Microstructure Transformations in a Press Hardening Steel during Tailored Thermomechanical Processing

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Microstructure transformation due to thermomechanical processing has an acute effect on the macroscopic properties of low-carbon steels. This effect includes viscoplastic deformation and phase transformations. Hot forming processes such as press hardening are particularly affected. Most engineering applications require a combination of high strength and sufficient residual ductility, which can be achieved by the development of graded microstructures. Herein, the evolution of phase transformations is investigated by linking experiments and simulations to produce graded microstructures. For this purpose, an extended material model is proposed to represent the evolution of phase transformations under inhomogeneous heating and cooling strategies. On the experimental side, phase transformations are identified during thermomechanical treatment of flat steel specimens using digital image correlation and thermal imaging. Based on the experimental results, the material parameters are identified, and the simulation model is validated. On the numerical side an algorithm for the finite-element simulation of phase transformations in low-carbon steels is proposed. The evolution of phase transformations is presented for the simulation of a tensile specimen using the finite-element method.

1. Introduction

The material properties of engineering components are strongly influenced by their microstructure. Especially in the hot forming of steels with integrated heat treatment, macroscopic material properties are subject to drastic change due to extensive structural transformations. These include various mechanisms, such as recrystallisation, recovery, and the development of phase transformations. For the thermomechanical processing of steels, a precise knowledge and prediction of such microstructural mechanisms is essential to achieve the desired macroscopic material properties, and in turn to grade the microstructures and adjust the material properties. High strength coupled with high energy absorption and sufficient ductility can be achieved for most engineering components. The difficulty lies in controlling the process parameters during thermomechanical processes.

For the numerical simulation of phase transformations, various multiphase models from the literature can be used. These approaches are divided mainly into macroscopic continuum mechanical models and microscopic phase field models. Due to the computational complexity of phase field models and their general inapplicability to large geometries, a continuum mechanical model with internal state variables is preferable, the most important of which are described subsequently.

Continuum mechanical models describe material behavior with internal variables at the microstructural level. Several continuum mechanical models have been proposed. Most models describe two-phase systems that capture the evolution of austenite and martensite and are often developed in the framework of small deformations (e.g., see previous studies [1–3]). For the present purpose, approaches within large deformation theory are more suitable (e.g., Hallberg et al. [4,5]). Multiphase models that consider more than two phases have been proposed, for example, by Mahnken and Schmeidt. [6] Furthermore, in the evolution of bainite, a distinction can be made between lower and upper bainite, as suggested in Mahnken et al. [7] Beyond upper and lower bainite, also granular, inverse, columnar, and coalesced bainite can occur, which is not considered in continuum mechanical models.

For 22MnB5 steel, cooling above the critical rate of 25 K s⁻¹ leads to an entirely martensitic microstructure, which is responsible for the high strength of the material, as shown by Naderi et al. [8] Lower cooling rates result in the formation of a relatively soft microstructure, consisting of ferrite, pearlite, and bainite. The phase transformations of these are strongly influenced by hot deformation. A hot deformation degree equal to or greater than 10% leads to a shift of the ferritic, pearlitic, and bainitic areas to shorter cooling times and higher temperatures, as found by Nietz et al. [9] Schaper et al. [10] and Nikravesh et al. [11]. Austenite deformation leads to the generation of...
more dislocations, which delay martensitic transformation, accelerate carbon diffusion, and cause an increase in nucleation sites, as shown by Naderi et al. and Zhou et al. In addition, the martensite self-temper during cooling of the press-hardened parts, resulting in a hardness that is 50 HV lower compared to that of water-quenched 22MnB5 parts with a hardness of about 500 HV (see Nishibata and Kojima).

The characterization of the material properties after the press hardening process requires a high experimental effort involving expensive working hours and equipment such as the deformation dilatometer shown in Bambach et al.

The characterization of phase transformations for various thermal and deformational conditions require a high experimental effort involving a high amount of samples, expensive working hours, and equipment such as a deformation dilatometer.

In Haupt a non-contact characterization method for determining phase transformations during the thermomechanical treatment of flat steel samples was presented. The benefit is that the analysis of a tailored treatment process with a graded austenitization temperature or strain distribution is possible with only one specimen. This is the method used in this study.

In this work, experimental and numerical examinations of 22MnB5 steel are conducted. The experimental characterization of the 22MnB5 steel provides the necessary data for the development and parameterization of the numerical model. The macroscopic material model of Mahnken et al. is taken as a starting point for further developments. The main objectives and contributions of this work are: 1) to develop a multiphase model that takes into account the transformation of the initial ferritic–pearlitic microstructure into austenite, and the formation of ferrite, pearlite, bainite, and martensite during the tailored temperature treatment; 2) to determine microstructural transformations experimentally by means of hot tensile tests followed by forced cooling; 3) to identify material parameters for the proposed model; and 4) to validate the proposed model with the experimental results performing finite-element simulations for hot tensile tests with tailored temperature treatment.

Within this context, this work focuses on the microstructural development of the steel 22MnB5, the most important microstructural mechanism studied being phase transformations. Both numerical and experimental investigations are performed. The overarching goal is to provide a fully functional constitutive model for the simulation of hot forming processes.

2. Thermodynamic Framework for Multiphase Continua

The thermodynamic framework for multiphase simulations proposed by Mahnken et al. is extended to also cover the development of ferrite and pearlite phases in addition to bainite and martensite. This broader framework is briefly presented subsequently and the equations for the evolution of the ferrite and pearlite phases are proposed.

2.1. Kinematics

The constitutive equations are based on the large strain theory. At each material point, the deformation gradient $\mathbf{F}$ is introduced, which maps the line segments $d\mathbf{x}$ of the reference configuration $B_0$ to the line segments $d\mathbf{x}$ of the current configuration $\mathcal{B}_0$. Based on the multiplicative splitting, the deformation gradient

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_i$$

is obtained, where $\mathbf{F}_e$ and $\mathbf{F}_i$ represent the elastic and plastic parts of the deformation gradient, respectively. The velocity gradient $\mathbf{L}$ with respect to the intermediate configuration is additively split as

$$\mathbf{L} := \mathbf{L}_e + \mathbf{L}_i,$$

where

$$\mathbf{L}_e := \mathbf{F}_e^{-1} \cdot \dot{\mathbf{F}}_e$$

$$\mathbf{L}_i := \mathbf{F}_i \cdot \mathbf{F}_i^{-1} = -\mathbf{F}_i \cdot \dot{\mathbf{F}}_i^{-1}$$

and where $\mathbf{L}_e$ and $\mathbf{L}_i$ are the elastic and inelastic part of the velocity gradient, respectively. The kinematics follow the same general approach as in Mahnken et al.

2.2. Balance Relations

The macroscopic modeling of steel is considered in the following as having a mixture of several phases, where interactions between the phases are not considered. In contrast to general mixtures, the phases do not diffuse but coexist. In the reference macroscopic configuration the carbon content is assumed to be constant. Following Haupt, the equilibrium relations with respect to the reference configuration $B_0$ are defined as

$$\rho_0 \dot{\mathbf{u}} - \text{Div}[\mathbf{F} \cdot \mathbf{S}] = \rho_0 \dot{\mathbf{f}}$$

$$\rho_0 \dot{\mathbf{e}} + \text{Div}\mathbf{b}_0 = \mathcal{P} + \rho_0 \dot{\mathbf{r}}_0$$

$$-\rho_0 \dot{\mathbf{e}} + \rho_0 \dot{\mathbf{b}}_0 + \mathbf{S} : \dot{\mathbf{E}} - \frac{1}{\theta} \mathbf{q}_0 : \text{Grad} \theta \geq 0$$

where $\rho_0$ is the density in the reference configuration, $\mathbf{u}$ is the displacement vector, $\mathbf{E}$ is the Green strain tensor, $\theta$ is the absolute temperature, $\mathbf{S}$ is the second Piola–Kirchhoff stress tensor, $\eta$ is the entropy, $\mathbf{f}$ is the mass density of external forces, $\mathbf{e}$ is the mass density of the internal energy, $\mathbf{q}_0$ is the heat-flux density vector, $\mathcal{P}$ is the stress power, and $\mathbf{r}_0$ is the mass density of the heat supply. The inequality Equation (3.3) is commonly referred to as the Clausius–Duhem inequality and is the central equation for proving thermodynamic consistency.

The phase fractions $z_i$ for all phases $i = 1, \ldots, n_z$ are introduced in vectorial form as

$$\mathbf{z} = [z_1, z_2, \ldots, z_{n_z}]$$

$$\sum_{i=1}^{n_z} z_i = 1$$

$$z_i \geq 0$$

where $n_z$ is the maximum number of phases.

As diffusion of the $z_i$ phases is excluded, the Clausius–Duhem inequality applies for the current case. Formally, a distinction must be made between mass phase fractions and volume phase...
fractions. However, because the difference between mass and volume fractions is considered negligible due to the small difference in the densities of the steel phases, the term phase fractions is used from now on. The stress power in the energy balance Equation (3.2) and the Clausius–Duhamel inequality Equation (3.3) is defined as the dual pairing of conjugate stress and strain tensor quantities, as shown in Haupt.[15] After an inelastic advance from the reference to the intermediate configuration, the stress power is defined as

\[ \mathcal{P} = S : E = \mathbf{M} : \mathbf{\Gamma} \]  

where the Green strain tensor is

\[ E = \frac{1}{2} (F^T \cdot F - 1) \]

In addition, in Equation (5) the Mandel stress tensor \( \mathbf{M} \) is defined as \( \mathbf{M} = \mathbf{C}_e \cdot \mathbf{S} \), where \( \mathbf{C}_e \) is the elastic right Cauchy–Green tensor and where \( \mathbf{S} = \mathbf{F}_1 \cdot \mathbf{S} \cdot \mathbf{F}_1^T \).

The Helmholtz energy \( \Psi \) is assumed as

\[ \Psi = \Psi[\mathbf{C}_e, \mathbf{\eta}, \mathbf{\xi}, \mathbf{\theta}] \]

where \( \mathbf{\eta} = (\eta_1, \ldots, \eta_n) \) is the internal variables of the strain hardening mode and \( \mathbf{\xi} \) is the phase fraction introduced in Equation (4). Both of them are internal variables. Following Haupt[7] and using the additive decomposition (Equation (2.1)) and the stress power (Equation (5)) in addition to the identity

\[ \frac{\partial \Psi}{\partial C_e} : \mathbf{\hat{C}}_e = 2(\mathbf{C}_e : \frac{\partial \Psi}{\partial C_e}) : \mathbf{\hat{C}}_e \]

the Clausius–Duhamel inequality with quantities with respect to the intermediate configuration is defined as

\[ \theta_i = \left( \frac{1}{\rho_0} \mathbf{M} - 2 \mathbf{C}_e \cdot \frac{\partial \Psi}{\partial C_e} \right) : \mathbf{\Gamma}_i + 2 \mathbf{C}_e \cdot \frac{\partial \Psi}{\partial C_e} : \mathbf{\hat{C}}_e - \frac{\partial \Psi}{\partial \mathbf{\eta}} \mathbf{\hat{\eta}} - \frac{\partial \Psi}{\partial \mathbf{\xi}} \mathbf{\hat{\xi}} - \left( \eta + \frac{\partial \Psi}{\partial \mathbf{\theta}} \right) \mathbf{\theta} - \frac{1}{\rho_0} \mathbf{q}_0 \cdot \text{Grad} \theta \geq 0 \]  

The thermodynamic forces \( \mathbf{Q} = [Q_1, Q_2, \ldots, Q_n] \) and \( \mathbf{Z} = [Z_1, Z_2, \ldots, Z_n] \) are defined, resulting in a set of constitutive relations given as

\[ \mathbf{M} = \rho_0 \mathbf{C}_e \frac{\partial \Psi}{\partial C_e} \]

\[ \eta = - \frac{\partial \Psi}{\partial \mathbf{\theta}} \]

\[ \mathbf{Q} = \rho_0 \frac{\partial \Psi}{\partial \mathbf{\eta}} \]

\[ \mathbf{Z} = \rho_0 \frac{\partial \Psi}{\partial \mathbf{\xi}} \]

The thermodynamic forces \( \mathbf{Q} \) and \( \mathbf{Z} \) describe the hardening stress and the chemical forces for phase transformation, respectively. Considering the constitutive relations in Equation (10) and (9), the following inequalities are obtained

\[ D^p = \mathbf{M} : \mathbf{\Gamma}_i - Q_i - Z_i \]

\[ D^\theta = - \frac{1}{\mathbf{C}_0} \mathbf{q}_0 \cdot \text{Grad} \theta \]

This sufficiently validates the Clausius–Duhamel inequality. The term \( D^p \) represents dissipation caused by phase transformation and the term \( D^\theta \) represents dissipation caused by thermal evolution. The heat flux vector with respect to the reference configuration \( \mathbf{\theta}_0 \) is derived from Fourier’s law as

\[ \mathbf{q}_0 = - \lambda_0 (\text{det} \mathbf{F}) \mathbf{C}^{-1} \cdot \text{Grad} \theta \]

where \( \mathbf{C} = \mathbf{F}^T \mathbf{F} \)

\[ \lambda_0 \] being the heat conduction coefficient.

The evolution equations for viscosity involving phase transformations are

\[ \mathbf{L}_p = \mathbf{L}_p[\mathbf{K}] \]

\[ \dot{\mathbf{q}} = \dot{\mathbf{\eta}}[\mathbf{K}] \]

\[ \dot{\mathbf{\xi}} = \dot{\mathbf{\xi}}[\mathbf{K}] \]

so that thermodynamic consistency is given in agreement with the dissipations Equation (11). The evolution of the hardening variables and the internal variables is described in terms of the generalized vector \( \mathbf{K} \), which is composed of the Mandel stress tensor \( \mathbf{M} \), the hardening variable \( \mathbf{Q} \), and the chemical forces \( \mathbf{Z} \), which are conjugate to the variables \( \dot{\mathbf{q}} \) and \( \dot{\mathbf{\xi}} \), respectively.

### 3. A Prototype Model

The general model proposed in Section 2 is now specified to 22MnB5 steel. Suggestions are made for the Helmholtz energy and the evolution of the internal variables based on the general thermodynamic framework. For proof of thermodynamic consistency, we refer to Mahnken et al.[7] Although material science does not consider pearlite, bainite, and martensite as phases but as separate microstructures, constitutive modeling views the microstructure as a mixture of several phases. Five phases are included in the tensile test: 1) ferrite, 2) austenite, 3) pearlite, 4) bainite, and 5) martensite.

In addition to the phases considered by Mahnken et al., a pearlite phase is added, and, in contrast to Mahnken et al.,[7] the formation of ferrite from austenite is recorded. Thus, the total number of phases given in Equation (4) is \( n_z = 5 \).

#### 3.1. Helmholtz Free Energy

The Helmholtz energy represents the energy storage due to small reversible deformations in the crystal lattice as well as inelastic deformations as described by Rahniecki and Bruns.[16] In addition, it represents dislocations or energy changes caused by interfacial effects. The Helmholtz energy \( \Psi \) is proposed as
\[ \Psi = \Psi^\text{el}[\mathbf{C}_e, \mathbf{z}, \theta] + \Psi^\text{pl}[\theta] + \Psi^\text{ch}[\mathbf{z}, \theta] + \Psi^\text{chem}[\mathbf{z}], \]

where

\[ \Psi^\text{el} = \frac{1}{2\rho_0} K[\theta] (\ln J_e)^2 + \frac{G[\theta]}{4\rho_0} (\text{tr} \ln \mathbf{C}_e)^2 \]

\[ - \frac{3K[\theta]}{\rho_0} \left( \sum_{i=1}^{5} \alpha_i[\theta] z_{0i} \right) \Delta \theta \ln J_e - \frac{3K[\theta]}{\rho_0} \sum_{i=1}^{5} \left( \rho_i[\theta_0] - 1 \right) z_i \ln J_e \]

\[ \Psi^\text{pl} = \int_0^\theta c_\text{d}[\theta] d\theta - \theta \int_0^\theta c_\text{d}[\theta] d\theta \]

\[ \Psi^\text{ch} = \sum_{i=1}^{5} \left( z_i - z_{0i} \right) \phi_{\text{ch},i}[\theta] \]  

\[ Q_1 = \rho_0 \frac{\partial \Psi}{\partial q_1} = Q_0 b q_1 \]

\[ Q_2 = \rho_0 \frac{\partial \Psi}{\partial q_2} = H q_2 \]

\[ Z_i = \rho_0 \frac{\partial \Psi}{\partial z_i} = -K[\theta] \left( \rho_i[\theta_0] - 1 \right) \ln J_e + \rho_0 \phi_{\text{ch},i}[\theta], \]

where \( Q_0 \) is an initial hardening stress.

### 3.3. Evolution Equations for Viscoplasticity

The additive decomposition of the velocity gradient \( \mathbf{L}_v \) is defined as

\[ \mathbf{L}_v = \mathbf{L}_p + \mathbf{L}_t \]

where \( \mathbf{L}_p \) and \( \mathbf{L}_t \) are the viscoplastic and transformation parts, respectively (see, e.g., Hallberg et al.\(^{[10]} \)). This is a consequence of introducing separate potentials for plasticity and phase transformations, as in Equation (3.1).

The viscoplastic part \( \mathbf{L}_p \) is defined by the common flow rule

\[ \mathbf{L}_p = \lambda \sqrt{\frac{2}{3}} \mathbf{N} \]

\[ \lambda = \left( \frac{\langle \phi \rangle}{D} \right)^m \]

\[ \phi = \sigma_v - (Y[\theta] + Q_1 + Q_2) \]

\[ \sigma_v = \sqrt{\frac{1}{2} \mathbf{M}^\text{dev}} \]

\[ \mathbf{M}^\text{dev} = \mathbf{M} - \frac{1}{3} \mathbf{M} : \mathbf{I} \mathbf{I} \]

where \( \lambda \) is the viscoplastic multiplier, \( \phi \) is the overstress function, \( D > 0 \) is the scalar drag stress, \( \sigma_v \) is the von Mises equivalent stress, and \( \mathbf{N} \) is the normalized Mandel tensor. The scalar \( Y[\theta] \) represents an initial barrier for inelastic behavior and the scalars \( Q_1 \) and \( Q_2 \) are macroscopic flow stresses defined as

\[ Q = Q_1 + Q_2 = Q_0 (1 - \exp[-b q_1]) + H v \]

The macroscopic yield stresses are derived from the internal hardening variable \( q_i \), as proposed by Haupt.\(^{[7]} \) Transformation-induced plasticity is assumed to be caused by martensitic and bainitic transformation. Thus, the velocity gradient \( \mathbf{L}_t \) for the transformation-induced plasticity is given as

\[ \mathbf{L}_t = \frac{3}{2} \int_0^\theta K_{\text{bpm}}(\sigma_v)(\mathbf{M}^\text{dev})^t + \frac{3}{2} \int_0^\theta K_{\text{bpm}}(\sigma_v)(\mathbf{M}^\text{dev})^t \]

based on the work of Leblond.\(^{[17]} \)
From Equation (18.1) the relation for the plastic multiplier is derived as

\[ \lambda = \sqrt{\frac{2}{3} \Gamma_p} (\Gamma_p)^3 = \varepsilon_i , \quad (21) \]

and for the barrier for inelastic behavior \( Y[\theta] \) is used

\[ Y[\theta] = Y_0 + c_Y (\theta - \theta_v) , \quad (22) \]

where \( Y_0 \) is the temperature-independent yield stress.

### 3.4. Evolution of Phase Fractions

The hot forming process under consideration covers several interdependent phase transformations. Many approaches have been taken toward phase transformations in steels. Reference is made to Böhm et al.\[19\] and Wolff et al.\[20\] Specific formulations for all five phases are given subsequently.

Initially, the material is considered to be purely ferritic. The development of the phase fractions is based on the ferritic state. Thus, the initial condition is set to

\[ z_0 = [1, 0, 0, 0, 0]^T . \quad (23) \]

Although the initial state of the real material is not completely ferritic, the pearlitic phase dissolves completely during austenitization and is therefore not considered at the beginning of the simulation. The ferritic phase does not necessarily dissolve completely, but may be retained during the cooling phase at temperatures in the intercritical range.

#### 3.4.1. Formation of Ferrite

It is assumed that ferrite formation follows the general Johnson–Mehl–Avrami–Kolmogorov model for time- and temperature-dependent phase transformations, as proposed by Kolmogorov\[20\] and Avrami\[21\].

Based on Schaper et al.\[10\], the function for the ferrite fraction is

\[ z_1(t) = 1 - \exp(-k_1 \left( \frac{t}{t_1} \right)^n_1) , \quad (24) \]

where \( k_1 \) is a material parameter, \( n_1 \) is the Avrami exponent, \( t_1 \) is a constant parameter, and \( t \) is the duration of the phase transformation (see, e.g., Schaper et al.\[10\] and Avrami\[21\]). By deriving Equation (24) with respect to time \( t \) and rearranging the result, the evolution equation for the formation of ferrite from austenite is

\[ \dot{z}_1 = (1 - z_1) \frac{k_1 n_1}{t_1} \left( -\frac{\ln(1 - z_1)}{k_1} \right) \left( \frac{n_1}{m_1} \right) \left( \frac{\theta_1 - \theta}{m_1} \right) H[\theta - \theta_1] H[\theta_1 - \theta] . \quad (25) \]

To limit the generation of ferrite to the appropriate temperature frame, the Heaviside functions \( H \) include \( H[s] = 1 \) for \( s > 0 \) and \( H[s] = 0 \). Otherwise, \( \theta_1 \) is the ferrite start temperature and \( \theta_3 \) is the pearlite start temperature. The effect of the austenitization temperature is included through the use of the material parameter \( \theta^* \) and the austenitization temperature \( \dot{\theta} \) divided by the material constant \( m_1 \).

#### 3.4.2. Formation of Austenite

Austenite is assumed to form only from the initial ferritic state during heating prior to hot forming. Austenite is expected to be the starting point for all other phases without retransformation. Thus, the sum of the other formed phases cannot exceed the amount of austenite created during heating. A simple approach for the evolution of austenite is used based on LeBlond and Deveaux\[22\] and Wolff et al.

\[ z_2 = \mu_{12} (z_1 - z_2) H[\theta - \theta_2] H[\theta_1 - \theta] - z_1 - z_4 - z_5 \quad (26) \]

where \( \theta_1 \) is the austenite starting temperature and \( \mu_{12} > 0 \) is a constant. Because the development of phase fractions takes place within certain temperature ranges, the Heavyside function \( H \) is used as a switch.

#### 3.4.3. Formation of Pearlite

As with the phase fraction of ferrite in Equation (24), the Johnson–Mehl–Avrami–Kolmogorov approach is used for the evolution of pearlite, based on Schaper et al.\[10\] and Avrami\[21\]. The function for the pearlite phase fraction is

\[ z_3(t) = 1 - \exp\left(-k_1 \left( \frac{t}{t_3} \right)^n_3 \right) , \quad (27) \]

where \( k_3 \) is a material parameter, \( n_3 \) is the Avrami exponent, \( t_3 \) is a constant parameter, and \( t \) is the duration of the transformation. Derived from Equation (27), the evolution equation for pearlite is

\[ \dot{z}_3 = (1 - z_3) \frac{k_3 n_3}{t_3} \left( -\frac{\ln(1 - z_3)}{k_3} \right) \left( \frac{n_3}{m_4} \right) \left( \frac{\theta_3 - \theta}{m_4} \right) H[\theta - \theta_3] H[\theta_3 - \theta] . \quad (28) \]

As with ferrite, the temperature frame for transformation is controlled by Heavyside functions. The influence of the austenitizing temperature is determined by the difference between a newly introduced material parameter \( \theta^* \) and the austenitization \( \dot{\theta} \) temperature divided by the material constant \( m_4 \).

#### 3.4.4. Formation of Bainite

Bainite forms from austenite only during moderate cooling. In contrast to martensitic transformations, bainitic transformation develops by diffusion processes. A distinction is made between upper bainite for high temperatures with carbide precipitation from austenite and lower bainite for lower temperatures with carbide precipitation in ferrite and austenite (see, e.g., Bhadresia\[23\]).

The approach adopted was originally published in Garrett et al.\[11\] and extended by Haupt\[24\] and Mahnken et al.\[25\]. A more detailed description can be found there.

The formation of bainite is related to nucleation and nucleus growth. The homogenized radius of a nucleus is introduced as the internal variable \( r \). According to Garrett et al.\[13\] the formation...
of bainite requires an incubation period. Accordingly, bainite development is tied to the barrier term \( r^* \) and bainite begins to develop when the radius of bainite particles \( r \) is larger than the required particle radius \( r^* \).

The evolution equation for \( r \) is derived in Haupt\(^7\) and distinguishes between upper and lower bainite. For the complete derivation, see Haupt.\(^9\) The equations for upper and lower bainite formation are combined to give the following equations for the radius of the bainite grains

\[
r = \alpha_2 \exp \left[ -\frac{\theta - \theta^*[e_\theta]}{B_3} \right] \exp[-\beta_2 e_\gamma] H[\theta - \theta^*] + \alpha_3 \exp \left[ -\frac{\theta^*[e_\theta] - \theta}{B_4} \right] \exp[-\beta_3 e_\gamma] H[\theta^* - \theta - \beta_3]
\]

where \( \alpha_2 = \alpha_3, \beta_2 = \beta_3, B_3, \) and \( B_1 \) are material parameters.

Following Garrett et al.,\(^1\) Mahnken et al.,\(^24\) and Haupt,\(^7\) the evolution of the bainite phase fraction considering the incubation time is calculated as follows

\[
\dot{z}_4 = A_5 \exp \left[ \frac{\theta^*[e_\theta] - \theta}{B_4} \right] \exp \left[ \frac{-G}{R \theta} \right] \left( \frac{r - r^*}{r} \right)^n
\]

\[
z_4 = \left( \frac{\theta^* - \theta}{m_4} \right) H[\theta^* - \theta - \beta_3]
\]

where \( \theta^* \) is the austenitization temperature, and \( m_4 \) is the material parameter, \( r \) is the critical value of \( r^* \). The \( \theta \) is the reference temperature, and \( G^* \) is the activation energy, which is calculated from

\[
G^* = \frac{A_1 \theta_0 \Delta \theta^{0.5}}{(\Delta \theta Q^*)^2 + A_4 \theta_0 e_{\sigma}}
\]

where \( A_1, A_4, \) and \( Q^* \) are constant material parameters.

### 3.4.5. Formation of Martensite

Martensite forms from austenite as a result of high cooling rates. The most common approach to modeling martensite is the Koistinen–Marburger approach, as shown by Wolff et al.,\(^19\) The evolution equation for \( z_5 \) is

\[
\dot{z}_5 = \left( \frac{\theta}{k_0} \right) (z_5 - z_1 - z_3 - z_4 - z_5) H[\theta_5 - \theta]
\]

where \( k_0 > 0 \) is the Koistinen–Marburger parameter and \( \theta_5 \) is the martensite start temperature. Although the martensite starting temperature depends on the stress, this relationship was disregarded because Mahnken et al.,\(^23\) showed that the dependence is almost nonexistence small.

### 3.5. Numerical Implementation

The constitutive relations for viscoplasticaity and phase transformations, together with the linear momentum in Equation (3), form an initial boundary value problem. This is solved using the finite element method for discretization in space combined with a suitable integration method for discretization in time.

The solving of boundary value problems by means of the finite element method is well documented in the literature and thus is not discussed in depth here (see, e.g., previous studies,\(^26,27\)).

Regarding the time integration of the constitutive equations, we refer to our own earlier work, as well as Mahnken and Schneider\(^8\) and Mahnken et al.,\(^20\) Here, the spectral decomposition of the right Cauchy–Green tensor, the local iteration for the implicit time integration of the Von Mises plasticity, and the spatial algorithmic tangent operator for the iterative solution of the equilibrium condition are described in detail.

Moreover, the internal variables such as the phase proportions \( z_i \) for each phase are integrated using an explicit Euler method. To reduce the corresponding time integration error, adaptive time stepping is performed (see, e.g., Mahnken and Stein\(^29\)). In this way, the resulting time integration scheme is semi-implicit.

### 4. Experimental Section

#### 4.1. Material, Specimen Geometry, and Preparation

The material investigated was an uncoated 22MnB5 sheet of 2 thickness with a chemical composition as shown in Table 1. The specimens for the uniaxial hot tensile tests were cut along the rolling direction of the sheet by wire-cut electrical discharge machining (EDM).

All test specimens had a dog-bone-shaped geometry as shown in Figure 1a and were sandblasted and degreased before being painted with a high-temperature black varnish. To perform a strain measurement via digital image correlation (DIC) technology during thermomechanical treatment, a white speckle pattern was added over the black paint using a high-temperature varnish. After thermomechanical treatment, small tensile specimens were cut by wire-cut EDM from the larger specimen as shown in Figure 1b. In addition, samples were taken of the tapered area for metallographic analysis and hardness tests (hatched area in Figure 1b).

#### 4.2. Thermomechanical Treatment with DIC and Thermal Imaging

First, the steel was austenitized at 850 or 900 °C, followed by an optional hot deformation at the respective austenization temperatures. The hot tensile tests were conducted after a soaking time of 300 s at a tensile speed of 1 mm s\(^{-1}\) until a total elongation of 10% or 20% was reached. Furthermore, undeformed samples were tested with the same temperature ramp. The specimens were then slowly cooled to room temperature in ambient air or quenched with compressed air. A Nikon digital camera was used to take pictures for the DIC evaluation. Furthermore, Infratec’s thermal imaging camera VarioCAM HD head 980 was
used to record the temperature change during the thermomechanical treatment of the samples. Images for the DIC analysis were taken with both cameras during soaking, forming, and cooling of the samples by automatic triggering at 1 Hz to measure the temperature and strain development. Pictures were taken until 250 were reached due to the measuring range of the thermal imaging camera. The GOM Correlate software was used to determine the local strain and temperature development during cooling of the specimens after an integration of the pictures of the thermal imaging and digital camera.

The experimental setup for the thermomechanical treatment of the flat steel specimens is shown in Figure 2. A homogenous temperature distribution with a maximum variation of $\pm 2.5^\circ$C on a length of 25 mm was reached in the middle of the specimen. A medium frequency generator from Trumpf Huttinger was used to heat the samples with a maximum power of 10 kW, a frequency of 250 kHz, and a heating rate of 20 K s$^{-1}$. A coupling distance of $\approx 2$ mm was set between the specimen and the frontal inductor, which was equipped with a circumferential U-shaped magnetic flux concentrator. The sample temperature was measured in a range 250–1000 $^\circ$C, which was predefined by the calibration of the camera. Due to the temperature-dependent change of the emission coefficient, a script was created by comparison measurements with a ratio pyrometer (step size 100 $^\circ$C). To eliminate any influence of surface radiation during the imaging sequences, an optical blue bandpass alter was applied to the digital camera. The experimental design is shown in Table 2.

For each condition in Table 2, three tests were conducted to obtain a sufficient statistical basis for the results.

4.3. Characterization of Phase Transformations and Mechanical Properties and Analysis of Material Microstructure

With the recorded data of strain evolution and temperature change throughout the thermomechanical treatment of the
specimens, the areas of interest were determined according to the parameters of Table 2. The data on temperature and strain change were then transferred to Excel for a phase transformation analysis. In Reitz et al.,[9] the method for the identification of phase transformations, used for all experiments conducted, was provided. To identify the starting temperature \( (A_C_{1}) \) and finishing temperature \( (A_C_{3}) \) of the ferrite-to-austenite transformation, three strain–temperature curves were analyzed and compared. The cooling rate was calculated similarly to the method used by Kumar et al.,[30] where 400 is divided by the time it takes to cool from 800 to 400 °C.

5. Experimental Results and Discussion

5.1. Phase Transformation Analysis and Microstructure

The results obtained for the thermomechanically machined samples at an austenitization temperature of 850 °C, which is 40 °C lower than the determined \( A_C_{3} \) temperature of 890 and 20 °C higher that the \( A_C_{1} \) temperature of 830 °C, are shown in Figure 3. Figure 3a,c displays the results for the start and end temperatures of the individual phase transformations and the resulting microstructure and phase fractions for cooling in ambient air, and Figure 3b,d shows the results for cooling with compressed air.

Table 2. Experimental plan for the thermomechanical treatment of the flat specimens.

| Condition | Austenitization temp. [°C] | Hot deformation [%] | Cooling          |
|-----------|-----------------------------|---------------------|------------------|
| S1        | 850                         | 0                   | Ambient air      |
| S2        | 850                         | 10                  | Compressed air   |
| S3        | 850                         | 20                  | Ambient air      |
| S4        | 850                         | 0                   | Compressed air   |
| S5        | 900                         | 10                  | Ambient air      |
| S6        | 900                         | 20                  | Compressed air   |
| S7        | 900                         | 0                   | Ambient air      |
| S8        | 10                          | 10                  | Compressed air   |
| S9        | 20                          | 20                  | Compressed air   |
| S10       | 900                         | 0                   | Compressed air   |
| S11       | 10                          | 10                  | Compressed air   |
| S12       | 20                          | 20                  | Compressed air   |

Figure 3. Transformation temperatures, microstructure, and phase fractions after austenitization at a temperature of 850 °C with subsequent cooling: a, c) cooling on ambient air with \( 8.5 \text{ K s}^{-1} \); b, d) cooling by compressed air with \( 29.5 \text{ K s}^{-1} \).
compressed air. Figure 3a shows that both the ferrite start temperature \( F_s \) and the ferrite end temperature \( F_f \) increase with the hot deformation strain. The cooling rate of all tested samples cooled in ambient air was 8.5 K s\(^{-1}\). With the end of the ferritic transformation, the pearlitic transformation began. The pearlite start temperature \( P_s \) increased with the hot deformation strain, while the pearlite end temperature \( P_f \) decreased. In both cases, the onset of transformations was shifted to faster cooling rates with increasing strain. An extended ferritic and pearlitic range could be observed, as also mentioned in previous studies.[1,13]

Figure 3b shows the results of the thermomechanically treated and air-quenched samples with a cooling rate of 29.5 K s\(^{-1}\). Bainitic transformation and martensitic transformation were observed in the undeformed sample S4. According to Abbasi et al.,[13] only martensitic transformation should occur at this high cooling rate and without deformation. This implies that austenitization below the \( \Delta C_3 \) temperature impacted the transformation kinetics of the investigated steel. Furthermore, ferritic transformation and pearlitic transformation were observed after performing a hot deformation of 10% and 20%, respectively. With increasing deformation strain, a higher \( F_s \) and a slightly higher \( P_s \) were determined. Moreover, the bainite starting temperature \( B_s \) was found to be highest after a hot deformation strain of 10%, and to decrease slightly with progressive strain up to 20%, as noted in Reitz et al.[9] for an austenitization temperature of 900 °C. Whereas the ferritic, pearlitic, and bainitic areas increased, the martensitic area decreased as a result of hot deformation. The deformation strain had no effect on the bainite end \( (B_f) \) or the martensite start temperature \( (M_s) \). Hot deformation shifts the bainitic transformation to faster cooling rates and higher temperatures, as shown in Schaper et al.[10] and Nikravesh et al.[11] Furthermore a reduced martensitic range was observed due to the increased final martensite temperature \( (M_f) \).

Figure 3c shows that after increasing the deformation strain from 10% to 20%, the ferrite volume fraction was about 10% larger. Nikravesh et al. found that hot deformation reduces the pearlite volume fraction at all cooling rates up to 20 K s\(^{-1}\), whereas the ferrite volume fraction is increased at higher cooling rates than 1 K s\(^{-1}\).[12] A larger ferritic region could be the reason why a higher ferrite volume fraction was observed at 20% elongation and no significant change in microstructure and phase fractions was found at 10% elongation compared to the undeformed condition. Comparing the micrographs and SEM images of Figure 4, a reduced pearlite volume fraction can be seen in Figure 4c in contrast to Figure 4a,b. Predominantly small pearlite grains occur in Figure 4f, and the micrographs of Figure 4d,e are similar.

After compressed air cooling, the martensite content decreased from 91% to 3% with increasing strain, whereas the bainite content rose from 4% to 72% (see Figure 3d). Since Figure 3b shows no ferritic transformation, the determined ferrite volume fraction of 5% for the undeformed sample S1 shown in Figure 3d (0%) was likely the result of untransformed residual ferrite due to austenitization in the intercritical temperature range. Furthermore, ferrite and pearlite formed during hot deformation and their content increased with increasing elongation. One reason for the observed change in microstructure and phase fractions shown in Figure 3d is the generation of dislocations during hot deformation within the austenitic region. Naderi et al.[8] found that these dislocations accelerate thermally activated phase transformations, which leads to a shift of ferrite and bainite to faster cooling rates. Here, the bainitic transformation is more strongly influenced than the ferritic transformation.

The microstructures of samples S4–S6 are shown in Figure 5. With increasing hot deformation, a higher number of ferritic grains is visible in Figure 5a–c. Bainitic needles can be found in Figure 5a. Although ferritic grains occur in Figure 5a–c, it was not possible to clearly distinguish between martensite,
bainite, and pearlite by optical microscopy. SEM images of the undeformed sample S4 showed a predominantly martensitic microstructure with a few ferritic grains, with many undissolved carbides visible within the ferrite (see Figure 5d). Furthermore, bainitic needles with small carbides inside could be identified. The SEM images of the thermomechanically processed samples S5 and S6, which were cooled with compressed air, showed a mixed structure of ferrite, pearlite, bainite, and martensite. The respective characteristic areas are shown in Figure 5e,f. Especially small pearlite grains of 600 nm were found within the ferrite and often at the grain boundaries (see Figure 6). A higher magnification of about 5000× was necessary to distinguish between the very small pearlite grains and carbides.

The results of the samples austenitized at 900 °C are shown in Figure 7. As in Figure 3, 7a,c shows the results for the start and end temperatures of each phase transformation as well as the resulting microstructure and the resulting phase fractions for cooling in ambient air, and Figure 7b,d shows the same for cooling with compressed air. When the austenitization temperature was increased from 850 to 900 °C, bainitic transformation was observed in addition to ferritic and pearlitic transformation at a cooling rate of 8.5 K s⁻¹ (see Figure 7a). For all three transformations, the slope increased after hot deformation, although no significant effect was observed for the Bs. As also indicated by Reitz et al., hot deformation of 10% resulted in a shift of the bainitic region to faster cooling rates, but further increasing the hot deformation to 20% led to a slight shift of the Bs to slower cooling rates. The growth of the Fs and Ps was less pronounced compared to Figure 3a. With increased hot deformation, larger ferritic and bainitic areas and a smaller pearlitic area were observed. This means that the assumption of a continuous shift of thermally activated phase transformations to faster cooling rates with increasing force level, as stated by Naderi et al., is not valid at a low strain level of 20%. A delayed bainitic transformation at a hot deformation of 20% was also found by Schaper et al. Figure 7b, in contrast to Figure 3b, shows martensitic transformation only for the undeformed sample S7, which was processed at a cooling rate of 29.5 K s⁻¹. Hot deformation of 10% and 20% additionally caused bainitic transformation. A slightly lower Ms is evident for the hot-formed samples S11 and S12, as previously determined by Naderi et al. The Ms had no particular tendency.

Naderi et al. explained that the increasing strain during hot deformation in the austenite phase becomes so great that it makes the movement of the glissile interfaces impossible and blocks the martensitic transformation. As a higher driving force is required, the martensitic transformation takes place at lower temperatures. Furthermore, the reduced Ms leads to a lower final amount of martensite, as found by Naderi et al.

In contrast to Figure 3d, 7d does not show a strong decrease of the martensite fraction. Another reason for this effect, apart from the aforementioned acceleration of thermally activated phase...
transformations by dislocations, could be the inhomogeneous carbon distribution within the austenite due to undissolved carbides, as Reitz et al.\cite{9} suggest. The microstructure of samples S7–S9 cooled in ambient air was not affected by hot deformation. A bainite content of \(\approx 52\%\), a ferrite content of \(\approx 35\%\), and a pearlite content of \(\approx 12\%\) were determined. Figure 8a–c shows micrographs for samples S7–S9, which were cooled at 900°C in ambient air after austenitization. All three images show a mixed microstructure. SEM analysis revealed a mixture of ferrite, bainite, and small pearlite islands (see Figure 8d–f), as shown in Figure 6.

The micrographs for specimens S10–S12, which were cooled with compressed air at a cooling rate of 29.5 K s\(^{-1}\), show a martensitic microstructure (see Figure 9a–c). The white grains in
Figure 9 represent self-tempered martensite, which is surrounded by martensite lancets (see Figure 9d).

SEM analysis for the undeformed sample S10 revealed a high content of self-tempered martensite, as shown in Figure 10. Figure 9b,c shows bainitic lancets in addition to martensitic lancets, but SEM images were necessary to distinguish between self-tempered martensite and bainite. The bainitic lancets are visible on the SEM images of the thermomechanically treated specimens S11 and S12 (see Figure 9e,f), which also had a high content of self-tempered martensite. In addition, hot deformation of 10% and 20% resulted in a finer microstructure with a smaller martensite cluster due to dynamic recrystallization (see Figure 9a–f). As noted by Nishibata and Kojima,[13] the fine cementite precipitates of self-tempered martensite have an acicular shape and are oriented in four directions. An example of the fine cementite precipitates detected is given in Figure 10.

5.2. Mechanical Properties

The results of the mechanical tests for all specimens austenitized at 850 and 900 °C are shown in Figure 11. For specimens S1–S3, which were cooled in ambient air (see Figure 11a, solid line), a higher hot deformation strain resulted in a small increase in UTS and a small decrease in EL, whereas the YS did not change significantly. In addition, the hardness did not fluctuate. The hardness of the undeformed and hot-worked specimens reached an average value of 190 HV1 (see Figure 11c), which is 10 HV higher than the hardness of the initial condition, which also consisted of a ferritic–pearlitic microstructure. For the air-cooled samples, shown by dashed lines in Figure 11a, decreasing UTS and YS were observed with increasing deformation strain. These results are consistent with the results of the microstructural analysis, which found a sharp decrease in martensite content responsible for the reduced strength properties. The EL for the undeformed sample S4 varied more compared to the hot deformed samples S5 and S6. The expected increase in EL due to the decreasing strength could be measured for a hot deformation of 20%, where almost no martensite was formed. That the hardness is reduced with increasing deformation strain confirms the results of the tensile tests and the microstructural analysis of the air-cooled specimens S4–S6, as shown in Figure 11c.

As shown in Figure 11b, samples S7–S9, which were cooled in ambient air, have an ≈150–200 MPa higher UTS and YS but lower EL compared to samples S1–S3, which were also cooled in ambient air but had a 50 °C lower austenitization temperature, as indicated with solid lines in Figure 11b. As the formation of bainite content was the reason for the higher strength properties at an austenitization temperature of 900 °C, the strength curve showed a slight downward trend at the lower temperature. This was also true for the hardness values, which were 15 HV
higher for the undeformed specimen S7 than for the hot-deformed specimens S8 and S9 (see Figure 11d).

The air-cooled samples S10–S12 had decreasing UTS and EL with increasing YS. A hot deformation of 20% resulted in a 50 MPa lower UTS and a 20 HV lower hardness (see Figure 11d) compared to the undeformed condition due to the reduced martensite content. At a hot deformation strain of 20%, the YS fluctuated more, but the tendency was for the YS to increase. The EL decreased slightly from 27% to 25% at a hot deformation of 10% and to about 21% at a hot deformation of 20%, with a higher variation of ±3% determined. One reason for the higher YS could be a finer microstructure due to dynamic recrystallization, which resulted in a smaller martensite package size, as shown by previous studies[32,33] and illustrated in Figure 9d-f. Xu et al.[33] also observed that the same martensite bundle thickness leads to unequal YS for differently loaded material. Furthermore, a lower $M_s$ resulted in a lower content of self-tempered martensite. The undeformed specimen S10, which consisted entirely of martensite, was found to have a higher elongation at fracture than the undeformed specimen S4, which was austenitized at a temperature that was 50 lower, due to the self-tempering of martensite.

6. Simulation Examples

In this section, we present two simulation examples of phase transformation that correspond to the constitutive modeling in Section 3. The first example applies the constitutive equations to a uniaxial loading case, to establish a basis for comparison between the numerical results and the experimental data provided in Section 5. The second example demonstrates the capability of the developed model by simulating a hot tensile test under inhomogeneous temperature loading. Particularly relevant is the distribution of phase fractions as a function of different heating strategies.

6.1. Comparison to Experiments

The first numerical example aims to verify the constitutive equations presented in Section 2 and 3. The objective is to show the performance of our model compared to the experimental results gathered in Section 5.

To this end, the material parameters were obtained by the process of parameter identification. The identified parameters are displayed in Table 3 and 4. In contrast to the usual optimization approach of minimizing the distance between experimental and
Table 3. Material parameters for phase transformation in steel 22MnB5 for cooling in ambient temperature.

| Function | Parameter | Value  | Unit  | Function | Parameter | Value  | Unit  |
|----------|-----------|--------|-------|----------|-----------|--------|-------|
| 2       | \( \theta_1 \) | 1.07E+03 | K     | 4       | \( \beta_1 \) | 1.90E-02 |       |
| 2       | \( k_1 \) | 6.93E-01 | –     | 4       | \( \beta_2 \) | 1.00E-01 | –     |
| 2       | \( n_1 \) | 5.50E+00 | –     | 4       | \( B_1 \) | 9.70E+00 | –     |
| 2       | \( t_1 \) | 1.04E+01 | –     | 4       | \( \gamma_1 \) | 5.88E+06 | –     |
| 2       | \( \mu_{12} \) | 1.08E-03 | –     | 4       | \( \gamma_2 \) | 9.35E-01 | –     |
| 2       | \( \mu_{12} \) | 6.05E-02 | –     | 4       | \( n_2 \) | 7.20E+00 | –     |
| 2       | \( \theta_3 \) | 9.74E+02 | K     | 4       | \( \gamma_3 \) | 6.40E+00 | –     |
| 2       | \( k_3 \) | 5.53E-01 | –     | 4       | \( R \) | 8.31E+00 | J mol K\(^{-1} \) |
| 2       | \( n_3 \) | 1.05E+01 | –     | 4       | \( Q^* \) | 3.08E+05 | –     |
| 2       | \( t_3 \) | 6.30E+00 | –     | 4       | \( \delta_3 \) | 1.20E+03 | –     |
| 2       | \( \theta_3 \) | 1.21E+03 | –     | 4       | \( m_4 \) | 3.10E+01 | –     |
| 2       | \( m_3 \) | 3.00E+01 | –     | 4       | \( \theta_3 \) | 6.78E+02 | K     |
| 2       | \( \theta_4 \) | 9.28E+02 | K     | 4       | \( k_5 \) | 6.05E-02 | –     |
| 2       | \( A_1 \) | 4.02E-04 | –     | –       | –       | –     | –     |
| 2       | \( A_2 \) | 2.21E-06 | –     | –       | –       | –     | –     |
| 2       | \( A_3 \) | 1.00E-04 | –     | –       | –       | –     | –     |
| 2       | \( A_4 \) | 3.30E-07 | –     | –       | –       | –     | –     |
| 2       | \( A_5 \) | 9.89E+02 | –     | –       | –       | –     | –     |
| 2       | \( a_6 \) | 9.00E-01 | –     | –       | –       | –     | –     |

The numerical results by a least-squares algorithm (see, e.g., Mahnken and Westermann\(^{[34]}\)), the parameters were obtained by a manual curve-fitting approach. For the fitting approach, the phase fractions after cooling and transformation temperatures shown in Figure 3 and 7 for both cooling strategies were used respectively. Because the cooling rate is not incorporated in the constitutive equations directly, two sets of material parameters are needed. Both sets of material parameters are used in the simulations. The loading conditions were based on the procedure of the experiments given in Table 2. Furthermore, the verified cases corresponded to specimens S3 and S9 as well as S6 and S12 with a total elongation at hot deformation of 20%. A homogeneous strain and stress distribution was assumed. The loading conditions are shown in Figure 12 for the austenitization temperatures \( T_1 = 850 \) and \( T_2 = 900 \).

The phase fractions \( z_i \) for both cooling strategies are shown in Figure 13. The numerical results for samples S3 and S9 are shown in Figure 13a,b, respectively. The solid lines represent the numerical results and the markers represent the phase fractions obtained from experiments, shown in Figure 3 and 7. After cooling in ambient air, the numerical analysis indicated a ferrite content of 76% and a pearlite content of 24%, while the experimental result showed 75% ferrite and 25% pearlite. Similarly, simulation and experimental results for sample S9, which was cooled in ambient air after austenitization at 900°C, were consistent with 35% ferrite, 12% pearlite, and 53% bainite. The results for samples S6 and S12 are shown in Figure 13c,d. At an austenitizing temperature of 850°C and after compressed-air cooling, the phase fractions were 15% ferrite, 10% pearlite, 72% bainite, and 3% martensite. Furthermore, at an austenitizing temperature of 900°C after compressed-air cooling, 3% bainite and 97% martensite were detected. The simulation results and the experimental results shown in Section 5 match. This becomes apparent in Figure 13. Here, the numerical results are displayed as solid lines and the experimental results are displayed by markers. The markers represent the phase fractions after cooling as well as at transformation start derived from the transformation start temperatures. The values are taken from Figure 3 and 7; thus the phase breaks in Figure 3 and 7 could be validated by the experiments quite well.

6.2. Finite-Element Simulation of a Hot Tensile Test with Tailored Thermomechanical Treatment

In the second example, a finite element simulation of a 2D tensile specimen was performed. The geometry and temperature distribution is shown in Figure 14. Point \( P_1 \) represents a temperature of 850°C and point \( P_2 \) a temperature of 900°C. The geometry was derived from Figure 1 to verify the simulation based on the hot tensile tests performed.

The phase fractions \( z_i \) for both cooling strategies after cooling were shown in Figure 15 and 16. As the austenitizing temperature decreased, the ferrite content increased, as shown in Figure 15a, until point \( P_1 \) reached a ferrite content of about 85%. A higher ferrite content with a higher percentage of non-transformed ferrite due to a decreasing austenitizing temperature is beneficial. Figure 15b shows that the final microstructure after thermomechanical treatment contained...
no retained austenite. The pearlite phase fraction shown in Figure 15c had a maximum of about 50% between point $P_1$ and $P_2$ and was reduced to 0% with a further increase in austenitizing temperature. The pearlite content within the sample area

Figure 12. Comparison to experiments—temperature and strain over time: a) sample S3 and S9 with austenitization at 850 and 900 °C along with a cooling of 8.5 K s$^{-1}$; (b) sample S6 and S12 annealing at 850 and 900 °C along with a cooling of 29.5 K s$^{-1}$.

Figure 13. Comparison to experiments—phase fractions over time during cooling, simulation results (solid lines), experimental data (markers): a) austenitization at 850 °C and cooling with 8.5 K s$^{-1}$, b) austenitization at 900 °C and cooling with 8.5 K s$^{-1}$, c) austenitization at 850 °C and cooling with 29.5 K s$^{-1}$, and d) austenitization at 900 °C and cooling with 29.5 K s$^{-1}$. 
with the lowest temperature was 15%. A phase composition close to the initial state was formed and the ferritic-pearlitic microstructure was consistent between simulation and experimental results. The bainitic phase began to develop only after intercritical austenitization at a temperature of about 850 °C, which is consistent with the experimental results shown in Figure 15d. Reitz et al. showed that a fully bainitic microstructure forms after austenitization at 950 °C, hot working of 20%,
and subsequent cooling in ambient air at 11 K s\(^{-1}\). The trend of an increasing bainitic area should be true, but further experimental tests should be performed to prove the phase compositions for other austenitizing temperatures. No martensite formed when cooled in ambient air, consistent with the experimental tests in Figure 15e. The final phase compositions of \(P_1\) and \(P_2\) after the tailored thermomechanical treatment are shown in Figure 17. At 850 °C (Figure 17a), a phase composition of 80% ferrite and 20% pearlite occurred, which is close to the composition in Figure 13a. The total ferritic phase fraction contained 5% nontransformed ferrite due to austenitization in the intercritical temperature range. A phase composition of 37% ferrite, 13% pearlite, and 50% bainite was the simulation result for an austenitizing temperature of 900 °C (Figure 17b), which is consistent with the experimental results in Figure 7c and the simulation results in Figure 13b.

Figure 16 shows the simulation results for the tailored thermomechanical treatment of a sample cooled by compressed air, where ferritic and pearlitic fractions are visible at an austenitizing temperature of lower than 850 °C, corresponding to the nontransformed fractions. A slightly stronger deformation takes place around 900 °C due to the temperature gradient. From \(P_2\), an increasing bainite and decreasing martensite content was calculated. In the area where almost no deformation occurs and the austenitizing temperature was above the \(A_{1}\) temperature, a fully martensitic microstructure developed. At a cooling rate of 29.5 K s\(^{-1}\), no retained austenite remained. The observed phase transformations during thermomechanical treatment of the flat specimen in this study were in agreement with previous publications.[8–10,35]

The final microstructure at point \(P_1\) consisted of 15% ferrite, 10% pearlite, 71% bainite, and 4% martensite, as shown in Figure 18a, and at \(P_2\) it consisted of 4% bainite and 96% martensite, as shown in Figure 18b. These results are consistent with those in Figure 7d, 3d, and 13c,d. In addition to the microstructural composition at points \(P_1\) and \(P_2\), the phase fractions between the two points were also of interest. The phase distribution at the midpoint between \(P_1\) and \(P_2\) when cooled in ambient air (see Figure 15) was 50% ferrite and 50% pearlite. Bainite developed only at an austenitizing temperature of 850 °C and martensite did not form at all.

The phase distribution between the two points when cooled with compressed air (see Figure 16) was composed of ≈50% bainite and 50% martensite. Beyond \(P_1\), both ferrite and
pearlite formed only at an austenitizing temperature below 850 °C. For both cooling strategies, the phase fractions increased linearly between the austenitization temperatures of 850 and 900 °C.

The distribution of the true strain $\varepsilon$ after complete cooling is shown in Figure 19. The true strain for cooling in ambient air and cooling with compressed air is shown in Figure 19a,b, respectively.
7. Conclusion

This study investigated the effects of different austenitization temperatures, hot deformation, and cooling conditions on phase transformation kinetics and the resulting phase composition. A multiphase model suitable for modeling multiphase continua was extended to capture the relevant five phases of 22MnB5 steel. The parameters of the model were identified in the simulation of the uniaxial loading case and applied to finite element simulations of tensile specimens hot deformed with a tailored temperature treatment. A noncontact characterization method was used to determine the phase transformations. The results can be summarized as follows. 1) The extended multiphase model is able to completely capture the evolution of ferrite, austenite, pearlite, bainite, and martensite for different austenitization temperatures and cooling strategies. 2) It was shown that the simulation model is suitable to predict the phase composition during a tailored thermomechanical treatment. To the knowledge of the authors, this has not been demonstrated before. Different temperature ranges were taken into account with multiple sets of material parameters. 3) Austenitization of the flat specimens at 850 °C, i.e., in the intercritical range, did not result in bainite formation, which was the reason for the lower strength and hardness properties. A strong influence of the cooling strategies on the bainitic transformation was found. At a high cooling rate of about 29.5 K s⁻¹, the formation of diffusion-induced phase transformations such as ferrite, pearlite, and bainite was accelerated more by increasing hot deformation than at the austenitization temperature of 900 °C. An inhomogeneous carbon distribution in combination with the aforementioned prevention of martensitic transformation could be the reason for this effect. 4) A hot deformation strain of 10% or 20% had the greatest effect on the intercritically austenitized specimens cooled with compressed air. Diffusion-activated phase transformations occurred earlier at increasing strains and at higher temperatures than in the undeformed specimens. The bainitic transformation showed the referenced differences with respect to the cooling rate at a hot deformation strain of 20%. 5) At an austenitizing temperature of 850 °C, a cooling rate above 29.5 K s⁻¹ is required to convert all austenite to martensite. A hot deformation reinforces this effect, as almost no martensite is formed beyond an elongation of 20%, and therefore much higher cooling rates are required to obtain a microstructure with a high martensite content. 6) The microstructure simulation of the flat steel sample subjected to tailored temperature treatment was consistent with the experimental results. 7) Thermomechanical processing of the samples cooled with compressed air showed a strong influence of hot deformation on the mechanical properties for the not fully austenitized material. The result was an ≈36% lower strength and hardness after hot deformation with a maximum elongation of 20%. Although the martensite content decreased significantly after hot deformation of 10%, an increase in ductility was only measurable after hot deformation of 20%, at which almost no more martensite could be detected. Full austenitization followed by compressed-air cooling lead to a slight decrease in UTS and hardness with an improvement in ductility due to the increasing bainite content. The observed increase in YS could be the result of dynamic recrystallization during hot deformation, as indicated by the discovered finer martensite clusters. The mechanical properties of the samples cooled in ambient air did not change significantly after thermomechanical treatment. The mechanical properties are strongly influenced by the microstructure and can be controlled by the austenitizing temperature, more precisely by the amount of austenite. 8) This investigation proved to be appropriate for the determination of phase transformations. The contents of the 12 samples could be used to parameterize the simulation tool for predicting the resulting mixed microstructure of a homogeneously and an inhomogeneously treated flat steel sample using the contactless characterization method. 9) Concerning future investigations, the proposed model is capable of predicting a wide variety of microstructure compositions. Meaningful research and improvements can be made on the following subjects: i) The complex microstructure of steels includes more micromechanical mechanisms apart from the phase transformation. Also, mechanisms such as recrystallization, recovery, and grain growth represent a major influence on the macroscopic material properties. During future investigations, especially recrystallization and the effect of the grain size on the flow stress have to be considered. To achieve this, the current material model may be coupled to the simulation of grain size evolution. ii) As the thermodynamic framework is formulated in a general sense, the simulation model can be applied to a variety of steel compositions. With the use of hot forming tensile tests, new parameters can be identified and the evolution of phase fractions in various steels can be predicted. iii) Proceeding from the elementary material investigations by numerical and experimental means, the obtained knowledge can be applied to more sophisticated hot forming processes in the future. On this occasion, the investigation of hot press hardening and the targeted adjustment of macroscopic material properties is of interest. iv) With the contactless characterization method, an investigation of graded thermomechanically treated flat steel specimen could be studied. These techniques enable us to investigate the influence of different austenitization temperatures and/or strain gradients on the microstructure and hardness with only one specimen. Considerably more data can be obtained from one sample.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

Keywords
digital image correlation, graded microstructure, low-carbon steel, phase transformations, thermomechanical treatment
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