Modeling of variant-interaction during bainitic phase transformation

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Abstract. In our research, we develop a thermodynamically consistent multi-scale model for phase transformations from austenite into \( n \) possible bainite variants. Each material point of the macroscopic configuration represents a polycrystal which describes the mesoscopic configuration. The microscopic configuration consists of an agglomeration of variants which is attached to each single crystal of the mesoscopic configuration. In addition, the model allows simulation of the macroscopic effects of volume change due to phase transformation as well as transformation-induced plasticity (TRIP). In this paper we present the results of recent work in the context of this model, which is concerned with the extension of the model for an effect of variant-interaction between the different crystallographic variants of bainite. For this reason we make use of the theory of transformation hardening. Thereby we are able to include an effect of preferential variant formation. This leads to the simultaneous formation of a selection of variants while the evolution of crystallographic unfavorable variants is handicapped or even completely suppressed. This extension of the model aims for the fact that in general not every crystallographic variant of bainite forms within a single austenite grain.

1. Introduction
The bainite phase transformation is of specific industrial relevance, especially in manufacturing processes which include hot-forming and quenching of large components. During this treatment most parts of the workpiece are subjected to cooling rates which are appropriate to yield a substantial amount of bainite in the final product. This leads to a notable influence on the product properties.

For a good overview on the research concerning the issues relevant to this work, we explicitly refer to the introduction of [1] and all references therein, since the present work is an extension to this publication. As to the nature of bainitic transformation it says “The crystallographic structure of the bainitic product phase features many different allotropic variants similar to what is known for martensite. In fact, the same crystallographic framework as for martensite can also be used in the case of bainite. A viable material model describing the mechanics of bainitic transformation must capture both the diffusive nature of the process as well as the multi-variant product phase formation. In addition, as one of the macroscopic characteristic features of low alloyed steels, phase transformations under moderate deviatoric stresses far from the yield stress lead to a permanent macroscopic inelastic deformation commonly termed transformation induced plasticity (TRIP).”

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In this paper we are concerned with the effect of variant-interaction during bainite transformation on the micro-scale of the material. During this transformation, preferential variant formation and variant interaction can be observed. To include these effects in our material model, we resort to the theory of transformation hardening. Concerning these topics of variant-interaction, interaction matrices and transformation hardening, we exemplarily refer to [2-6] among others. As a consequence the volume-fractions of the already evolved bainite variants have an influence on the subsequent bainite transformation. This ansatz may lead to the partial suppression of several variants and further to the remaining of retained austenite at the end of the transformation. This is reasonable, because in general, the bainite transformation is not complete and the different variants do not always evolve in equal volume-fractions, due to several influencing factors, e.g. chemical composition of the considered steel or thermo-mechanical loading.

The general and thermodynamic framework presented in this paper has already been published in [1]. Main aspects of the modeling section have been transferred to this article in order to provide a sufficient basis and the main equations of the material model. We skip the derivation of a special form of the Clausius-Duhem inequality, the heat-conduction equation and prove of thermodynamic consistency. For closer details related to the aforementioned topics as well as to the modeling part in general, we refer to [1].

The structure of this paper is as follows: Section 2 presents the general constitutive framework, the main equations and the extension of the material model to the simulation of variant-interaction during the bainitic phase-transformation. In section 3, we give a brief numerical example in order to show the effect of the variant-interaction during the bainite-transformation in a crystal-grain. We conclude the paper with a brief summary and outlook in section 4.

2. Modeling and Multi-scale framework

2.1. Thermodynamic framework on the macro-scale

The constitutive equations in this work are formulated within a geometrically linear theory. To this end the displacement gradient $\mathbf{u} \otimes \nabla$ is introduced at each material point $P$ with position vector $\mathbf{x}$ of the macroscopic configuration $\mathcal{B}$ in figure 1. Here, within a cartesian frame with base vectors $\mathbf{e}_i, i = 1, 2, 3$ and coordinates $x_i, i = 1, 2, 3$, the nabla operator is defined as $\nabla := \partial / \partial x_i \mathbf{e}_i$. This defines the strain tensor of the geometrically linear theory

$$\epsilon := \text{sym} \{ \mathbf{u} \otimes \nabla \}.$$  \hspace{1cm} (1)

In our multi-scale model, illustrated in figure 1, the material is regarded as a coexisting mixture of its polycrystals as well as of its phases, here bainite and austenite. The macroscopic temperature $\theta$ in a body point is the average temperature inside the polycrystal. In this way we assume the same temperature in each single grain of a polycrystal on the mesoscale.

Figure 1. Multi-scale model: a) Macroscopic configuration $\mathcal{B}$, b) Mesoscopic configuration consisting of a polycrystal with volume fractions $\xi^i$ and c) Microscopic configuration of a single crystal grain with variants $\lambda^{ij}$; the temperature $\theta$ is regarded as a homogenized quantity.
The carbon diffusion at the mesoscopic and microscopic levels, i.e. inside of a single crystal and between grains of the polycrystal during the phase transformation (see e.g. [7]), is not taken into account by the model under consideration. The balance relations are (e.g. [8])

1. \( \dot{\varphi} u - \text{Div}[\sigma] = \varphi_0 f \),  \hspace{1cm} \text{(linear momentum)}
2. \( \varphi_0 \dot{\varepsilon} + \text{Div}[\varphi_0 q_0] = \sigma : \varepsilon + \varphi_0 r_0 \),  \hspace{1cm} \text{(energy)}
3. \( -\varphi_0 \dot{\theta} + \varphi_0 \theta \dot{\eta} + \sigma : \dot{\varepsilon} - \frac{1}{\varphi_0} q_0 \text{Grad} \theta \geq 0 \).  \hspace{1cm} \text{(entropy)}

In this notation we use: \( \varphi_0 \) - density, \( u \) - displacement vector, \( \varepsilon \) – strain tensor of equation (1), \( \theta \) - absolute temperature, \( \sigma \) - (symmetric) Cauchy stress tensor, \( f \) - mass density of external forces, \( \varepsilon \) - mass density of the internal energy, \( \eta \) - entropy, \( q_0 \) - heat-flux density vector, \( r_0 \) - mass density of heat supply. The dot above an argument denotes its time derivative. We also recall that the inequality (2.3) is known as the Clausius-Duhem inequality. These equations are completed by suitable boundary and initial conditions for the displacement vector \( u \) and for the temperature \( \theta \) (for details see [1]).

Using the Legendre-transform \( \Psi = e - \theta \eta \) between the internal energy \( e \) and the Helmholtz free energy \( \Psi \), the Clausius-Duhem inequality (2.3) becomes

\[ \theta \gamma = \frac{1}{\varphi_0} \varphi_0 - \Psi - \theta \eta - \frac{1}{\varphi_0} q_0 \text{Grad} \theta \geq 0. \]  \hspace{1cm} (4)

\( \theta \gamma \) is the (mass density of) internal dissipation, \( \gamma \) is the (mass density of) entropy-production rate. The stress-power \( \varphi \) is given as a dual-pairing of the Cauchy stress \( \sigma \) and the strain-rate \( \varepsilon \)

\[ \varphi = \sigma : \varepsilon. \]  \hspace{1cm} (5)

2.2. Meso-micro relations

According to figure 1.b), a mesoscopic configuration, consisting of a polycrystal, is attached to each material point of the macroscopic configuration. Following [9] the polycrystal consists of \( N \) crystals. The volume fraction of the crystal with orientation \( i \) is denoted by \( \xi_i \), and all polycrystals on the mesoscale satisfy the normalization condition \( \sum_{i=1}^{N} \xi_i = 1 \).

In the following we assume constant volume fractions for all crystals, which means \( \xi_i = 0 \). Each crystal on the microscale has \( n \) variants, and the index \( j \) ranges from 0 for the austenite to the number \( n \) of bainitic variants. The volume fractions of austenite \( \lambda_{i0} \) and bainitic variants \( \lambda_{ij}, j = 1, ..., n, i = 1, ..., N \) satisfy mass conservation, and each variant ranges between zero and one. In summary we have the constraints for all \( i \in \{1, ..., N\} \) and \( j \in \{1, ..., n\} \)

\[ 1. \sum_{j=0}^{n} \lambda_{ij} = 1, \quad 2. \lambda_{ij} \geq 0. \]  \hspace{1cm} (6)

The austenitization of a low alloyed steel is possible only above the equilibrium temperature \( A_{c1} \). Therefore, for a temperature below \( A_{c1} \) and above \( M_s \) (martensite start temperature) austenite can transform into ferrite, pearlite and bainite. A reverse transformation in that temperature regime is not to be expected. To focus on the prototypical situation, we only consider the transformation from austenite to bainite. The evolution of its variants is subjected to the following constraints:

\[ 1. \sum_{j=0}^{n} \dot{\lambda}_{ij} = 0 \quad 2. \text{Austenite:} \dot{\lambda}_{i0} \leq 0 \quad 2. \text{Bainite:} \dot{\lambda}_{ij} \geq 0. \]  \hspace{1cm} (7)

In addition, we assume the following additive decomposition of the total mesoscopic strain tensor in the \( j \)th variant of the \( i \)th crystal:

\[ \varepsilon_{ij} = \varepsilon_{el}^{ij} + \varepsilon_{th}^{ij} + \varepsilon_{pl}^{ij} + \eta_{tr}^{ij}, \]  \hspace{1cm} (8)

so that \( \varepsilon_{ij} \) consists of an elastic part \( \varepsilon_{el}^{ij} \), a thermal part \( \varepsilon_{th}^{ij} \), a plastic part \( \varepsilon_{pl}^{ij} \) and a rotated transformation part \( \eta_{tr}^{ij} \). \( \varepsilon_{th}^{ij} \) represents the thermal expansion and is given by \( \varepsilon_{th}^{ij} = (\theta - \theta_0) A_{ij}^{th} \), where \( \theta_0 \) is a reference temperature and \( A_{ij}^{th} \) are the thermal expansion tensors associated with the \( i \)th crystal and with the \( j \)th variant (bainite: \( j > 0 \), austenite: \( j = 0 \)). \( \varepsilon_{pl}^{ij} \) in equation (8) refers to the
inelastic strains arising from the viscoplastic material behavior. The associated evolution equations are given in section 2.6. The rotated transformation strain tensor \( \boldsymbol{\eta}_{tr}^{ij} \) in (8) is obtained from
\[
1. \quad \eta_{tr}^{ij} = (R_i)^T \eta_{tr}^j R_i, \quad \text{where} \quad 2. \quad \eta_{tr}^j = U_j - I .
\]
Here, \( R_i \in SO_3 \), \( i = 1, ..., N \), is a rotation tensor, \( \eta_{tr}^j \) is the linearized transformation strain tensor from austenite to the \( j \)th bainite variant, \( U_j \) is the symmetric transformation tensor and \( I \) is the identity tensor. The austenite is taken as a reference configuration with transformation strain \( \eta_{tr}^j = 0 \).

2.3. Macro-meso relations
For later exposition we assume the following relations between macroscopic and mesoscopic strains:
\[
1. \quad \varepsilon := \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{el}^{ij}, \quad 2. \quad \varepsilon_{el} := \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{el}^{ij}, \quad 3. \quad \varepsilon_{th} := \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{th}^{ij},
\]
\[
4. \quad \varepsilon_{pl} := \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{pl}^{ij}, \quad 5. \quad \varepsilon_{eff} := \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \eta_{tr}^{ij} .
\]
Here, \( \varepsilon \) is the macroscopic strain tensor from equation (1). \( \varepsilon_{el}, \varepsilon_{th}, \varepsilon_{pl} \) and \( \varepsilon_{eff} \) are the effective elastic, thermal, the effective plastic strain and the effective eigenstrain tensor, respectively. We make the assumption of a constant stress \( \sigma \), then by inserting the effective strain (10.1) into (5), the stress power in (5) is obtained as
\[
P = \sigma : \dot{\varepsilon} = \sigma : \frac{d}{dt} \left( \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{el}^{ij} \right) = \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \sigma : \dot{\varepsilon}^{ij} + \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \varepsilon_{eff}^{ij} .
\]

2.4. Helmholtz free energy
We assume a quadratic functional for the Helmholtz free energy, where, analogously to equation (9), the elasticity constants \( C_{tuvw}^i \) of the \( j \)th variant of crystal \( i \) are transformed as \( C_{tuvw}^{ij} = R_i R_i^T R_j R_j^T R_w R_w^T C_{tuvw}^i \) such that the energy density of variant \( j \) of crystal \( i \) is defined as
\[
1. \quad \psi_{el}^{ij}[\xi_{el}^i, q_k^j, \theta] = \psi_{el}^{ij} + \psi_{pl}^{ij} + \psi_{ch}^{ij} , \quad \text{where} \quad 2. \quad \psi_{el}^{ij}[\xi_{el}^i] = \frac{1}{2} \sum_{k=0}^1 \xi_{el}^{ij} q_k^j C_{el}^{ij}, \quad 3. \quad \psi_{pl}^{ij}[q_k^j] = \frac{1}{2} \sum_{k=0}^1 q_k^j H^{ij} q_k^j + \frac{1}{2} \sum_{k=0}^1 q_k^j H^{ij} q_k^j ,
\]
\[
4. \quad \psi_{ch}^{ij}[\theta] = \phi_{ch}^{ij} + \Delta \phi_{ch}^{ij} \theta ,
\]
and the total Helmholtz free energy is defined as a weighted sum
\[
1. \quad \psi[\xi_{el}^{ij}, q_k^j, \theta, \lambda^{ij}, \xi^i] = \psi_{el}^{eff} + \psi_{pl}^{eff} + \psi_{ch}^{eff} + \psi_{\theta}^{eff} + \psi_{\theta}^{eff} , \quad \text{where} \quad 2. \quad \psi_{el}^{eff}[\xi_{el}^{ij}, \lambda^{ij}, \xi^i] = \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \psi_{el}^{eff}[\xi_{el}^i], \quad 3. \quad \psi_{pl}^{eff}[q_k^j, \lambda^{ij}, \xi^i] = \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \psi_{pl}^{eff}[q_k^j, \lambda^{ij}, \xi^i],
\]
\[
4. \quad \psi_{ch}^{eff}[\theta, \lambda^{ij}, \xi^i] = \sum_{i=1}^N \xi^i \sum_{j=0}^\infty \lambda^{ij} \psi_{ch}^{eff}[\theta, \lambda^{ij}, \xi^i] , \quad \text{and} \quad 5. \quad \psi_{\theta}^{eff}[\theta] = \int_{\theta_0}^{\theta} c_d[\theta] d\theta - \int_{\theta_0}^{\theta} c_d[\theta] d\theta .
\]
\( H^{ij}, q_0^j \) and \( b^j \) are material parameters associated to the hardening variables, \( q_0^j \) and \( q_2^j \), used for the modelling of combined linear and nonlinear hardening. Further, \( \phi_{ch}^{ij} \) describes a constant chemical energy, \( \Delta \phi_{ch}^{ij} \) a temperature dependent part and \( c_d \) the specific heat capacity.

2.5. Thermodynamic forces
The thermodynamic forces are obtained by standard procedure from the Clausius-Duhem inequality in (4) under use of (8) and (11). With the Helmholtz free energy from (13), the macroscopic Cauchy stress tensor for variant \( j \) of crystal \( i \) results as:
We point out, that the assumption of a constant stress \( \sigma \) over the polycrystal is equivalent to the use of a Reuss-type lower bound. Taking the weighted sum of (14.2) over all crystals and variants results into

\[
\sum_{l=1}^{N_i} \xi^l \sum_{j=0}^{N_j} \lambda^{lj} (\mathcal{C}^{lj})^{-1} \sigma = \sum_{l=1}^{N_i} \xi^l \sum_{j=0}^{N_j} \lambda^{lj} \mathcal{E}^{lj}.
\]

Then, by use of the definitions (10) for the effective strains and the effective compliance tensor \((\mathcal{C}_{eff})^{-1} := \sum_{l=1}^{N_i} \xi^l \sum_{j=0}^{N_j} \lambda^{lj} (\mathcal{C}^{lj})^{-1}\), equation (15) is written as

\[
\sigma = \mathcal{C}_{eff} : \mathcal{E}_{el}.
\]

We further identify the hardening stresses and chemical forces for phase-transformation as:

\[
\begin{align*}
1. & \quad Q_1^{ij} = \varrho_0 \frac{\partial \mathcal{W}}{\partial q^i_1} = q_0^j b^j q_1^{ij}, \quad Q_2^{ij} = \varrho_0 \frac{\partial \mathcal{W}}{\partial q^j_2} = H^j q_2^{ij}, \quad \text{and} \\
2. & \quad \Lambda^{ij} = \varrho_0 \frac{\partial \mathcal{W}}{\partial \lambda^{ij}} - \xi^i \sigma \mathcal{E}^{ij} \\
& \quad = -\xi^i \left( \frac{1}{2} \sigma : (\mathcal{C}^{ij})^{-1} : \sigma + \sigma : (\mathcal{E}^{ij} + \mathcal{E}^{ij}_{th} + \mathcal{E}^{ij}_{pl} + \eta^{ij}_{tr}) - \varrho_0 \psi^{ij}_{pl} - \varrho_0 (\phi^{ij}_{ch} + \Delta \phi^{ij}_{ch} \theta) \right).
\end{align*}
\]

2.6. Evolution equations: Phase transformation combined with variant interaction
Contrary to martensitic displacive transformations, bainitic phase transformations are accompanied by diffusion processes making the bainite formation time dependent. Concerning the formulation of evolution equations for phase transformation, we resort to the methods of viscoplasticity. Therefore, we formulate evolution equations for the bainitic variants of Perzyna-type as follows:

\[
\begin{align*}
1. & \quad \text{Evolution of bainitic variants} \quad \dot{\lambda}^{ij}_i = \frac{1}{\nu_{tr}} (\Phi^{ij}_{tr} n_{tr} (H_s [\lambda^{i0}, \lambda^{ij}]) n_{tr}, \quad i, j > 0 \\
2. & \quad \text{Evolution of austenite} \quad \dot{\lambda}^{i0}_i = -\sum_{j=1}^{n} \lambda^{ij}_j \\
3. & \quad \text{Overstress function} \quad \Phi^{ij}_{tr} = (\Lambda^{i0} - \Lambda^{ij}) - (f_c + \alpha_{vi} V^{ij}) \\
4. & \quad \text{Saturation function} \quad H_s [\lambda^{i0}, \lambda^{ij}] = (\lambda^{i0})^s (\lambda^{ij})^{s_2}.
\end{align*}
\]

The function \( \langle x \rangle \) is defined as \( \langle x \rangle = x \) for \( x > 0 \), \( \langle x \rangle = 0 \) for \( x \leq 0 \) ("Maclaury brackets"). It guarantees that the relation \( \dot{\lambda}^{ij}_i \geq 0 \) is always fulfilled. In addition, the overstress function \( \Phi^{ij}_{tr} \) in (18.1) ensures that the bainitic variants only start to form out of the austenite if the difference between the free enthalpies of austenite and bainite exceeds an energetic barrier \( f_c \). The evolution of austenite is calculated from the constraint (7.1) as the negative sum over the rates of bainite fractions. The speed of growth for bainite is dependent on the saturation \( H_s \) in equation (18.4). On the one hand it ensures that for a decreasing amount of austenite the formation of bainite is slowed down. On the other hand small amounts of bainite lead to a slow formation of bainitic variants in the beginning of the simulation. This approach adopts the main ideas of the classical theory by Johnson-Mehl-Avrami-Kolmogorov for diffusion-controlled isothermal phase transformations (see e.g. [10]). The typical S-shape of the curves can be seen in the results of the numerical example in section 3.

For modeling of variant interaction, an influence factor \( V^{ij} \) is introduced, which can raise the energetic barrier in \( \Phi^{ij}_{tr} \) needed for the evolution of the different variants. Further, the parameter \( \alpha_{vi} \) is used to control the overall strength of the interaction effect. For \( \alpha_{vi} = 0 \) the variant interaction is deactivated. The influence factor is defined as

\[
V^{ij} := \sum_{k=1}^{n} \lambda^{ik} \mathcal{E}^{kj}_{vi},
\]
where $e_{vi}^{kj}$ is a factor which describes the influence of variant $k$ on the evolution of variant $j$. Therefore, if variant $k$ hinders the evolution of variant $j$, the value of $e_{vi}^{kj}$ will be larger compared to the value of another variant, which is more likely to form besides variant $j$. The influence of variant $k$ is then automatically controlled with help of its volume-fraction $\lambda_{ik}$ in equation (19). At this point it has to be discussed, which values are suitable for the factors $e_{vi}^{kj}$ in order to lead to a realistic result.

All material parameters for the description of the evolution of bainite variants are summarized as $\kappa_{tr}^j = [v_{tr}, n_{tr}, \bar{f}_c, s_1, s_2, \phi_{ch}^{ij}, \Delta\phi_{ch}^{ij}, \alpha_{vi}]$. At this point we use the same set of material-parameters for all variants, resulting in only one set of parameters for the evolution of variants.

**Remark.** For simulation of inelastic behavior of the constituents, time dependent viscoplasticity combined with non-linear isotropic hardening is used. Since the focus of this paper is on the variant-interaction, we do not further elaborate on the specific issue (details in: [1] and [11]).

### 3. Numerical Example

#### 3.1. Numerical implementation

For the numerical implementation of the constitutive equations in section 2, we make use of a two-step staggered algorithm (see figure 2). It consists of the following two steps:

- **Step I** Calculation of variants $\lambda_{ij}$ with a projected Newton algorithm, combined with an active-set-strategy, where the viscoplastic strains $\varepsilon_{pl}^{ij}$ are constants.
- **Step II** Calculation of viscoplasticity with a Newton iteration and radial return method, where the variants $\lambda_{ij}$ are constants.

A description of the algorithm in Step I can be found in [12]. Basic principles of the algorithm in Step II can be found e.g. in [13].

![Numerical implementation: two-step-staggered algorithm.](image)

**Figure 2.** Numerical implementation: two-step-staggered algorithm.

![Variant selection: schematic of thermo-mechanical loading (dotted line: temperature, dashed line: stress).](image)

**Figure 3.** Variant selection: schematic of thermo-mechanical loading (dotted line: temperature, dashed line: stress).
3.2. Variant selection: Variant-interaction during bainitic phase transformation in a single crystal

In this example the calculations are performed for a single grain, subjected to an external stress field and a constant temperature, as shown exemplarily in figure 3. We note that the grain counter \( i \) is now equal to one while the variant counter \( j \) may be any number from 1 to 24. The zone marked with cyan color in figure 3 represents the process of austenitization and the following cooling-phase needed for initiation of the bainitic transformation.

We assume that the material has been cooled down to a temperature of 340 °C with a moderate cooling-rate, making the formation of bainite possible. This is the point where our simulation starts. The temperature is supposed to be at the constant value of 340 °C and external stresses are applied to the crystal. It should be noted that the single element level considerations mainly serve the purpose of demonstrating the algorithm’s capability of capturing the effect of variant-interaction. Therefore viscoplasticity has not been taken into account at this stage which would be difficult to deal with in a stress-controlled analysis at a single material point for a weakly hardening material. However, viscoplasticity would be accounted for at the next level, i.e. at the level of a polycrystal, e.g. by means of a representative volume element. A respective example has been given in [1].

Figure 4. Variant selection: for a mechanical loading of \( \sigma_x = 250 \, MPa \); a) without variant-interaction (\( a_{\text{vintr}} = 0 \)); b) with variant-interaction (\( a_{\text{vintr}} = 125 \))

For reasons of clarity, we present results of simulations considering the evolution of only three bainitic variants. The material parameters are chosen as in [1], except for \( n_{trr} \), which is set to 2.5. The variant-interaction factors are chosen as follows, using matrix formulation:

\[
E_{vi} = \begin{bmatrix}
e_{v1}^{11} & e_{v1}^{12} & e_{v1}^{13} \\
e_{v1}^{21} & e_{v1}^{22} & e_{v1}^{23} \\
e_{v1}^{31} & e_{v1}^{32} & e_{v1}^{33}
\end{bmatrix} = \begin{bmatrix}
0.01 & 0.5 & 0.75 \\
0.5 & 0.01 & 0.25 \\
0.75 & 0.25 & 0.01
\end{bmatrix}.
\]

The transformation strain tensors for the variants are set to:

\[
U_{i} = \begin{bmatrix}
U_{xx} & U_{yy} & U_{zz} & U_{xy} & U_{xz} & U_{yz}
\end{bmatrix}
\]

\[
U_0 = \begin{bmatrix}
1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0
\end{bmatrix}
\]

\[
U_1 = \begin{bmatrix}
1.0296 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0
\end{bmatrix}
\]

\[
U_2 = \begin{bmatrix}
1.0 & 1.0296 & 1.0 & 0.0 & 0.0 & -0.186
\end{bmatrix}
\]

\[
U_3 = \begin{bmatrix}
1.0 & 1.0 & 1.0296 & 0.0 & 0.186 & 0.0
\end{bmatrix}
\]

Figure 4 a) shows the results for variant evolution without variant-interaction, i.e. for \( a_{\text{vintr}} = 0 \), under an external mechanical loading of \( \sigma_x = 250 \, MPa \). Here, the loading in x-direction leads to a preferred transformation of the austenite into the first bainitic variant (BV1). The other two variants (BV2 and BV3) only evolve to low, equal amounts. In comparison to this, figure 4 b) presents results for a simulation considering variant-interaction (\( a_{\text{vintr}} = 125 \)). The results show a more balanced evolution of the different variants. Although the variant BV1 again is the first one to evolve, the variant-
interaction factor $e_{vi}$, in combination with the relatively high overall strength of the interaction $a_{vint} = 125$, hinders the evolution at the later stages of the transformation, allowing the evolution of the other two variants. Further, we point out, that the model is now capable of simulating transformations with a remaining volume-fraction of austenite. This is a reasonable extension, since general experiments often show a specific amount of untransformed retained austenite.

In figure 5, we compare several simulations for different values of $a_{vint}$. These results show the influence of the overall strength of the variant-interaction on the evolution of the bainitic variants.

![Figure 5. Variant selection: influence of the overall strength of the variant-interaction on the evolution of the bainitic variants](image)

4. Summary and Outlook
In this paper, we extended a model for bainitic variant evolution by a mechanism for variant-interaction. This is achieved with an ansatz adopted from the theory of transformation hardening. With this extension, we obtain an effective tool for simulating the influence of the different variants belonging to each other, potentially hindering or preventing the evolution of crystallographically unfavorable variants.

The variant-interaction factors in the presented numerical example have been merely chosen to clarify the capabilities of the model. Future work should include the determination of proper values, reflecting the real variant-interaction. Preceding this task, we will have to identify the true transformation strain tensors of the bainitic variants. Further steps could be the modeling of mesoscopic carbon diffusion and the dissolution of austenite into bainitic ferrite and carbides.

5. References
[1] Mahnken R, Schneider A, Antretter T, Ehlenbröker U and Wolff M 2015 *Int. J. Solids Struct.* 54 156-71
[2] Franciosi P 1985 *Acta Metall.* 33 1601-12
[3] Siredey N, Patoor E, Berveiller M and Eberhardt A 1999 *Int. J. Solids Struct.* 36 4289-315
[4] Niclaeys C, Ben Zineb T, Arbab-Chirani S and Patoor E 2002 *Int. J. Plast.* 18 1619-47
[5] Kundu S and Bhadeshia H K D H 2007 *Scripta Mater.* 57 869-72
[6] Gérard C, Cailletaud G and Bacroix B 2013 *Int. J. Plast.* 42 194-212
[7] Bhadeshia H K D H 2003 *Bainite in Steels, Transformations, Microstructure and Properties* (Cambridge: University Press)
[8] Haupt P 2002 *Continuum Mechanics and Theory of Materials* (Berlin: Springer)
[9] Hackl K and Heinen R 2008 *Continuum Mech. Thermodyn.* 19 499-510
[10] Avrami M 1940 *J. Chem. Phys.* 8 212-24
[11] Lemaitre J and Chaboche J L 1990 *Mechanics of Solid Materials* (Cambridge: University Press)
[12] Mahnken R and Wilmanns S 2011 *Comput. Mater. Sci.* 50 2535-48
[13] Simo J C and Hughes T J R 1998 Computational inelasticity In: *Interdisciplinary Applied Mathematics. Mechanics and Materials* (Berlin: Springer)
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