure for examining Mn concentration variations within the parent grain.

Spatial relationship between Mn gradients and bainitic ferrite. Fig. 3(d) combines a magnified forescatter-detector (FSD)-enhanced image (corresponding to the blue rectangle in (b)) of the selected region with three EDS line profiles. The profiles reveal local Mn variations across distances of several hundred nanometres. The concentration ranges discussed below are approximate values read from the averaged trends, since individual raw-data points exhibit larger fluctuations.

Line scan 1 samples the neighborhood of a broad side and the tapered end of the selected plate-like bainitic ferrite grain. Along this path, the Mn concentration increases from approximately 4–5 wt.-% to a maximum of approximately 8–9 wt.-%, showing that the plate is adjacent to a region of increasing Mn content. Line scan 2 traverses the selected grain and extends into its surroundings. Its averaged profile contains an Mn-lean interval of approximately 5.5–6 wt.-%, followed by an increase to approximately 8–8.5 wt.-% outside the outlined plate. Together, these profiles associate the selected plate-like bainitic ferrite grain with an Mn-lean region, adjoining higher-Mn region near its broad side and tapered end. The Mn chemical contrast is expressed as spatially extended concentration gradients.

The longer line scan 3 extends over approximately $1.2 \mu\text{m}$ within the same inferred prior-austenite region. Its averaged profile contains multiple Mn-rich maxima of approximately 7–8 wt.-% separated by Mn-lean intervals of approximately 3–4.5 wt.-%. Thus, the sampled region is chemically subdivided into several Mn-rich and Mn-lean zones connected by gradients, rather than containing only one isolated enrichment next to the selected plate. Similar chemical gradients in additional prior-austenite regions are presented in Fig. S3 of the Supplementary Material, indicating that this Mn heterogeneity is not restricted to the single region shown in Fig. 3(d).

These correlative measurements establish the spatial relationship between the selected plate-like bainitic ferrite grain and Mn gradients across distances of several hundred nanometres. To complement this local correlation with three-dimensional nanoscale chemical information, APT was used to compare the initial ART710 condition with 710-F260 after the complete heat-treatment cycle. The APT tips sample separate local volumes rather than the particular grain examined by correlative STEM-TKD-EDS.

APT characterization of Mn heterogeneities. In Fig. 4 the APT results for the ART710 and 710-F260 conditions are compared in (a) and (b), respectively. The elemental atom maps of both tips are provided in Fig. S4 of the Supplementary Material. In ART710, Mn and C partition preferentially to austenite, while Cr also shows moderate enrichment in this phase. Fig. 4(a) shows C atoms together with a 5.5 at.-% Mn iso-concentration surface delineating the ferrite/austenite interfacial region. Several Mo-enriched particles are additionally visualized using 1 at.-% Mo iso-concentration surfaces. The concentration profiles along ROI 1 quantify the initial elemental partitioning and localized interfacial enrichment. The ferrite plateau contains 2.33 ± 0.25 at.-% Mn, 0.70 ± 0.17 at.-% C, 4.05 ± 0.30 at.-% Si, and 90.80 ± 0.44 at.-% Fe. The corresponding austenite plateau contains 7.49 ± 0.38 at.-% Mn, 1.66 ± 0.20 at.-% C, 3.45 ± 0.23 at.-% Si, and 84.93 ± 0.37 at.-% Fe. The Cr concentration increases from 0.85 ± 0.11 at.-% in ferrite to 1.38 ± 0.11 at.-% in austenite, whereas Mo and Nb remain below 1 at.-% in the phase interiors. In addition to this phase-to-phase partitioning, a localized Mn-enriched layer is resolved on the austenite side adjacent to the interface. Its mean Mn concentration is 9.47 ± 0.77 at.-%, with a maximum of 9.98 ± 0.35 at.-% at approximately 7.2 nm along ROI 1, about 2.5 percentage points above the adjacent austenite plateau. The apparent thickness of this Mn chemical boundary is approximately 1–2 nm along the profiling direction. Such interfacial Mn enrichment is consistent with previous APT observations of nanoscale Mn heterogeneity near austenite-containing interfaces in medium-Mn steels [75,76].

Fig. 4(b) shows the APT tip from the 710-F260 condition after flash austenitization, isothermal holding at 260 °C for 2 h, and final quenching. Fe atoms are shown together with a 10 at.-% Mn iso-concentration

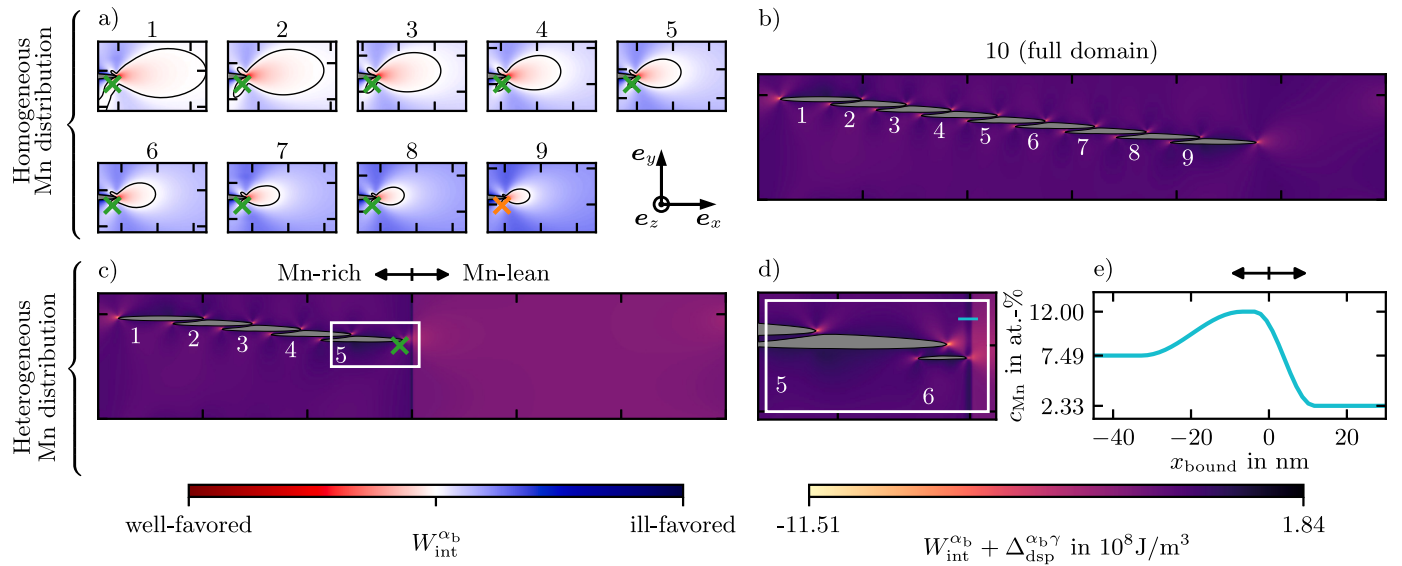


Fig. 5. Consecutive growth of bainitic sub-units with a homogeneous Mn distribution (a)–(b), and with a chemical heterogeneous Mn field including an Mn-rich, an Mn-lean region and an Mn gradient (c)–(e). The elastic favorability at each sub-unit tip is found to decrease as the number of sub-units present in the simulation domain increases (a). The nuclei are placed in the same relative position with respect to the preceding sub-unit tip. In this configuration, the tenth sub-unit (initial position marked in 9) is not able to grow and ultimately vanishes (b). The displacive driving force $\Delta_{dsp}^{a_b/\gamma}$ is reduced in Mn-rich regions (c). The position of the nucleus of the sixth sub-unit is marked with a green cross. As demonstrated in (d), the growth of the sixth sub-unit is stopped where the Mn content increases. The Mn gradient acts as an obstacle to further growth. The Mn profile extracted along the blue line in (d) is shown in (e). The white rectangles in (c) and (d) indicate the same area in the simulation domain.

surface to visualize the local Mn distribution. This iso-surface marks a selected concentration level within the continuous Mn gradient and does not identify a phase interface or a sharp compositional boundary. The average concentrations in ROI 2 are 9.84 ± 1.20 at.-% Mn, 1.46 ± 0.44 at.-% C, 3.16 ± 0.20 at.-% Si, 1.27 ± 0.09 at.-% Cr, 0.49 ± 0.07 at.-% Mo, 0.02 ± 0.01 at.-% Nb, and 83.56 ± 1.59 at.-% Fe. The Mn concentration remains above the nominal value of 5.97 at.-% throughout the profile, while the average C concentration also exceeds the nominal value of 0.91 at.-%. The Mn enrichment and elevated average C content are consistent with a region of retained austenite or martensite formed from solute-enriched prior austenite. The main feature of ROI 2 is an extended Mn concentration gradient. The Mn content decreases overall from approximately 12.0 to 7.4 at.-% over a sampled distance of approximately 18 nm. C is also heterogeneous, ranging from approximately 0.74 to 2.29 at.-%. Unlike the narrow Mn peak in ART710, ROI 2 exhibits a gradual variation in Mn concentration over the sampled region.

Taken together, the EDS and APT results establish the presence of Mn heterogeneity in the examined regions after the complete 710-F260 heat-treatment cycle, while the ART710 APT measurement identifies the initial interfacial Mn enrichment and phase-to-phase partitioning. The measured Mn concentration ranges provide an experimental basis for the prescribed chemical heterogeneity described in Section 4. The origin and retention of the gradients, and their possible implications for bainitic ferrite growth, are discussed in Section 5.3.

5.2. Simulation results

Pure shear vs. shear-dominated transformation strains with dilation. The minor dilatation contribution in the shear-dominated transformation strain causes an asymmetric elastic interaction field with respect to the habit plane. It is highlighted, that the interaction contour is applicable exclusively to the growth of identical variants and does not extend to complementary ones, cf., e.g., [30]. In Fig. 2, a comparative analysis is presented of the elastic interaction $W_{int}^{\alpha_b}$ of a sub-unit that is subject to

a pure shear transformation strain (b) and shear-dominated dilatation transformation strain (c). In the latter case, the asymmetry in elastic interaction with respect to the habit plane is evident. Due to this asymmetry, the growth of a secondary sub-unit of the same variant is more favorable on one side of the tip than on the other when dilatation strains are considered. For the purpose of confirming the asymmetry, the growth of a secondary sub-unit is compared in two locations that are marked in Fig. 2(c). Given that the magnitude of the displacive driving force remains within a modest margin above a critical value, the elastic interaction prevents growth on one side of the tip (orange cross) and supports growth on the other (green cross). In both cases, the obtained interaction fields remain consistent with the theoretical considerations, cf., e.g., [14], and previous simulation studies [30], which have shown that the stress field at the sub-unit tip will favor nucleation of the same variant.

Sheaf formation. In Fig. 5, the results of a simulation study on a bainitic sheaf are illustrated. New sub-unit nuclei are manually placed in the simulation domain, after the preceding unit reached a volume threshold. Each newly introduced nucleus is permitted to grow until it reaches a prescribed volume threshold (or until it shrinks and vanishes). Upon attainment of this threshold, the next nucleus is placed in the same relative position with respect to the tip of the preceding sub-unit. This procedure is iteratively continued until the growth terminates. In this setup, the tenth nucleus eventually vanishes. In Fig. 5(a), the elastic favorability is plotted surrounding the tip of each sub-unit at the final time step of each successive simulation. A green cross marks the location of the center of the sub-subsequent sub-unit. As elucidated in the preceding paragraph, the elastic favorability is asymmetric with respect to the habit plane. Consequently, the nuclei are always placed on the same side of the preceding sub-unit. It is evident that the energetically favorable region progressively decreases in spatial extent for each newly formed nucleus, until the marked position lies outside this region. The zoomed-in views in (a) are shown at a constant spatial scale across all simulation steps. As illustrated in Fig. 5(b), following

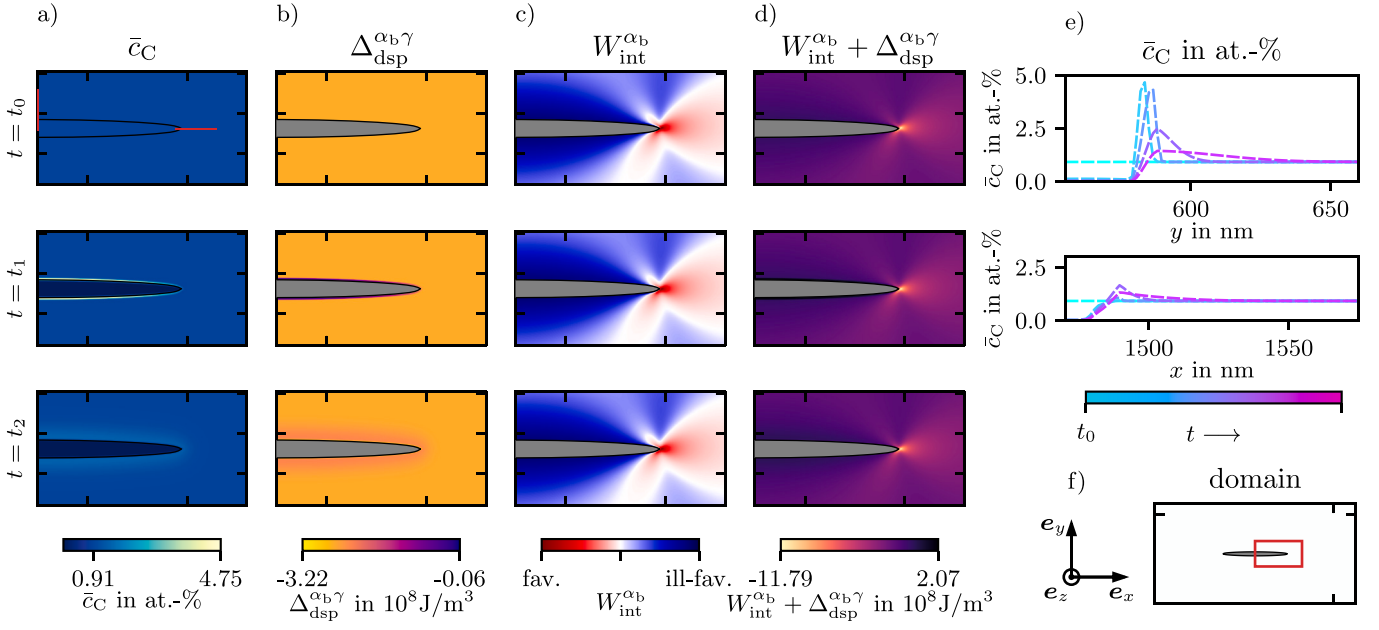


Fig. 6. Impact of C partitioning on sub-unit growth. Due to a substantially lower diffusivity in austenite a C pile-up at the interface is present at the interface which diffuses slowly into the surrounding austenite (a). The C pile up decreases the displacive driving force (b). Only minor changes in the elastic interaction contribution are present due to the C partitioning (c). The combined effect of displacive driving force and elastic interaction (d) reveals a reduction along the broad side of the bainite sub-unit. As shown in (e), the C pile-up is significantly higher along the broad face of the interface than across the tip (paths are indicated by red lines in (a)). A thin black line marks the corresponding sharp interface between austenite and sub-unit. In (f), the region of interest is indicated in red. Subfigures (a)–(d) show a magnified view of this region.

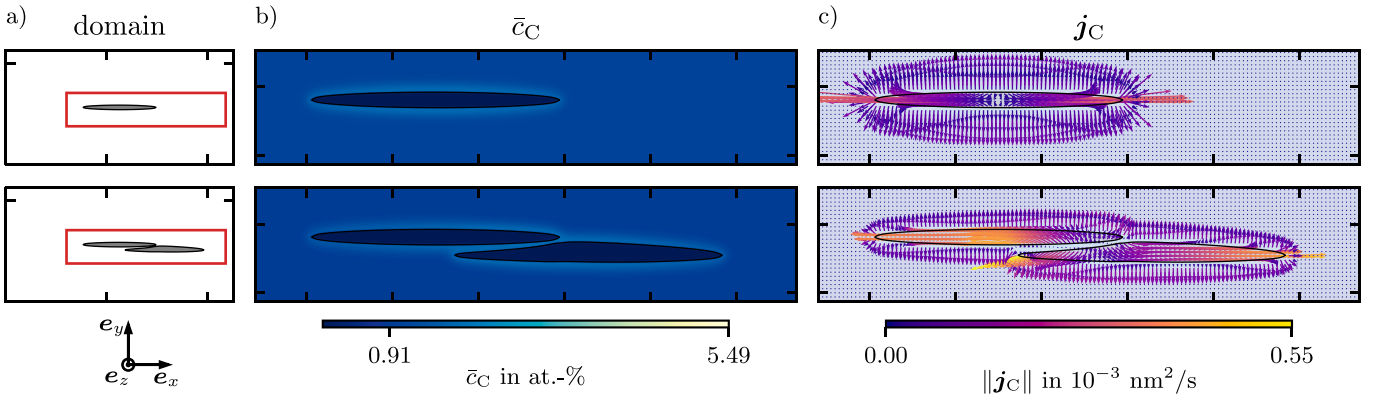


Fig. 7. Comparison of C partitioning with one (upper row) and two sub-units (lower row) at an arbitrary timestep. In (a), the region of interest is highlighted in red. In this area, the C concentration field \$\bar{c}_C\$ is visualized in (b). In (c), the C flux vectors \$j_C\$ are illustrated. The impact of one sub-unit on the other is readily apparent.

the placement of a tenth nucleus, the full computational domain reveals the absence of a tenth sub-unit, which instead undergoes a process of shrinkage and subsequent disappearance. The driving force is evaluated based on the local C and Mn concentration as introduced in Fig. 1(a) using Eq. (14). This study indicates that, while the displacive driving force and the transformation strains are equivalent for each bainitic sub-unit, the growth terminates ultimately due to the elastic interaction. The angle of the sheaf with respect to the habit plane depends on the nucleus position, as well as the termination of sub-unit growth.

Chemical heterogeneity. A subsequent investigation is conducted to ascertain the impact of chemical heterogeneities on the growth of bainitic sub-units and sheaves. Guided by the findings of the APT, a chemical gradient is artificially introduced into the system through the

prescription of an Mn concentration field. This field comprises an Mn-rich and an Mn-lean region with an additional Mn-concentration peak, consistent with the maximum Mn concentration identified by APT measurements of the 710-F260 condition. The Mn profile extracted along the blue line in Fig. 5(d) is shown in Fig. 5(e). The local increase in Mn results in the local reduction of the displacive driving force as evident in Fig. 1(a). The chemical gradient acts as an obstacle for further growth. As shown in Fig. 5(c)–(d), the sixth sub-unit is not able to grow beyond the Mn-enriched region and the chemical gradient. The simulation results show that when a propagating sheaf encounters such a chemical gradient, the associated decrease in displacive driving force can lead to the complete arrest of the transformation front.

Carbon partitioning. In Fig. 6, the impact of C partitioning on the driving force is investigated. The C first accumulates at the interface

due to substantially smaller diffusivity in austenite. Over a longer time, the C is distributed in the austenite, cf. Fig. 6(a). In Fig. 6(b), it is evident, how this impacts the displacive driving force $\Delta G_{\text{dsp}}^{\text{b}}/V$. In regions of elevated C content, the displacive driving force becomes close to zero and is therefore not sufficient to allow growth. The elastic interaction is impacted only slightly, cf. Fig. 6(c). However, in the illustration of the combination in Fig. 6(d), it is clear to see, that the driving force promoting growth is decreased along the broad sides of the sub-unit. Moreover, in Fig. 6(e), the C profiles along the red lines illustrated in Fig. 6(a) are depicted. It is evident, that due to the strong curvature at the tip, less C is partitioned there. In Fig. 7, the C partitioning is compared for a single sub-unit (upper row) and two neighboring sub-units (lower row) at an arbitrary timestep during the partitioning simulation in terms of the local C concentration c_{C} , Fig. 7(b), and the corresponding C flux vectors j_{C} , Fig. 7(c). The presence of a second sub-unit results in pronounced alterations to the C flux field, as reflected by changes in both magnitude and direction of the flux vectors.

5.3. Linked discussion of simulation and experimental results

Origins and persistence of Mn heterogeneities. The experimental observations reveal strong Mn heterogeneities in the final microstructure after flash austenitization, isothermal holding, and final quenching. The internal Mn gradients in 710-F260 may originate from two forms of chemical heterogeneity in ART710: localized Mn-enriched chemical boundaries near ferrite/austenite interfaces and the Mn redistribution between Mn-rich austenite and Mn-lean ferrite (Fig. 4(a)). During the high-temperature part of the flash cycle, Mn diffusion may broaden the interfacial Mn enrichments and smooth the transitions between neighboring Mn-rich and Mn-lean regions without complete homogenization [47]. Migration of phase and grain boundaries during austenitization may also leave inherited compositional variations within larger austenite grains [46]. Both forms of initial heterogeneity may therefore contribute to the final intragranular gradients, but their relative contributions cannot be distinguished by the present EDS and APT measurements. Although the APT and EDS profiles of 710-F260 were measured after final quenching, substantial Mn redistribution by lattice diffusion is not expected during the 260 °C hold. This interpretation is consistent with APT observations showing no measurable partitioning of substitutional elements during bainitic transformation at 200 °C and 300 °C [77]. Further Mn redistribution during final cooling is expected to be even more limited, and martensite formation does not require diffusional redistribution of substitutional solutes [47,69]. The measured Mn gradients are therefore more likely inherited from the chemical state at the start of bainitization than generated during growth of the selected bainitic ferrite plate. The measurements do not establish the exact Mn profile at the peak austenitization temperature. This inference concerns Mn rather than C, which can redistribute by partitioning during low-temperature heat treatment [69,77].

Linking Mn heterogeneities to growth arrest. These intragranular Mn variations provide a basis for examining a local chemical growth-limiting mechanism. At a given temperature and C content, increasing Mn stabilizes austenite relative to ferrite and reduces the displacive driving force for bainitic transformation [39]. Growth towards an Mn-enriched region may therefore become less favorable before the transformation front reaches a PAGB. The observed spatial relationship between the selected plate and an internal Mn gradient is consistent with this possibility. However, prior-austenite grain size affects bainitic morphology and effective grain size [78], while the grain-boundary structure also influences bainite nucleation [79]. Grain-size effects are therefore not restricted to direct impingement on a PAGB. Although the selected plate is smaller than its parent grain and its tapered end lies beside an internal Mn gradient, out-of-plane PAGBs may also have constrained its growth. The observed spatial correlation is therefore treated as motivation for testing a local chemical growth-limiting

mechanism, not as evidence that Mn heterogeneity is the dominant factor controlling the final morphology of bainitic ferrite. The present measurements do not determine the relative contributions of prior-austenite grain size and Mn heterogeneity, and a dominant grain-size contribution remains possible. The final-state observations also do not directly record growth arrest or separate the contributions of preferential nucleation in Mn-lean regions, C redistribution, local stresses, and impingement. Through-thickness averaging over the finite lamella thickness limits the assignment of chemical variations to individual interfaces. In addition, the ART710 and 710-F260 measurements also do not track the evolution of the same Mn chemical boundary. The experiments therefore establish Mn heterogeneity and its local spatial relationship with bainitic ferrite, while the simulations assess whether a prescribed Mn field can suppress further growth under controlled conditions.

Simulation-experiment synergy. The simulations are designed to isolate the impact of Mn heterogeneities on bainitic sub-unit growth by prescribing the Mn field while keeping all other input parameters constant. Within the prescribed model conditions, Mn heterogeneity modifies the local growth conditions of bainitic ferrite. Additional simulations on a single sub-unit demonstrate, consistent with earlier findings, that the tip region of a bainitic sub-unit is energetically favored for the nucleation of subsequent sub-unit, cf., e.g., [30]. Moreover, the simulations indicate that the introduction of a small dilatational strain component leads to a side preference for the nucleation and growth of subsequent sub-units. This effect is directly incorporated into the modeling of sheaf growth. The central conclusion is that an Mn-enriched region can stop an advancing bainitic ferrite front when the local transformation driving force falls below the critical value necessary for growth. This behavior is consistent with thermodynamic and dilatometric studies showing that increasing Mn content lowers the displacive driving force for bainite formation and slows, or even suppresses, the bainitic transformation [39]. In the present simulation study, the Mn-rich region is introduced based on APT observations and acts as a barrier through its effect on the local energy balance. Interface motion is allowed only when the displacive driving force is large enough to compensate the interfacial and elastic energy associated with the transformation. Mn-enriched regions locally stabilize the parent austenite, while C rejected from bainitic sub-units into the surrounding austenite further reduces the local driving force as shown by simulations. Similar C-enrichment effects in the retained austenite are central to the incomplete bainite reaction and the stabilization of residual austenite [37]. In a chemically homogeneous alloy, this limitation appears mainly as a global restriction on the transformed fraction. In a chemically heterogeneous alloy, the same type of thermodynamic constraint can become spatially localized and Mn-enriched regions and steep Mn gradients act as chemical barriers. The simulations therefore indicate that the experimentally observed Mn heterogeneity can lead to local growth arrest of bainitic ferrite, which is expected to contribute to a refinement of the final bcc microstructure. The main contribution of this work lies in the combined use of experiments and simulations, where the experiments evidence chemical heterogeneities and the simulations enable the isolation of a chemical heterogeneity effect that is not directly accessible experimentally. The results show that retained Mn heterogeneity can act as an internal growth-limiting feature for bainitic ferrite when the local composition lowers the transformation driving force enough to violate the growth criterion. This supports the broader idea of using chemical heterogeneity as an active microstructural design variable [46].

6. Summary and conclusion

Summary. This work investigates the growth of bainitic sub-units within a multiphase-field framework, in close relation to experimental observations of microstructural evolution. A particular emphasis is placed on the role of transformation strains, chemical heterogeneities,

and carbon redistribution following growth. Electron backscatter diffraction provides an overview of the final 710-F260 phase distribution and bcc-domain morphology. Correlative scanning transmission electron microscopy, transmission Kikuchi diffraction, and energy-dispersive X-ray spectroscopy relate the selected plate-like bainitic ferrite grain to surrounding manganese gradients, while atom-probe tomography characterizes the initial interfacial manganese chemical boundary in ART710 and nanoscale manganese gradients after the complete 710-F260 cycle. Through simulations the growth of a single bainitic sub-unit is analyzed by comparing a pure shear transformation strain with a shear-dominated transformation strain that additionally incorporates a small volumetric strain component. Building on these results, the successive addition of sub-units and the resulting sheaf structure are examined. The influence of manganese-enriched regions on bainitic transformation is investigated by combining experiments and simulations. To this end atom-probe tomography-derived chemical boundaries are introduced into the phase-field simulations and the impact of the experimentally observed manganese gradients on bainitic transformation are investigated in a controlled modeling setup. Furthermore, the impact of carbon partitioning on the driving force is evaluated within a fully coupled chemo-mechanical framework. A combined chemo-mechanical criterion for the driving force is formulated and used to investigate the interplay between elastic and chemical fields.

Conclusion. The simulations confirm earlier findings that the tip region of a bainitic sub-unit is energetically favored for the nucleation of subsequent sub-units owing to elastic driving forces. In addition, carbon partitioning is found to occur preferentially through the broad side of the sub-unit, resulting in a smaller reduction of the displacive driving force at the tip, thereby further promoting nucleation in this region. This preferential nucleation promotes the directional growth of bainitic sheaves and provides an explanation for their characteristic elongated morphology. The inclusion of a dilatational component of the transformation strains introduces an asymmetry with respect to the habit plane, leading to an asymmetric distribution of the elastic driving forces and consequently influencing the preferred sites for subsequent sub-unit formation. Furthermore, with each successive addition of a bainitic sub-unit, the elastically favored region at the sheaf tip decreases in size under the imposed boundary conditions. Consequently, the driving force promoting the nucleation and growth of the subsequent sub-unit is progressively reduced, making continued sheaf growth increasingly unfavorable. The simulations incorporating atom-probe tomography-derived chemical heterogeneities demonstrate that manganese-enriched regions can promote earlier growth arrest of bainitic sheaves and thereby provide a plausible mechanism for microstructural refinement. Overall, the experiments establish manganese heterogeneity and its local spatial relationship with bainitic ferrite, while the simulations show that such heterogeneity can act as an internal growth-limiting feature under the prescribed conditions. These findings support the use of chemical heterogeneity as a microstructural design parameter.

CRediT authorship contribution statement

Thea Kannenberg: Writing – original draft, Visualization (Simulation), Validation, Software (Simulation), Methodology, Investigation, Formal analysis (Simulation), Conceptualization. **Bowen Zou:** Writing – original draft (Experiment), Visualization (Experiment), Methodology, Investigation, Formal analysis (Experiment), Data curation (Experiment), Conceptualization. **Wenwen Song:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **Daniel Schneider:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work the authors used DeepL (DeepL SE) and ChatGPT (OpenAI) in order to improve readability and clarity of the manuscript. No content was generated by these tools. After using these tools, the authors reviewed and edited the content and take full responsibility for the content of the published article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

TK and BZ gratefully acknowledge the financial support of the German Research Foundation (DFG) within the project “Giga-NANOBAIN” (Proj. No. 490856143). TK acknowledges support by the Joachim Herz Foundation and expresses gratitude to E. Schoof and P. G. K. Amos for their preliminary work that contributed to this study. BZ and WS also express their gratitude to Y. Li and B. Gault for their support with the APT specimen measurements during their time at the Max Planck Institute for Sustainable Materials (MPI-SusMat). DS gratefully acknowledges scientific discussion within the Helmholtz programme MSE, no. 43.31.01.

Appendix A. Interface stabilization

A balanced ratio of terms building the diffuse interface and the driving forces is required for numerical accuracy. While this can be achieved for small interface widths, computational constraints in large-scale simulations necessitate interface widths exceeding the physical scale. In this case, the physical interfacial energy alone is insufficient to ensure a stable interface. To compensate for this, an additional stabilization term $\Delta_{\text{stab}}^{\alpha\beta}$ is introduced in Eq. (6) reading

$$\begin{aligned} \Delta_{\text{stab}}^{\alpha\beta} = & -\gamma_{\text{stab}} \epsilon \left(\Delta \phi_{\alpha} - \|\nabla \phi_{\alpha}\| \operatorname{div} \left(\frac{\nabla \phi_{\alpha}}{\|\nabla \phi_{\alpha}\|} \right) \right. \\ & \left. - \Delta \phi_{\beta} + \|\nabla \phi_{\beta}\| \operatorname{div} \left(\frac{\nabla \phi_{\beta}}{\|\nabla \phi_{\beta}\|} \right) \right) \\ & - \gamma_{\text{stab}} \frac{16}{\epsilon \pi^2} (\phi_{\alpha} - \phi_{\beta}), \end{aligned} \quad (20)$$

cf. [52, Eqs. (31)–(32)], where Δ denotes the Laplace operator. The associated interface parameter γ_{stab} is used to tune the strength of the artificial interface stabilization. However, this additional contribution acts solely in the interface-normal direction. Consequently, it has no energetic contribution to the equilibrium state, i.e., the additional contribution does not contribute to curvature minimization, cf., e.g., [52]. A correct interplay of gradient and potential energy is ensured. A more detailed description is given in [32,52]. Similar stabilization methods are presented in [80,81].

Appendix B. Visualization of anisotropy in the elastic energy density

The polar plot in Fig. 2(a) relates anisotropic eigenstrains to the isotropic elastic energy employing an orientation-dependent elastic energy function $B(\mathbf{n})$ introduced in [67]. This approach has been employed, e.g., in [28,82]. The function $B(\mathbf{n})$ is given by

$$B(\mathbf{n}) = C_{ijkl} \bar{\epsilon}_{ij} \bar{\epsilon}_{kl} - n_i \bar{\sigma}_{ij} \Omega_{jl} \bar{\sigma}_{lm} n_m, \quad (21)$$

cf., e.g., [67, Eq. (8.1.2)], where $\tilde{\sigma}_{ij} = C_{ijkl}\tilde{\epsilon}_{kl}$ and the inverse Green function tensor reads

$$(\mathbf{\Omega}^{-1}(\mathbf{n})) = C_{ijkl}n_kn_l\mathbf{e}_i \otimes \mathbf{e}_j, \quad (22)$$

cf., e.g., [67, Eq. (8.1.3)], where $\mathbf{n}$ represents a normal vector. For the purpose of the polar plot visualization in Fig. 2(a) only, homogeneous elastic moduli are assumed, the phase-field simulations retain the actual modulus contrast. Given the modest stiffness difference and the qualitative purpose of this figure, this simplification suffices to illustrate the asymmetry introduced by dilatational eigenstrains with respect to the habit plane.

Appendix C. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.mtla.2026.102906>.

Data availability

Data will be made available upon reasonable request.

References

- [1] H.K.D.H. Bhadeshia, R.W.K. Honeycombe, *Steels: Microstructure and Properties*, fourth ed., Elsevier Butterworth-Heinemann, Oxford, UK, 2017.
- [2] F. Caballero, Carbide-free bainite in steels, in: *Phase Transformations in Steels*, in: Woodhead Publishing Series in Metals and Surface Engineering, 1, Woodhead Publishing, 2012, pp. 436–467.
- [3] C. Garcia-Mateo, F.G. Caballero, T. Sourmail, J. Cornide, V. Smanio, R. Elvira, Composition design of nanocrystalline bainitic steels by diffusionless solid reaction, *Met. Mater. Int.* 20 (3) (2014) 405–415.
- [4] Y. Huang, X.-l. Zhang, W.-n. Liu, X.-m. Wang, J.-k. Han, Microstructure and mechanical properties of NANOBAIN steel, *J. Iron Steel Res. Int.* 23 (3) (2016) 253–260.
- [5] H.K.D.H. Bhadeshia, in: K.H.J. Buschow, R.W. Cahn, M.C. Flemings, B. Ilschner, E.J. Kramer, S. Mahajan (Eds.), *Novel Steels for Rails*, Elsevier Science, Amsterdam New York, 2002.
- [6] F.G. Caballero, J. Pujante, T. Sourmail, R. Rementeria, D. De-Castro, P. Dierckx, G. Ramfrez, C. Sidoroff-Coicaud, P. Valizadeh Moghaddam, E. Vuorinen, Advanced heat treatments and complex ferritic structures for bearing steels, *Metals* 9 (11) (2019) 1137.
- [7] W.T. Reynolds Jr., H.I. Aaronson, G. Spanos, A summary of the present diffusionist views on bainite, *Mater. Trans. JIM* 32 (8) (1991) 737–746.
- [8] A. Borgenstam, M. Hillert, J. Ågren, Metallographic evidence of carbon diffusion in the growth of bainite, *Acta Mater.* 57 (11) (2009) 3242–3252.
- [9] H.K.D.H. Bhadeshia, D. Edmonds, The mechanism of bainite formation in steels, *Acta Metall.* 28 (9) (1980) 1265–1273.
- [10] R.F. Hehemann, K.R. Kinsman, H.I. Aaronson, A debate on the bainite reaction, *Met. Trans.* 3 (5) (1972) 1077–1094.
- [11] L.C.D. Fielding, The bainite controversy, *Mater. Sci. Technol.* 29 (4) (2013) 383–399.
- [12] H.K.D.H. Bhadeshia, *Bainite in Steels: Theory and Practice*, third ed., Maney Publishing, Leeds, UK, 2015.
- [13] H.K.D.H. Bhadeshia, *Bainite : Overall transformation kinetics*, *Le J. de Phys. Colloq.* 43 (C4) (1982) C4–443–C4–448.
- [14] H.K.D.H. Bhadeshia, J.W. Christian, Bainite in steels, *Met. Trans. A* 21 (3) (1990) 767–797.
- [15] H.K.D.H. Bhadeshia, Mechanism of the bainite transformation: A turning point, *Met. Mater. Trans. A* (2025).
- [16] N. Moelans, B. Blanpain, P. Wollants, An introduction to phase-field modeling of microstructure evolution, *Calphad* 32 (2) (2008) 268–294.
- [17] I. Steinbach, Phase-field models in materials science, *Modelling Simul. Mater. Sci. Eng.* 17 (7) (2009) 073001.
- [18] D. Tourret, H. Liu, J. Llorca, Phase-field modeling of microstructure evolution: Recent applications, perspectives and challenges, *Prog. Mater. Sci.* 123 (2022) 100810.
- [19] A. Prah, D. Schneider, B. Nestler, A continuum thermodynamic approach to the phase-field method: the order parameter as internal state variable, *Contin. Mech. Thermodyn.* 37 (4) (2025) 55.
- [20] A. Prah, A. Elmhazy, D. Schneider, B. Nestler, The multiphase-field method based on internal state variables, *Contin. Mech. Thermodyn.* 38 (3) (2026) 47.
- [21] T.T. Arif, R.S. Qin, A phase-field model for bainitic transformation, *Comput. Mater. Sci.* 77 (2013) 230–235.
- [22] T.T. Arif, R.S. Qin, A phase-field model for the formation of martensite and bainite, *Adv. Mater. Res.* 922 (2014) 31–36.
- [23] M. Toloui, M. Militzer, Phase field modeling of the simultaneous formation of bainite and ferrite in TRIP steel, *Acta Mater.* 144 (2018) 786–800.
- [24] W. Song, U. Prah, Y. Ma, W. Bleck, Multiphase-field simulation of cementite precipitation during isothermal lower bainitic transformation, *Steel Res. Int.* 89 (8) (2018) 1800028.
- [25] M. Düsing, R. Mahnken, Simulation of lower bainitic transformation with the phase-field method considering carbide formation, *Comput. Mater. Sci.* 111 (2016) 91–100.
- [26] M. Düsing, R. Mahnken, A coupled phase field/diffusion model for upper and lower bainitic transformation, *Int. J. Solids Struct.* 135 (2018) 172–183.
- [27] M. Düsing, R. Mahnken, A coupled phase field/diffusional/mechanical framework for simulation of upper and lower bainitic transformation, *Int. J. Solids Struct.* 162 (2019) 45–59.
- [28] P.G.K. Amos, E. Schoof, D. Schneider, B. Nestler, Chemo-elastic phase-field simulation of the cooperative growth of mutually-accommodating Widmanstätten plates, *J. Alloys Compd.* 767 (2018) 1141–1154.
- [29] C. Hüter, M. Lin, D. Schicchi, M. Hunkel, U. Prah, R. Spatschek, A multiscale perspective on the kinetics of solid state transformations with application to bainite formation, *AIMS Mater. Sci.* 2 (4) (2015) 319–345.
- [30] E. Schoof, P. Kubendran Amos, D. Schneider, B. Nestler, Influence of stress-free transformation strain on the autocatalytic growth of bainite: A multiphase-field analysis, *Materialia* 9 (2020) 100620.
- [31] H. Salama, M.A. Ali, O. Shchyglo, I. Steinbach, Phase-field simulation framework for modeling martensite and bainite formation in steel, *Comput. Mater. Sci.* 241 (2024) 113033.
- [32] E. Schoof, Chemomechanische Modellierung der Wärmebehandlung von Stählen mit der Phasenfeldmethode, in: *Schriftenreihe des Instituts für Angewandte Materialien*, 93, KIT Scientific Publishing, Karlsruhe, 2021.
- [33] F.G. Caballero, H.K.D.H. Bhadeshia, K.J.A. Mawella, D.G. Jones, P. Brown, Very strong low temperature bainite, *Mater. Sci. Technol.* 18 (3) (2002) 279–284.
- [34] V. Ruiz-Jimenez, J.A. Jimenez, F.G. Caballero, C. Garcia-Mateo, Bainitic ferrite plate thickness evolution in two nanostructured steels, *Materials* 14 (15) (2021) 4347.
- [35] S. Singh, H. Bhadeshia, Estimation of bainite plate-thickness in low-alloy steels, *Mater. Sci. Eng.: A* 245 (1) (1998) 72–79.
- [36] C. Garcia-Mateo, F.G. Caballero, H.K.D.H. Bhadeshia, Development of hard bainite, *ISIJ Int.* 43 (8) (2003) 1238–1243.
- [37] C. Goulas, M.G. Mecozzi, J. Sietsma, Bainite formation in medium-carbon low-silicon spring steels accounting for chemical segregation, *Met. Mater. Trans. A* 47 (2016) 3077–3087.
- [38] N.E. Tenaglia, J.M. Massone, R.E. Boeri, J.G. Speer, Effect of microsegregation on carbide-free bainitic transformation in a high-silicon cast steel, *Mater. Sci. Technol.* 36 (6) (2020) 690–698.
- [39] M. Morawiec, J. Opara, C. Garcia-Mateo, J.A. Jimenez, A. Grajcar, Effect of Mn on the chemical driving force and bainite transformation kinetics in medium-manganese alloys, *J. Therm. Anal. Calorim.* 148 (2023) 1567–1576.
- [40] J. Abraham Mathews, J. Sietsma, R. Petrov, M. Santofimia, Influence of chemical segregation on bainitic microstructures in a carburized bearing steel, *Mater. Des.* 223 (2022) 111232.
- [41] L. Huang, F. Liu, M. Huang, Accelerating bainite transformation by concurrent pearlite formation in a medium Mn steel: Experiments and modelling, *J. Mater. Sci. Technol.* 176 (2024) 211–223.
- [42] J.H. Kim, G. Gu, S.-H. Hong, C.J. Yu, M. Koo, E.Y. Kim, A. Zargaran, J.S. Lee, D.-W. Suh, Acceleration of bainitic transformation in 0.28C-3.8Mn-1.5Si steel utilizing chemical heterogeneity, *Scr. Mater.* 239 (2024) 115779.
- [43] J. Yan, X. Zhang, H. Liu, G. Miyamoto, Z. Cao, Y. Zhang, Y. Pei, P. Shi, J. Chen, T. Furuha, Enhancing ductility of the TRIP aided bainitic ferrite steel by Mn heterogeneity introduced via reversion: Towards the 3rd generation, *Scr. Mater.* 252 (2024) 116241.
- [44] C. Liu, D. Sun, C. Chen, B. Lv, X. Wang, Z. Yang, F. Zhang, Constructing multi-scale retained austenite makes bainitic steel better mechanical properties by introducing weak chemical heterogeneity, *Mater. Res. Lett.* 12 (9) (2024) 653–660.
- [45] B. Zou, M. Zapf, T. Kannenberg, D. Schneider, Y. Wang, X. Shen, U. Prah, W. Song, In situ synchrotron X-ray diffraction study of flash austenitization and process design insights in medium-manganese steels for energy applications, *JOM* (2026).
- [46] R. Ding, Y. Yao, B. Sun, G. Liu, J. He, T. Li, X. Wan, Z. Dai, D. Ponge, D. Raabe, C. Zhang, A. Godfrey, G. Miyamoto, T. Furuha, Z. Yang, S. van der Zwaag, H. Chen, Chemical boundary engineering: A new route toward lean, ultrastrong yet ductile steels, *Sci. Adv.* 6 (13) (2020) eaay1430.
- [47] Y. Wang, R. Ding, C. Franke, T. Li, X. Rong, P. Wen, Z. Yang, H. Chen, Flash annealing of a chemically heterogeneous medium Mn steel, *Scr. Mater.* 242 (2024) 115923.
- [48] V.L. Ginzburg, On the theory of superconductivity, *Il Nuovo Cimento* 2 (6) (1955) 1234–1250.
- [49] B. Nestler, H. Garcke, B. Stinner, Multicomponent alloy solidification: Phase-field modeling and simulations, *Phys. Rev. E* 71 (4) (2005) 041609.
- [50] I. Steinbach, F. Pezzolla, A generalized field method for multiphase transformations using interface fields, *Phys. D: Nonlinear Phenom.* 134 (4) (1999) 385–393.

- [51] P.W. Hoffrogge, S. Daubner, D. Schneider, B. Nestler, B. Zhou, J. Eiken, Triple junction benchmark for multiphase-field models combining capillary and bulk driving forces, *Modelling Simul. Mater. Sci. Eng.* 33 (1) (2025) 015001.
- [52] E. Schoof, D. Schneider, N. Streichhan, T. Mittnacht, M. Selzer, B. Nestler, Multiphase-field modeling of martensitic phase transformation in a dual-phase microstructure, *Int. J. Solids Struct.* 134 (2018) 181–194.
- [53] H. Goldstein, C.P. Poole, J.L. Saffko, *Classical Mechanics*, third ed., Addison Wesley, San Francisco, 2002.
- [54] A. Durga, P. Wollants, N. Moelans, Evaluation of interfacial excess contributions in different phase-field models for elastically inhomogeneous systems, *Modelling Simul. Mater. Sci. Eng.* 21 (5) (2013) 055018.
- [55] J. Mosler, O. Shchyglo, H.M. Hojjat, A novel homogenization method for phase field approaches based on partial rank-one relaxation, *J. Mech. Phys. Solids* 68 (2014) 251–266.
- [56] D. Schneider, F. Schwab, E. Schoof, A. Reiter, C. Herrmann, M. Selzer, T. Böhlke, B. Nestler, On the stress calculation within phase-field approaches: A model for finite deformations, *Comput. Mech.* 60 (2) (2017) 203–217.
- [57] B. Svendsen, P. Shanthraj, D. Raabe, Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids, *J. Mech. Phys. Solids* 112 (2018) 619–636.
- [58] T. Kannenberg, A. Prahs, B. Svendsen, B. Nestler, D. Schneider, Coupling approaches in chemo-mechanical multiphase-field models, *Int. J. Mech. Sci.* 303 (2025) 110569.
- [59] T. Kannenberg, A. Prahs, B. Svendsen, B. Nestler, D. Schneider, Chemo-mechanical benchmark for phase-field approaches, *Modelling Simul. Mater. Sci. Eng.* 33 (1) (2025) 015004.
- [60] T. Kannenberg, A. Prahs, B. Nestler, D. Schneider, A chemo-mechanically fully coupled multiphase-field model for multicomponent systems accounting for balance equations on singular surfaces, *PAMM* 26 (1) (2026) e70090.
- [61] O. Mustak, E. Evcil, C. Simsir, Simulation of through-hardening of SAE 52100 steel bearings – Part I: Determination of material properties, *Mater. Und Werkst.* 47 (8) (2016) 735–745.
- [62] J. Ågren, Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels, *Acta Metall.* 30 (4) (1982) 841–851.
- [63] J. Ågren, A revised expression for the diffusivity of carbon in binary Fe3C austenite, *Scr. Metall.* 20 (11) (1986) 1507–1510.
- [64] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-calc & DICTRA, computational tools for materials science, *Calphad* 26 (2) (2002) 273–312.
- [65] P.G.K. Amos, L.T. Mushongera, B. Nestler, Phase-field analysis of volume-diffusion controlled shape-instabilities in metallic systems-I: 2-dimensional plate-like structures, *Comput. Mater. Sci.* 144 (2018) 363–373.
- [66] N. Luzginova, L. Zhao, J. Sietsma, Bainite formation kinetics in high carbon alloyed steel, *Mater. Sci. Eng.: A* 481–482 (2008) 766–769.
- [67] A.G. Khachaturyan, *Theory of Structural Transformations in Solids*, Wiley, New York, 1983.
- [68] H.K.D.H. Bhadeshia, D.V. Edmonds, The bainite transformation in a silicon steel, *Met. Trans. A* 10 (7) (1979) 895–907.
- [69] J. Speer, D. Matlock, B. De Cooman, J. Schroth, Carbon partitioning into austenite after martensite transformation, *Acta Mater.* 51 (9) (2003) 2611–2622.
- [70] Y. Li, S. Chen, C. Wang, D.S. Martín, W. Xu, Modeling retained austenite in Q&P steels accounting for the bainitic transformation and correction of its mismatch on optimal conditions, *Acta Mater.* 188 (2020) 528–538.
- [71] P.G.K. Amos, E. Schoof, N. Streichan, D. Schneider, B. Nestler, Phase-field analysis of quenching and partitioning in a polycrystalline Fe-C system under constrained-carbon equilibrium condition, *Comput. Mater. Sci.* 159 (2019) 281–296.
- [72] J. Hötzer, A. Reiter, H. Hierl, P. Steinmetz, M. Selzer, B. Nestler, The parallel multi-physics phase-field framework Pace3D, *J. Comput. Sci.* 26 (2018) 1–12.
- [73] B. Hu, X. Shen, Q. Guo, Q. Wen, X. Tu, C. Ding, F. Ding, W. Song, H. Luo, Yielding behavior of triplex medium Mn steel alternated with cooling strategies altering martensite/ferrite interfacial feature, *J. Mater. Sci. Technol.* 126 (2022) 60–70.
- [74] J.R. Michael, L.A. Giannuzzi, M.G. Burke, X.L. Zhong, Mechanism of FIB-induced phase transformation in austenitic steel, *Microsc. Microanal.* 28 (1) (2022) 70–82.
- [75] O. Dmitrieva, D. Ponge, G. Inden, J. Millán, P. Choi, J. Sietsma, D. Raabe, Chemical gradients across phase boundaries between martensite and austenite in steel studied by atom probe tomography and simulation, *Acta Mater.* 59 (1) (2011) 364–374.
- [76] X. Shen, H. Qiao, W. Song, W. Bleck, Near-atomic scale characterization of Mn-gradient in reverted austenite in hot-rolled medium-Mn steels, *Steel Res. Int.* 94 (11) (2023) 2300145.
- [77] F.G. Caballero, M.K. Miller, S.S. Babu, C. Garcia-Mateo, Atomic scale observations of bainite transformation in a high carbon high silicon steel, *Acta Mater.* 55 (1) (2007) 381–390.
- [78] H. Zhao, B.P. Wynne, E.J. Palmiere, Effect of austenite grain size on the bainitic ferrite morphology and grain refinement of a pipeline steel after continuous cooling, *Mater. Charact.* 123 (2017) 128–136.
- [79] A.M. Ravi, A. Kumar, M. Herbig, J. Sietsma, M.J. Santofimia, Impact of austenite grain boundaries and ferrite nucleation on bainite formation in steels, *Acta Mater.* 188 (2020) 424–434.
- [80] C.C. Chen, H.K. Lin, C.W. Lan, Phase field modeling with large interface thickness and undercooling, *J. Cryst. Growth* 385 (2014) 121–126.
- [81] V. Feyen, N. Moelans, Quantitative high driving force phase-field model for multi-grain structures, *Acta Mater.* 256 (2023) 119087.
- [82] M. Cottura, B. Appolaire, A. Finel, Y. Le Bouar, Phase field study of acicular growth: Role of elasticity in Widmanstätten structure, *Acta Mater.* 72 (2014) 200–210.