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A comprehensive model of thermo-elasto-plasticity with phase transitions in steel

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A comprehensive model of thermo-elasto-plasticity with phase transitions in steel

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Abstract

This work deals with mathematical modeling of processes involved in the quenching process of steel. It is the aim to provide a comprehensive model of thermo-elasto-plasticity with phase transitions in steel for small deformations, which integrates the complex behavior of steel materials in general models of thermo-elasto-plasticity and deals with the modeling of the mathematical problem of linear thermo-elasto-plasticity, taking into account phase transitions and transformation-induced plasticity. Moreover, the qualitative behavior of the solution is illustrated for the Jominy-End-Quench-Test in a simple numerical simulation.

Kurzfassung

Diese Arbeit befasst sich mit der mathematischen Modellierung von Abschreckprozessen bei Stahlbauteilen. Das Ziel ist es, ein Gesamtmodell für kleine Deformationen bereitzustellen, welches das komplexe physikalische Materialverhalten von Stahl in allgemeinere Modelle der Thermo-Elasto-Plastizität einbindet und somit das mathematische Problem der linearen Thermo-Elasto-Plastizität unter Berücksichtigung von Phasentransformationen und Umwandlungsplastizität beschreibt. Darüberhinaus ist das qualitative Lösungsverhalten für ein Beispielproblem anhand des Jominy-End-Abschreck-Tests dargestellt.

Keywords

Steel, material behavior, distortion engineering, phase transitions, TRIP, coupling of TRIP and plasticity, Jominy-End-Quench-Test

AMS subject classifications

35Q72, 74A15, 74C05, 74F05, 74N99

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Contents

1 Introduction

Today, steel is one of the most common materials in industry. The world steel production, with more than 1.3 billion tons produced annually, takes the second place behind cement. Steel and iron materials are used in various areas, very often with high quality requirements according geometry, structure, surface finish, hardness and other properties of the components for questions of production and processing of modern steels. This creates a major challenge for the prediction of the material behavior, i.e. stress, strain and phase composition.
The modeling and the simulation of essential effects can help to gain a deeper understanding of the material behavior. An important goal is to minimize the distortion at the end of the production process, i.e. the unwanted or undesirable deviation from the norm geometry.
Controlling distortion in the manufacturing process, especially in heat treatment processes of steel, remains a complex problem even today for the significant distortion potential of steel workpieces, and the costs of compensating distortion failures of wrought component parts are considerably large. Therefore it is a major interest to understand the causes of distortion in every production step in detail, cf. [HKLM02, WBBD12].

1.1 Steel

Steel is an iron-carbon alloy with a carbon content between 0.002% and 2.1% by weight. It is (in the solid state) a polycrystalline material. Macroscopic phenomena in steel are the possible solid-solid phase transformations, which are strongly influenced by the history of the temperature and the carbon content (cf. e.g. [Dah93, WW04, BT06]). Phase transitions, which occur during the heat treatment of steel materials, e.g. heating and quenching, are connected with volume changes and heat effects. This results in a time- and temperature-dependent stress distribution and deformation, which are crucial for the result of heat treatment processes.
Another important phenomenon is the transformation-induced plasticity (TRIP) with appears in connection with phase transformations. TRIP already occurs under deviatoric stresses and leads to permanent deformation at relatively low stress, even if the yield stress of the softer phase is not reached. This effect cannot be explained by classical plasticity at the macroscopic level of modeling (cf. e.g. [Mit87, FST96, Fis97, FRW$^+$00, DL06, DLZ06]).

1.2 Heat treatment processes

The condition in which workpieces and tools made of steel are processed fulfills rarely the needs arising from the intended purpose. Therefore, it is necessary to change the condition of the steel material, e.g. by heat treatment, in order to modify the material properties w.r.t. the different conditions needed in the specific application (cf. e.g. [Hor92, Koh94] for details). Such hardening treatments set up large internal strains in the metal and cause distortion of steel components during the production process.

1.3 Literature review: Coupled models for material behavior of steel

Some references that exist associated with the problem of interest are given afterwards. More detailed information are given in [Boe12a].
For coupled models dealing with the material behavior of steel there exists literature in a smaller scale. Problems of thermo-elasticity are treated in [Wei09], modeling of elasto-plastic problems can be found in [Pal98, Lub02]. In connection with phase transitions a thermo-plastic problem is discussed in [DB04a] and the coupling with an elasto-plastic problem can be found in [DB04b]. In [IW85] stress, temperature and phase transitions are coupled. TRIP and plasticity are considered in [TP06]. Coupled models of thermo-elasto-plasticity with phase transitions and TRIP are discussed in [WB03, WBS05, WBT11] for small deformations. An important contribution to the modeling of thermo-elasto-plasticity with phase transitions and TRIP of the material behavior of steel and the basis of this work are [WBH08, WBMS11]. In [MWSB12] a corresponding model is formulated within a thermodynamic framework at large strains. Coupled models that neglect the classical plasticity are discussed in e.g. [WBS04, WB06, WBS06, WBB07]. For such models dimensional analysis (cf. [WBF08]), carbon diffusion (cf. [WABM06]) and creep (cf. [WB10, BWD$^+$11]) are investigated.

1.4 Scope

This work is concerned with mathematical modeling of thermo-elasto-plasticity with phase transitions in steel of processes involved in the quenching process of steel workpieces. Therefore, it is positioned in the overlap of two scientific disciplines: applied mathematics and materials science. The considered physical processes are heat conduction, phase transformations, thermo-elasticity, classical plasticity and TRIP.
Stress- and strain-dependent phase transformations, TRIP and its interactions with classical plasticity are important phenomena of both theoretical and practical interest in the material

behavior, as they may cause distortion of steel work-pieces. Therefore the idea came up to integrate the complex behavior of steel materials (especially the phase transformations and TRIP) in general models of thermo-elasto-plasticity as a prototypical example for heat treatment processes of steel components (cf. [WBH08, WBMS11] for instance). The steel is assumed as a co-existing mixture of its phases (or components), while diffusion processes are not considered in this work. Usually, diffusion of the phases is not designated in macroscopic models and the (macroscopic) carbon diffusion is primarily interesting in order to investigate special heat treatment processes, like carburizing (or carbonization, cf. [Lie09]). In this case, the model has to be extended by adding an equation describing the carbon concentration (cf. [WABM06] for an ansatz).
The main objective of this work is the formulation of a (mathematical) model of TRIP and their interaction with classical plasticity in the framework of small deformations. To sum up, the results provide a theoretical basis for further mathematical investigation or the efficient implementation of numerical algorithms suitable for real-world applications.

1.5 Outline

After the introduction in the first section, the modeling and the simulation are contained in sec. 2 and sec. 3, followed by a discussion and outlook in the last section. In sec. 1, some citations for well-known models for material behavior of steel are provided. The aim of sec. 2 is to formulate the model of linear thermo-elasto-plasticity with phase transitions and TRIP, describing the material behavior of steel in the context of macroscopic continuum mechanics and to discuss the capabilities. Due to the possible interaction (coupling) of transformation-induced and classical plasticity, the usual approach in plasticity without phase transformations has to be modified substantially. Numerical simulations of the fully coupled problem are illustrated in sec. 3 via the Jominy-End-Quench-Test.

2 Modeling of material behavior of steel

This section deals with the formulation of a complex (macroscopic) model of the material behavior of steel including specific phenomena like stress-dependent phase transitions, TRIP and the possible interaction with classical plasticity developed in [WBH08, WBMS11] for small deformations.

2.1 Governing equations

A material body will be identified with its reference configuration $\Omega \subset \mathbb{R}^3$. In the framework of small deformations we have the well-known balance equations for linear momentum and energy:

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} - \operatorname{div}(\boldsymbol{\sigma}) = \mathbf{f}, \tag{1}$$

$$\rho_0 \frac{\partial e}{\partial t} + \operatorname{div}(\mathbf{q}) = \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + r. \tag{2}$$

Moreover, the second law of thermodynamics is applied in the form of the Clausius-Duhem inequality:

$$-\rho_0 \frac{\partial \psi}{\partial t} - \rho_0 \eta \frac{\partial \theta}{\partial t} + \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} - \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta \geq 0. \tag{3}$$

The relations (1) – (3) have to be fulfilled in the space-time domain $\Omega \times]0, T[$, $T \in \mathbb{R}$. The notations are standard: ρ_0 – bulk density in the reference configuration, i.e. for $t = 0$, $\mathbf{u}$ – displacement vector, $\boldsymbol{\varepsilon}$ – (linearized) Green strain tensor, θ – absolute temperature, $\boldsymbol{\sigma}$ – Cauchy

stress tensor, $\mathbf{f}$ – volume density of external forces, e – mass density of internal energy, $\mathbf{q}$ – heat flux, r – volume density of heat supply, ψ – mass density of free (or Helmholtz) energy, η – mass density of entropy. Note the relations:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{u}) := \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right), \qquad \mathbf{u} = (u_1, u_2, u_3)^T \qquad \text{and} \tag{4}$$

$$\psi := e - \theta\eta. \tag{5}$$

2.2 Phase transitions

The evolution of phase fractions is given by the ODEs

$$\frac{\partial p_i}{\partial t} = \gamma_i\big(\mathbf{p}, \theta, \frac{\partial\theta}{\partial t}, \boldsymbol{\sigma}, \boldsymbol{\xi}\big) \qquad (i = 1, \dots, m) \qquad (m \geq 2) \tag{6}$$

In general, the phase evolution may depend on internal variables labeled by $\boldsymbol{\xi}$. Here, $\mathbf{p}$ denotes $(p_1, \dots, p_m)$. Moreover, the phase (mass) fractions p_i of the ith phase $(i = 1, \dots, m)$ have to fulfill the subsequent balance and non-negativity relations

$$\sum_{i=1}^{m} p_i = 1, \qquad p_i \geq 0 \qquad \text{for} \qquad i = 1, \dots, m \tag{7}$$

which implies $\sum_{i=1}^{m} \gamma_i = 0$. More detailed information are given in sec. 2.10.

2.3 Decomposition of the strain tensor

As usual in the theory of small deformations (using geometric linearization), the linearized Green strain tensor $\boldsymbol{\varepsilon}$ is decomposed into the following three components

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{te} + \boldsymbol{\varepsilon}_{trip} + \boldsymbol{\varepsilon}_{cp}, \tag{8}$$

where $\boldsymbol{\varepsilon}_{te}$ – thermoelastic strain (including (isotropic) density variations due to temperature changes and phase transformations), $\boldsymbol{\varepsilon}_{trip}$ – (non-isotropic) strain due to TRIP and $\boldsymbol{\varepsilon}_{cp}$ – strain due to (classical) plasticity. Because of the two mechanisms for plasticity (interaction between classical plasticity and TRIP), the considered model is an concrete example of a so-called two-mechanism model (cf. [WT08, WBT10, Saï11, WBT11] for multi-mechanism models). Sometimes, $\boldsymbol{\varepsilon}_{te}$ is also split up into a pure elastic part, a pure thermal part and a part only due to phase changes. Viscosity and creep effects are not taken into account. In principal, they could be considered analogously with some modifications (cf. e.g. [WB10, BWD$^+$11, KBW12, WBBK12]). As usual, the inelastic strains are assumed to be volume-preserving, i.e.

$$\operatorname{tr}(\boldsymbol{\varepsilon}_{trip}) = 0 \implies \boldsymbol{\varepsilon}_{trip} = \boldsymbol{\varepsilon}^*_{trip} \qquad \text{and} \qquad \operatorname{tr}(\boldsymbol{\varepsilon}_{cp}) = 0 \implies \boldsymbol{\varepsilon}_{cp} = \boldsymbol{\varepsilon}^*_{cp}. \tag{9}$$

We remark that classical plasticity and TRIP act by the stress deviator on the deformation. For later on, the accumulated plastic and TRIP strain are given via:

$$s_{cp} := \int_0^t \sqrt{\frac{2}{3}\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial\tau} : \frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial\tau}}\,\mathrm{d}\tau \qquad \text{and} \qquad s_{trip} := \int_0^t \sqrt{\frac{2}{3}\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial\tau} : \frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial\tau}}\,\mathrm{d}\tau. \tag{10}$$

2.4 Thermo-elasticity relation

The material law (11) is a generalization of the so-called Duhamel-Neumann's law (or generalized Hooke's law) of the classical (linear) thermo-elasticity for isotropic bodies, cf. e.g. [WBH08, WBMS11]. The last term in (11) takes the density changes as a result of phase transitions into account. In order to separate this part from the thermal expansion, the phase densities appear at the initial temperature. The stress tensor $\boldsymbol{\sigma}$ and the thermoelastic part $\boldsymbol{\varepsilon}_{te}$ of the strain tensor are connected by the law of thermo-elasticity taking density changes due to phase transformations into account:

$$\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon}^*_{te} + K\mathrm{tr}(\boldsymbol{\varepsilon}_{te})\mathrm{Id} - 3K_\alpha\,(\theta-\theta_0)\,\mathrm{Id} - K\sum_{i=1}^{m}\left(\frac{\rho_0}{\rho_i(\theta_0)}-1\right)p_i\mathrm{Id}, \tag{11}$$

where μ – shear modulus, K – compression (bulk) modulus, $K_\alpha := K\alpha$ – modulus taking compression and linear heat-dilatation of the bulk material into account, $\rho_i(\theta_0)$ – density of the ith phase phase at initial temperature θ_0, i.e. at $t = 0$. The deviator $\boldsymbol{\varepsilon}^*_{te} := \boldsymbol{\varepsilon}_{te} - \frac{1}{3}\mathrm{tr}(\boldsymbol{\varepsilon}_{te})\mathrm{Id}$ can be written as $\boldsymbol{\varepsilon}^*_{te} = \boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}_{trip} - \boldsymbol{\varepsilon}_{cp}$, using (8). Alternatively, the last two terms in (11) may be written as a sum

$$\frac{1}{3}\frac{\rho_0-\rho(\theta)}{\rho_0}\mathrm{Id} = \alpha\,(\theta-\theta_0)\,\mathrm{Id} + \frac{1}{3}\frac{\rho_0-\rho(\theta_0)}{\rho_0}\mathrm{Id}, \tag{12}$$

where $\rho(\theta)$ – current density related to the current temperature using (7) and a mixture rule for density, cf. [WBD03]. The stress in (11) can be alternatively defined by using Young's modulus and Poisson's ratio or the Lamé constants instead of using bulk and shear modulus. We have

$$\lambda := K - \frac{2\mu}{3}, \qquad \nu := \frac{3K-2\mu}{2(3K+\mu)}, \qquad E := \frac{9K\mu}{3K+\mu}, \tag{13}$$

where λ – Lamé's first coefficient, ν – Poission's ration and E – Young's modulus.

2.5 Plasticity

Using the von Mises criterion (cf. [LC90, Lem01] for generalizations), the material behavior is constrained by

$$F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) := \sqrt{\frac{3}{2}\left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right) : \left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right)} - (R_0 + R) \le 0, \tag{14}$$

which is a restriction on the deviator of the effective stress $\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}$. The notations are: F – yield function, $\boldsymbol{\sigma}$ – stress deviator, $\mathbf{X}_{cp}$ – back-stress associated with plasticity (with $\mathrm{tr}(\mathbf{X}_{cp}) = 0$, cf. e.g. [WBT10] for details), R_0 – initial radius of the yield sphere in the stress space (or initial yield stress), R – its possible increment due to isotropic hardening. The evolution of the plastic strain $\boldsymbol{\varepsilon}_{cp}$ is governed by the flow rule:

$$\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t} = \Lambda\,\left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right), \tag{15}$$

where the plastic multiplier Λ has to fulfill

$$\Lambda = 0, \quad \text{if} \quad F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) < 0 \quad \text{and} \tag{16}$$

$$\Lambda \ge 0, \quad \text{if} \quad F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) = 0 \quad \text{(yield condition)}. \tag{17}$$

Thus, plastic deformation is only possible, if the yield condition (17) is fulfilled. The relation (15) – (17) is equivalent to a variational inequality, cf. sec. 2.12.

2.6 Transformation-induced plasticity (TRIP)

Phase transformations under non-vanishing deviatoric (non-isotropic) stress yield a permanent deviatoric deformation which cannot be described by classical plasticity at the macroscopic level. It is assumed that TRIP has no yield condition and that its evolution can be described by

$$\frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} = b\,\left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{trip}\right), \tag{18}$$

where $\mathbf{X}_{trip}$ – back-stress associated with TRIP (with $\mathrm{tr}(\mathbf{X}_{cp}) = 0$, cf. e.g. [WBT10] for details) and $b \geq 0$ depends essentially on the phase evolution. One proposal for TRIP in the multi-phase case (based on the Franitza-Mitter-Leblond ansatz, cf. e.g. [WBS09]) is:

$$b = \frac{3}{2}\sum_{i=1}^{m} \kappa_i \frac{\partial \phi_i}{\partial p_i}\,(p_i)\,\max\left\{\frac{\partial p_i}{\partial t}, 0\right\} \tag{19}$$

where κ_i – Greenwood-Johnson parameter (may depend on temperature and stress direction, cf. e.g. [WBH08]) and $\phi_i \in C^{0,1}([0,1]) \cap C^1(]0,1[)$ – saturation function of the ith phase satisfying

$$\kappa_i \geq 0, \qquad \phi(0) = 0, \qquad \phi(1) = 1, \qquad \frac{\partial \phi_i}{\partial p_i}(p) \geq 0 \ \text{ f.a. } \ 0 < p < 1. \tag{20}$$

The function ϕ_i describes the dependence of the transformed phase fraction p_i on the strain due to TRIP. Cf. sec. 2.11 for an equivalent formulation of (18).

Remark 1 (Proposals for saturation functions). There are various proposals for saturation functions in the literature (cf. [WBDL03]), partially based on experiments, partially derived from theoretical considerations:

$$\begin{aligned}
&\phi(p) = p && \text{(Tanaka)},\\
&\phi(p) = p(2-p) && \text{(Desalos, Denis)},\\
&\phi(p) = p(1-\ln(p)) && \text{(Leblond)},\\
&\phi(p) = p(3-2\sqrt{p}) && \text{(Abrassart)}.
\end{aligned}$$

2.7 Isotropic and kinematic hardening

For further investigations, it is very useful to get more information about the isotropic hardening variable R. The following ansatz is suggested in [WBH08, WBMS11]:

$$R(t) = \gamma_{cp}\left(s_{cp}(t) - \int_0^t \frac{\beta_{cp}}{\gamma_{cp}} R \frac{\partial s_{cp}}{\partial s}(s)\,\mathrm{d}s\right) \tag{21}$$

as well as the linear ODE (differentiating (21))

$$\frac{\partial R}{\partial t} = \gamma_{cp}\frac{\partial s_{cp}}{\partial t} - \left(\beta \frac{\partial s_{cp}}{\partial t} - \frac{\frac{\partial \gamma_{cp}}{\partial t}}{\gamma_{cp}}\right) R. \tag{22}$$

Clearly, the solution of the ODE (22) (for the initial value $R(0) = 0$) reads as

$$R(t) = \gamma_{cp}\int_0^t \frac{\partial s_{cp}}{\partial s}\exp\left(-\int_0^s \beta_{cp}\frac{\partial s_{cp}}{\partial \tau}\,\mathrm{d}\tau\right)\mathrm{d}s. \tag{23}$$

Moreover, one gets the following estimate

$$0 \leq R = R(t) \leq \frac{\gamma_{cp}}{\min(\beta_{cp})}\Big(1 - \exp\big(-\min(\beta_{cp})s_{cp}\big)\Big). \tag{24}$$

In general, the parameters β_{cp} and γ_{cp} depend on the temperature and the phase fractions. Therefore, R is a slope of s_{cp} for constant β_{cp} and γ_{cp}, i.e. $R = \frac{\gamma_{cp}}{\beta_{cp}}\Big(1 - \exp\big(-\beta_{cp} s_{cp}\big)\Big)$. The curve R has its decline γ_{cp} and its saturation value is $\frac{\gamma_{cp}}{\beta_{cp}}$. Besides this, R is an increasing function of s_{cp}, as one expects in isotropic hardening (cf. [WBH08]): $0 \le R \le \frac{\gamma_{cp}}{\beta_{cp}}$, $0 \le \frac{\partial R}{\partial t} \le \gamma_{cp} \frac{\partial s_{cp}}{\partial t}$.

The general model leads to the following equations for the back-stresses, cf. [WBH08, WBMS11]:

$$\mathbf{X}_{cp}(t) = c_{cp}\left(\boldsymbol{\varepsilon}_{cp} - \int_0^t \frac{a_{cp}}{c_{cp}} \mathbf{X}_{cp} \frac{\partial s_{cp}}{\partial s}\,\mathrm{d}s\right) + c_{int}\left(\boldsymbol{\varepsilon}_{trip} - \int_0^t \frac{a_{trip}}{c_{trip}} \mathbf{X}_{trip} \frac{\partial s_{trip}}{\partial s}\,\mathrm{d}s\right), \tag{25}$$

$$\mathbf{X}_{trip}(t) = c_{int}\left(\boldsymbol{\varepsilon}_{cp} - \int_0^t \frac{a_{cp}}{c_{cp}} \mathbf{X}_{cp} \frac{\partial s_{cp}}{\partial s}\,\mathrm{d}s\right) + c_{trip}\left(\boldsymbol{\varepsilon}_{trip} - \int_0^t \frac{a_{trip}}{c_{trip}} \mathbf{X}_{trip} \frac{\partial s_{trip}}{\partial s}\,\mathrm{d}s\right). \tag{26}$$

These relations may be understood as generalizations of the well-known Armstrong-Frederick equations in plasticity (cf. [LC90, JK96, Hau02]). For a constant coefficient c_{cp} and without TRIP, from (25) follows the classical Armstrong-Frederick equation for non-linear hardening:

$$\frac{\partial \mathbf{X}_{cp}}{\partial t} = c_{cp} \frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} - a_{cp} \mathbf{X}_{cp} \frac{\partial s_{cp}}{\partial t}. \tag{27}$$

In a similar manner, for constant c_{trip} and without classical plasticity, from (26) follows an analogon for TRIP

$$\frac{\partial \mathbf{X}_{trip}}{\partial t} = c_{trip} \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} - a_{trip} \mathbf{X}_{trip} \frac{\partial s_{trip}}{\partial t}. \tag{28}$$

For a given evolution of θ, $\mathbf{p}$, $\boldsymbol{\varepsilon}_{cp}$ and $\boldsymbol{\varepsilon}_{trip}$ (and therefore s_{cp} and s_{trip}), (25) and (26) are a coupled system of Volterra integral equations with a unique solution $(\mathbf{X}_{cp}, \mathbf{X}_{trip})$ (in the class of continuous functions under suitable conditions). It is well-known, that in the case of purely classical plasticity the Armstrong-Frederick equation (27) leads to a bounded back-stress for given $\boldsymbol{\varepsilon}_{cp}$ (saturation effect, cf. e.g. [WBH08]). A similar result for the case of coupled back-stresses $\mathbf{X}_{cp}$ and $\mathbf{X}_{trip}$ is not obvious. For constant c_{cp}, c_{int}, c_{trip}, the differentiation of (25) and (26) yields the following coupled system of ODEs

$$\frac{\partial \mathbf{X}_{cp}}{\partial t} = c_{cp} \frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} - a_{cp} \mathbf{X}_{cp} \frac{\partial s_{cp}}{\partial t} + c_{int} \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} - \frac{c_{int} a_{trip}}{c_{trip}} \mathbf{X}_{trip} \frac{\partial s_{trip}}{\partial t}, \tag{29}$$

$$\frac{\partial \mathbf{X}_{trip}}{\partial t} = c_{int} \frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} - \frac{c_{int} a_{cp}}{c_{cp}} \mathbf{X}_{cp} \frac{\partial s_{cp}}{\partial t} + c_{trip} \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} - a_{trip} \mathbf{X}_{trip} \frac{\partial s_{trip}}{\partial t}. \tag{30}$$

This linear system of ODEs has a unique solution (for given evolution of $\boldsymbol{\varepsilon}_{cp}$ and $\boldsymbol{\varepsilon}_{trip}$). Using the results from the theory of ODEs, one obtains the following results:

Lemma 1 (Boundedness of the back-stresses)**.** *Under the assumptions c_{cp}, c_{int}, c_{trip}, a_{cp}, a_{trip} are constant, a_{cp}, $a_{trip} > 0$ and $c_{int}^2 < c_{cp}\, c_{trip}$ the back-stresses are bounded*

$$|\mathbf{X}_{cp}(\mathbf{x},t)| \le c < \infty, \qquad |\mathbf{X}_{trip}(\mathbf{x},t)| \le c < \infty \qquad \text{f.a. } (\mathbf{x},t) \in \Omega \times]0,T[$$

and

$$\|\boldsymbol{\sigma}^* - \mathbf{X}_{cp}^*\| \le c < \infty, \quad \|\boldsymbol{\sigma}^*\| \le c < \infty, \quad \|\boldsymbol{\sigma}^* - \mathbf{X}_{trip}^*\| \le c < \infty, \quad \|\boldsymbol{\varepsilon}_{te}^*\| \le c < \infty.$$

These results can also be obtained in case of general a_{cp}, a_{trip}, c_{cp}, c_{int} and c_{trip}. The global boundedness of $\mathbf{X}_{cp}$, $\mathbf{X}_{trip}$, R, $\boldsymbol{\sigma}^*$ and $\boldsymbol{\varepsilon}_{te}^*$ (uniformly w.r.t. $\boldsymbol{\varepsilon}_{cp}$, $\boldsymbol{\varepsilon}_{trip}$, s_{cp} and s_{trip}) is an important consequence of the general nonlinear hardening. In contrast to this, the case $a_{cp} = a_{trip} = \beta_{cp} = 0$ leads to a linear relation between $\mathbf{X}_{cp}$, $\mathbf{X}_{trip}$, $\boldsymbol{\varepsilon}_{cp}$, $\boldsymbol{\varepsilon}_{trip}$, R and s_{cp}. Thus, the model has an unbounded growth of the hardening variables for unbounded growing strains in this case. Moreover, the stress deviator might be growing unbounded, too.

Remark 2. The hardening variable R and the back-stresses $\mathbf{X}_{cp}$ and $\mathbf{X}_{trip}$ can be obtained as internal variables in a thermo-mechanical framework. R is a scalar having the character of a stress. The quantities $\mathbf{X}_{cp}$, $\mathbf{X}_{trip}$, and R may be considered as thermodynamic forces (cf. [WBH08] for details).

2.8 Initial and boundary conditions

Finally, the following initial conditions f.a. $\mathbf{x}$ in Ω are assumed:

$$\mathbf{u}(\mathbf{x},0)=\mathbf{u}_0(\mathbf{x}), \qquad \frac{\partial \mathbf{u}}{\partial t}(\mathbf{x},0)=\mathbf{u}_1(\mathbf{x}), \qquad \theta(\mathbf{x},0)=\theta_0(\mathbf{x}), \tag{31}$$

$$\boldsymbol{\varepsilon}_{trip}(\mathbf{x},0)=\mathbf{0}, \qquad \boldsymbol{\varepsilon}_{cp}(\mathbf{x},0)=\mathbf{0}, \qquad \boldsymbol{\xi}(\mathbf{x},0)=\boldsymbol{\xi}_0(\mathbf{x}), \tag{32}$$

$$\mathbf{p}(\mathbf{x},0)=\mathbf{p}_0(\mathbf{x}) \tag{33}$$

with

$$\sum_{i=1}^{m} p_{0i}=1, \qquad p_{0i}\geq 0 \qquad \text{for} \qquad i=1,\dots,m. \tag{34}$$

Furthermore, boundary conditions for $\mathbf{u}$ and θ have to be added. There are mixed boundary conditions for $\mathbf{u}$ assumed:

$$\mathbf{u}=\mathbf{0} \quad \text{f.a. points in } \Gamma_1, \qquad \boldsymbol{\sigma}\cdot\boldsymbol{\nu}_{\Gamma_2}=\mathbf{0} \quad \text{f.a. points in } \Gamma_2, \tag{35}$$

where Γ_1 and Γ_2 are mutually disjoint parts of the boundary of Ω s.t. $\text{meas}(\Gamma_1)>0$ and Γ_1 is closed and $\boldsymbol{\nu}_{\Gamma_2}$ is the outward unit normal vector on Γ_2 (this case without any boundary load is important e.g. in heat treatment processes, where no load is applied on the surface). Let the temperature fulfill the Robin condition

$$-\lambda_\theta \frac{\partial \theta}{\partial \boldsymbol{\nu}_\Gamma}=\delta\,(\theta-\theta_\Gamma) \text{ on } \partial\Omega\times]0,T[, \tag{36}$$

where λ_θ – heat conductivity, δ – heat-exchange coefficient, θ_Γ – temperature of the surrounding medium and $\boldsymbol{\nu}_\Gamma$ – outward unit normal vector to the boundary $\partial\Omega$.

2.9 Complete model of material behavior

Modeling the relevant interactions between temperature, mechanical behavior and phase transitions leads to an initial boundary value problem (IBVP) for a system of coupled nonlinear partial and ordinary differential equations and inequalities for the time and space-dependent temperature, displacement and phase fractions. Summarizing all the model equations needed to describe the evolution of displacement, temperature and phase fractions leads to the following IBVP: Find the displacement $\mathbf{u}:\Omega\times[0,T[\to\mathbb{R}^3$ s.t.

$$\begin{aligned}\rho_0\frac{\partial^2\mathbf{u}}{\partial t^2}-2\,\mathrm{div}\big(\mu\boldsymbol{\varepsilon}(\mathbf{u})\big)-\mathrm{grad}\big(\lambda\mathrm{div}(\mathbf{u})\big)+3\,\mathrm{grad}\big(K_\alpha(\theta-\theta_0)\big)+\\ +\mathrm{grad}\left(K\sum_{i=1}^{m}\left(\frac{\rho_0}{\rho_i(\theta_0)}-1\right)p_i\right)+2\,\mathrm{div}\big(\mu\boldsymbol{\varepsilon}_{trip}\big)+2\,\mathrm{div}\big(\mu\boldsymbol{\varepsilon}_{cp}\big)=\mathbf{f} \quad \text{in} \quad \Omega\times]0,T[,\end{aligned}$$

the temperature $\theta:\Omega\times[0,T[\to\mathbb{R}$ s.t.

$$\rho_0 c_e\frac{\partial\theta}{\partial t}-\mathrm{div}\big(\lambda_\theta\nabla\theta\big)=(\boldsymbol{\sigma}-\mathbf{X}_{cp}):\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t}+(\boldsymbol{\sigma}-\mathbf{X}_{trip}):\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial t}+$$

$$+\theta\frac{\partial\boldsymbol{\sigma}}{\partial\theta}:\frac{\partial\boldsymbol{\varepsilon}_{te}}{\partial t}+\theta\frac{\partial\mathbf{X}_{cp}}{\partial\theta}:\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t}+\theta\frac{\partial\mathbf{X}_{trip}}{\partial\theta}:\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial t}+\rho_0\sum_{i=2}^{m}L_i\frac{\partial p_i}{\partial t}+r\quad\text{in}\quad\Omega\times]0,T[$$

and the phase fractions $\mathbf{p}:\Omega\times[0,T[\to\mathbb{R}^m$ s.t.

$$\frac{\partial\mathbf{p}}{\partial t}=\boldsymbol{\gamma}\big(\mathbf{p},\theta,\frac{\partial\theta}{\partial t},\mathrm{tr}(\boldsymbol{\sigma}),\boldsymbol{\sigma}^*:\boldsymbol{\sigma}^*\big)\quad\text{in}\quad\Omega\times]0,T[$$

including the relations (4), (8), (14) in combination with (23) and

$$\begin{aligned}
\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t}&=\Lambda\left(\boldsymbol{\sigma}^*-\mathbf{X}^*_{cp}\right),\quad\Lambda\geq 0\text{ for }F=0\text{ and }\Lambda=0\text{ for }F<0 && \text{in}\quad\Omega\times]0,T[,\\
\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial t}&=\frac{3}{2}\left(\boldsymbol{\sigma}^*-\mathbf{X}^*_{trip}\right)\sum_{i=1}^{m}\kappa_i\frac{\partial\phi_i}{\partial p_i}(p_i)\max\left\{\frac{\partial p_i}{\partial t},0\right\} && \text{in}\quad\Omega\times]0,T[,\\
\frac{\partial\mathbf{X}_{cp}}{\partial t}&=c_{cp}\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t}-a_{cp}\mathbf{X}_{cp}\frac{\partial s_{cp}}{\partial t}+c_{int}\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial t}-\frac{c_{int}a_{trip}}{c_{trip}}\mathbf{X}_{trip}\frac{\partial s_{trip}}{\partial t} && \text{in}\quad\Omega\times]0,T[,\\
\frac{\partial\mathbf{X}_{trip}}{\partial t}&=c_{int}\frac{\partial\boldsymbol{\varepsilon}_{cp}}{\partial t}-\frac{c_{int}a_{cp}}{c_{cp}}\mathbf{X}_{cp}\frac{\partial s_{cp}}{\partial t}+c_{trip}\frac{\partial\boldsymbol{\varepsilon}_{trip}}{\partial t}-a_{trip}\mathbf{X}_{trip}\frac{\partial s_{trip}}{\partial t} && \text{in}\quad\Omega\times]0,T[
\end{aligned}$$

as well as initial values (31) – (33) and boundary values (35) – (36).

In [WBH08] (cf. also [MWSB12]) was proven that

Lemma 2 (Thermo-dynamic consistency)**.** *The presented bulk model is thermo-dynamic consistent, i.e. the dissipation inequality* (3) *is fulfilled (under reasonable assumptions).*

Remark 3. As in the theory of linear thermo-elasticity for small deformations commonly accepted, one obtains (cf. e.g. [JR00]) the following approximation of the thermo-mechanical dissipation

$$\theta\,\frac{\partial\boldsymbol{\sigma}}{\partial\theta}:\frac{\partial\boldsymbol{\varepsilon}_{te}}{\partial t}=-3\,K_\alpha\,\theta_0\,\mathrm{div}\left(\frac{\partial\mathbf{u}}{\partial t}\right),\tag{37}$$

where θ_0 denotes a (constant) reference temperature close to the actual temperature. Furthermore, the material parameters are assumed to be real constants.

2.10 General model for phase transitions in steel

Isothermal diffusive transformations are well described by the Johnson-Mehl-Avrami-Kolmogorov kinetics (cf. e.g. [WBB07]) and models for martensitic transformation are based on the Koistinen-Marburger equation (cf. [KM59]), but there are some essential open questions in modeling the non-isothermal transformation and phase transformations under stress. In [WBB07] one can find a good description of a phenomenological model for phase transformations, but there are a lot of proposals for modifications and generalizations of phenomenological models for phase transformations, cf. e.g. [LMDD85, Vis87, FBTO94, Höm95, MS02, WBS03, AGC04, BHSW04]. In this section, (6) is specialized in order to obtain applicable models for phase transformations for multi-phase simultaneous and consecutive reactions. In the context of macroscopic modeling, we consider steel as a coexisting mixture of m ($m\geq 2$) phases (or constituents), which differ in their micro-structure and have different material parameters. These phases are assumed to be continuously distributed in the model, so that the steel appears as a co-existing mixture of its phases (or components), while diffusion processes (of the phases) are neglected, i.e. they stay at their original places of formation. Moreover, we do not consider carbon diffusion, cf. [WABM06].

The considerations below are not only valid for phase transformations in steel, but also for general (chemical or other) reactions in coexisting mixtures without diffusion of the constituents. The following general model for phase transformations in steel is proposed in [WBB07]. The change of p_i in favor of p_j can be described by the transformation law

$$\frac{\partial p_i}{\partial t} = -\sum_{j=1}^{m} a_{ij} H(p_i) H(\bar{p}_{ij} - p_j) G_{ij} + \sum_{j=1}^{m} a_{ji} H(p_j) H(\bar{p}_{ji} - p_i) G_{ji}, \qquad i = 1, \dots, m. \tag{38}$$

where H – Heaviside function, $\bar{p}_{ij}$ – the equilibrium fraction (maximal possible fraction) $\bar{p}_i$ of the ith phase ($\bar{p}_{ij} = 0$ if the phase transformation does not occur), G_{ij} a switch function, taking into account that the transformation of the ith phase into the jth phase (for $i \neq j$, $i, j = 1, \dots, m$, abbr.: $i \to j$) takes place during a defined temperature interval and $-a_{ij}$ – transformation rate for the transformation $i \to j$. We specify the a_{ij}:

$$a_{ij} := (e_{ij}(\theta, \boldsymbol{\xi}) + p_j)^{r_{ij}(\theta,\boldsymbol{\xi})} \, (\bar{p}_{ij} - p_j)^{s_{ij}(\theta,\boldsymbol{\xi})} g_{ij}(\theta, \boldsymbol{\xi}) h_{ij} \left(\frac{\partial \theta}{\partial t} \right) \quad \text{for} \quad i, j = 1, \dots, m. \tag{39}$$

The parameters e_{ij}, r_{ij}, s_{ij} and g_{ij} have to fulfill $e_{ii} = r_{ii} = s_{ii} = g_{ii} = 0$ for $i = i, \dots, m$ and

$$e_{ij} \geq 0, \qquad r_{ij} \geq 0, \qquad s_{ij} \geq 0, \qquad g_{ij} \geq 0, \qquad h_{ij} \geq 0 \qquad \text{f.a. admissible arguments.}$$

Remark 4 (Leblond-Devaux proposal). A simple specialization of (38) consists of

$$\frac{\partial p_i}{\partial t} = -\mu_{ij} p_i, \tag{40}$$

where the non-negative μ_{ij} may depend on the same arguments as a_{ij} in (39). This means that the decomposition rate of i into j is proportional to the fraction of i available for decomposition. In case of only two present phases this leads to

$$\frac{\partial p_1}{\partial t} = -\mu_{12} p_1, \qquad p_1(0) = p_0 \qquad \text{and} \qquad \frac{\partial p_2}{\partial t} = \mu_{12} \left(\bar{p}_{12} - p_2 \right), \qquad p_2(0) = 0 \tag{41}$$

for the forming phase ($\bar{p}_{12} = 1$), which is a special case of the Leblond-Devaux proposal. Leblond and Devaux suggested applying the linear approach to martensitic transformation as well. Due to Koistinen and Marburger (cf. e.g. [WBDH08] and generalizations of (42) in [WFL07]), the martensite fraction forming from a given (austenite) fraction p_1 at the temperature θ less than the martensite start temperature θ_{ms} reads as

$$\bar{p}_{12}(\theta) = p_1 \left(t_{ms} \right) \left(1 - \exp \left(-\frac{\theta_{ms} - \theta}{\theta_{m0}} \right) \right). \tag{42}$$

2.11 Equivalent formulation of TRIP

Due (8) and (11) the following relations hold:

$$\boldsymbol{\sigma}^* = 2\mu \, \boldsymbol{\varepsilon}^*_{te} = 2\mu \left(\boldsymbol{\varepsilon}^*(\mathbf{u}) - \boldsymbol{\varepsilon}_{trip} - \boldsymbol{\varepsilon}_{cp} \right) \qquad \text{and} \qquad \operatorname{tr}(\boldsymbol{\sigma}) = 2\mu \operatorname{tr}(\boldsymbol{\varepsilon}(\mathbf{u})) = 2\mu \operatorname{div}(\mathbf{u}). \tag{43}$$

Now, the problem (18), $(32)_1$ can be formulated as an equivalent initial value problem:

$$\boldsymbol{\varepsilon}'_{trip}(t) = b(t) \big(2\mu \, \boldsymbol{\varepsilon}^*(\mathbf{u}(t)) - 2\mu \, \boldsymbol{\varepsilon}_{cp}(t) - \mathbf{X}^*_{trip} \big) - 2\mu \, b(t) \boldsymbol{\varepsilon}_{trip}(t), \qquad t \in]0, T[\tag{44}$$

$$\boldsymbol{\varepsilon}_{trip}(0) = \mathbf{0} \tag{45}$$

where b is defined as in (19) and $\mathbf{X}^*_{trip}$ is the solution of (26). Therefore, the solution reads as

$$\boldsymbol{\varepsilon}_{trip}(t) = \int_0^t b(s) \exp \left(-\int_s^t 2\mu \, b(\tau) \, \mathrm{d}\tau \right) \big(2\mu \, \boldsymbol{\varepsilon}^*(\mathbf{u}(s)) - 2\mu \, \boldsymbol{\varepsilon}_{cp}(s) - \mathbf{X}^*_{trip} \big) \, \mathrm{d}s \tag{46}$$

for $t \in [0, T[$.

2.12 Equivalent formulation of plasticity

For further mathematical investigation it is convenient to reformulate the described model, using a variational inequality (or rather a differential inclusion) in order to characterize the plastic deformation. The following (original) problem is to find the strain $\boldsymbol{\varepsilon}_{cp} : \Omega \times [0,T[\to \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ with $\mathrm{tr}(\boldsymbol{\varepsilon}_{cp}) = 0$, s.t.

$$\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t}(\mathbf{x},t) = \Lambda \left(\boldsymbol{\sigma}^*(\mathbf{x},t) - \mathbf{X}^*_{cp}(\mathbf{x},t)\right), \qquad (\mathbf{x},t) \in \Omega\times]0,T[, \tag{47}$$

$$\boldsymbol{\varepsilon}_{cp}(\mathbf{x},0) = \mathbf{0}, \qquad \mathbf{x} \in \Omega, \tag{48}$$

where the plastic multiplier Λ has to fulfill (16) – (17) f.a. $\boldsymbol{\sigma} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ with $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) \leq 0$. The plastic multiplier can also be expressed as $\Lambda = \frac{3}{2(R_0+R)} \frac{\partial s_{cp}}{\partial t}$, cf. [WBMS11]. Taking (47), (16) – (17) and the yield function (14) into account, (47) can be reformulated as

$$\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} = \frac{2}{3}\,\Lambda(R_0+R)\,\frac{\partial F}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) = \tilde{\Lambda}\,\frac{\partial F}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) \tag{49}$$

with a new multiplier $\tilde{\Lambda}$. This reformulation is often called 'normality rule', cf. [Mau92, Lub06]. We define $F : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ via (14) for given $\mathbf{X}_{cp}$ and for given constants $R_0, R \in \mathbb{R}^+$. The set of all admissible $\boldsymbol{\sigma}$ is convex (cf. [HR99]). We define

$$\begin{aligned} \mathbf{K}_F &:= \left\{\boldsymbol{\tau} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}, \mathrm{tr}(\boldsymbol{\tau}) = 0 : F(\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R) \leq 0\right\}, \\ \mathbf{K} &:= \left\{\boldsymbol{\tau} \in [L^2(\Omega)]^9 : \boldsymbol{\tau}(\mathbf{x}) \in \mathbf{K}_F \text{ f.a.a. } \mathbf{x} \in \Omega\right\}. \end{aligned} \tag{50}$$

Remark 5 (Time- or parameter-dependent $\mathbf{K}$). Due to the general time-dependence of R_0 and R, the set of admissible stresses varies in time, when considering a time-dependent process (cf. e.g. [HR99, HWR05, WBH08]). In [Mac92, CR06, BFM11] the yield function depends explicitly on the temperature. Therefore one defines F via

$$\begin{aligned} F(\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R; \theta, t) &:= \sqrt{\frac{3}{2}\left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right) : \left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right)} - \left(R_0 + R(\theta,t)\right), \\ \mathbf{K}_F(\theta,t) &:= \left\{\boldsymbol{\tau} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}},\, \mathrm{tr}(\boldsymbol{\tau}) = 0 : F(\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R; \theta, t) \leq 0\right\}, \\ \mathbf{K}(\theta,t) &:= \left\{\boldsymbol{\tau} \in [L^2(\Omega)]^9 : \boldsymbol{\tau}(\mathbf{x}) \in \mathbf{K}_F(\theta,t) \text{ f.a.a. } \mathbf{x} \in \Omega\right\}. \end{aligned} \tag{51}$$

In general, the function R is not monotone and therefore, the set of space- and time-dependent functions generated by $\mathbf{K}$ (i.e. all L^2-functions with values in $\mathbf{K}$ f.a.a. $t \in [0,T[$) is in general not convex.

The constraint in (47) – (48) resp. (16) – (17) is non-linear. An adequate tool for dealing with non-linear constraints for equations is a variational inequality (cf. e.g. [HR99]). Based on the identity $\mathbf{A}^* : \mathbf{B}^* = \mathbf{A}^* : \mathbf{B} = \mathbf{A} : \mathbf{B} - \frac{1}{3}\mathrm{tr}(\mathbf{A})\mathrm{tr}(\mathbf{B})$ for $\mathbf{A}, \mathbf{B} \in \mathbb{R}^9$, the relations (47) – (48), (17) and (14) are equivalent to the variational inequality

$$\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} : \left(\boldsymbol{\tau} - \boldsymbol{\sigma}\right) \leq 0 \qquad \text{in} \qquad \Omega\times]0,T[\tag{52}$$

f.a. $\boldsymbol{\tau} \in \mathbb{R}^9$ with $\boldsymbol{\tau} = \boldsymbol{\tau}^T$ and $F(\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R) \leq 0$, where $\boldsymbol{\sigma}$ has to fulfill (14).

Lemma 3. *The set* $\mathbf{K}$ *is nonempty and convex.*

Proof. Since $R_0 > 0$ and $R \geq 0$, one concludes that $\mathbf{0} \in \mathbf{K}_F$. Hence, $\mathbf{K}$ is nonempty. Furthermore, let $\boldsymbol{\sigma}, \boldsymbol{\tau} \in \mathbf{K}$ and $\lambda \in [0,1]$. Obviously, $\mathrm{tr}(\lambda\boldsymbol{\sigma} + (1-\lambda)\boldsymbol{\tau}) = 0$ for $\mathrm{tr}(\boldsymbol{\sigma}) = \mathrm{tr}(\boldsymbol{\tau}) = 0$ and $\lambda\boldsymbol{\sigma} + (1-\lambda)\boldsymbol{\tau} = (\lambda\boldsymbol{\sigma} + (1-\lambda)\boldsymbol{\tau})^T$ for $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$ and $\boldsymbol{\tau} = \boldsymbol{\tau}^T$. Moreover, the convexity of the function F completes the proof. □

Theorem 1 (Main result: Equivalent formulation of plasticity)**.** *For fixed* $\mathbf{X}_{cp}$*,* R_0 *and* R *let* $F = F(\boldsymbol{\sigma})$ *be a convex function* $\mathbb{R}^{3\times3} \to \mathbb{R}$*, which is differentiable in* $\mathbb{R}^{3\times3} \setminus \{\mathbf{0}\}$ *and fulfills* $F(\mathbf{0}) < 0$*. Moreover, let* $\frac{\partial F}{\partial \boldsymbol{\sigma}}(\boldsymbol{\tau}) \neq 0$ *f.a.* $\boldsymbol{\tau} \in \mathbb{R}^{3\times3}$ *with* $\boldsymbol{\tau} = \boldsymbol{\tau}^T$ *and* $F(\boldsymbol{\tau}) = 0$*. In addition, let* $\boldsymbol{\sigma}^*(0) \in \mathbf{K}$*. Assume* (14) *and* (50) *are given. Then, the normality rule* (49) *and the variational inequality* (52) *are equivalent.*

Proof. The proof of the main theorem is divided into two parts:

1. The normality rule (49) implies the variational inequality (52). Equation (52) is obviously fulfilled for $\Lambda = 0$. For $\Lambda > 0$ it follows $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) = 0$ and therefore $\frac{\partial F}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) = \frac{3\left(\boldsymbol{\sigma}^* - \mathbf{X}^*_{cp}\right)}{2(R_0+R)} \neq 0$. Thus, $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t}$ and $\frac{\partial F}{\partial \boldsymbol{\sigma}}$ are parallel and have the same orientation. Because of the convexity of $\mathbf{K}_F$, it follows $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} : \left(\boldsymbol{\tau}^* - \boldsymbol{\sigma}^*\right) \leq 0$ in $\Omega\times]0,T[$ f.a. $\boldsymbol{\tau} \in \mathbb{R}^{3\times3}$ with $\boldsymbol{\tau} = \boldsymbol{\tau}^T$ and $F(\boldsymbol{\tau}) \leq 0$, which is equivalent to (52).

2. On the other hand, the variational inequality (52) implies the normality rule (49). If $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) < 0$, then it follows $\boldsymbol{\sigma}^* \in \mathrm{Int}(\mathbf{K}_F)$ and (52) implies $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} = 0 = \tilde{\Lambda}\, \frac{\partial F}{\partial \boldsymbol{\sigma}}$ with $\tilde{\Lambda} = 0$, compatible with (17). Let $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) = 0$. Hence, $\boldsymbol{\sigma}^* \in \partial\mathbf{K}_F$. Putting $\boldsymbol{\tau} = \boldsymbol{\sigma} + \mathbf{v}$ with $\mathbf{v} : \frac{\partial F}{\partial \boldsymbol{\sigma}} \leq 0$ s.t. $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) \leq 0$ in (52) we have $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} : \mathbf{v} \leq 0$ f.a. $\mathbf{v}$ with $\mathbf{v} : \frac{\partial F}{\partial \boldsymbol{\sigma}} \leq 0$. Therefore, $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t}$ and $\frac{\partial F}{\partial \boldsymbol{\sigma}}$ are parallel and have the same orientation. Thus, (49) is valid.

□

As a result of the re-formulation via a variational inequality, the plastic multiplier is excluded. If $\boldsymbol{\sigma}$ fulfills (14) with a strong inequality, than (52) leads to $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} = \mathbf{0}$, i.e. there is no plastic deformation. If no plastic deformation occurs, the model of 'thermo-elasticity with phase transitions and TRIP without classical plasticity' (cf. e.g. [Boe07, Ker11, Boe12b]) is directly applicable. The (mathematical) problem of perfect plasticity is e.g. discussed in [ER04].

In order to prepare further mathematical investigations, one can reformulate the variational inequality as a differential inclusion. This approach is also used in [ASS01] for instance. There are at least two possibilities when dealing with the variational inequality (52). Either one can exclude $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t}$ via $\boldsymbol{\sigma}^*$ or vice versa.

1. Eliminating $\boldsymbol{\sigma}$ in the variational inequality: Using (8) and (43) one rewrites (52). This leads to a new variational inequality for $\boldsymbol{\varepsilon}^*_{te}$. For convenience we denote $\boldsymbol{\eta} := \boldsymbol{\varepsilon}^*_{te}$. Thus, we look for a function $\boldsymbol{\eta} : \Omega \times [0,T[\to \mathbb{R}^9$, s.t.

$$\begin{aligned} &\mathrm{tr}(\boldsymbol{\eta}) = 0, \quad F(2\mu\,\boldsymbol{\eta}, \mathbf{X}_{cp}, R_0, R) \leq 0 \\ &\frac{\partial \boldsymbol{\eta}}{\partial t} : \left(\boldsymbol{\tau} - \boldsymbol{\eta}\right) \geq \left(\varepsilon^*\left(\frac{\partial \mathbf{u}}{\partial t}\right) - \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t}\right) : \left(\boldsymbol{\tau} - \boldsymbol{\eta}\right) \end{aligned} \tag{53}$$

   f.a. $\boldsymbol{\tau} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}$ with $\boldsymbol{\tau} = \boldsymbol{\tau}^T$, $\mathrm{tr}(\boldsymbol{\tau}) = 0$ and $F(2\mu\,\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R) \leq 0$. Based on (8) and (43), $\boldsymbol{\varepsilon}_{te}$ is given by $\boldsymbol{\varepsilon}_{te} = \boldsymbol{\eta} + \frac{1}{3}\mathrm{tr}(\boldsymbol{\varepsilon}(\mathbf{u}))\mathrm{Id}$. Moreover, it holds

$$\boldsymbol{\varepsilon}_{cp} = \boldsymbol{\varepsilon}^*(\mathbf{u}) - \boldsymbol{\varepsilon}_{trip} - \boldsymbol{\eta} \qquad \text{and} \qquad \frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} = \boldsymbol{\varepsilon}^*\left(\frac{\partial \mathbf{u}}{\partial t}\right) - \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} - \frac{\partial \boldsymbol{\eta}}{\partial t}. \tag{54}$$

2. Eliminating $\boldsymbol{\varepsilon}_{cp}$ in the variational inequality: This approach is similar to the idea in [DL76]. In this particular situation one gets from (8) and (43) (for constant μ)

$$\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} = -\frac{1}{2\mu}\left(\frac{\partial \boldsymbol{\sigma}^*}{\partial t}\right) + \boldsymbol{\varepsilon}^*\left(\frac{\partial \mathbf{u}}{\partial t}\right) - \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} \tag{55}$$

Therefore, the inequality (52) reads as

$$\frac{1}{2\mu}\left(\frac{\partial \boldsymbol{\sigma}^*}{\partial t}\right) : \big(\boldsymbol{\tau}-\boldsymbol{\sigma}\big) - \boldsymbol{\varepsilon}^*\left(\frac{\partial \mathbf{u}}{\partial t}\right) : \big(\boldsymbol{\tau}-\boldsymbol{\sigma}\big) + \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t} : \big(\boldsymbol{\tau}-\boldsymbol{\sigma}\big) \geq 0 \tag{56}$$

f.a. $\boldsymbol{\tau} \in \mathbb{R}^9$ with $\boldsymbol{\tau} = \boldsymbol{\tau}^T$ and $F(\boldsymbol{\tau}, \mathbf{X}_{cp}, R_0, R) \leq 0$, where $\boldsymbol{\sigma}$ has to be symmetric and to fulfill the constraint $F(\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) \leq 0$. Note, that only in the special case without influence of $\boldsymbol{\varepsilon}_{cp}$ on $\boldsymbol{\varepsilon}_{trip}$, one can exclude $\frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t}$ from (56) without any return of $\boldsymbol{\varepsilon}_{cp}$ after substituting $\frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t}$ in (56). But, in the case of hardening, one re-imports $\boldsymbol{\varepsilon}_{cp}$ via the back-stress relations. That is why this approach seems to be inconvenient.

Remark 6 (Definition of a weak formulation of the variational inequality). The weak formulation of the variational inequality reads as: Find $\boldsymbol{\eta} \in W^{1,2}(0,T;[L^2(\Omega)]^9)$ with $\boldsymbol{\eta}(t) \in \mathbf{K}$ f.a.a. $t \in]0,T[$ s.t.

$$\int_\Omega \frac{\partial \boldsymbol{\eta}}{\partial t}(t) : \big(\boldsymbol{\sigma} - \boldsymbol{\eta}(t)\big)\,\mathrm{d}\mathbf{x} \geq \int_\Omega \left(\boldsymbol{\varepsilon}^*\left(\frac{\partial \mathbf{u}}{\partial t}(t)\right) - \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t}\right) : \big(\boldsymbol{\sigma} - \boldsymbol{\eta}(t)\big)\,\mathrm{d}\mathbf{x} \tag{57}$$

f.a. $\boldsymbol{\sigma} \in [L^2(\Omega)]^9$ with $\mathrm{tr}(\boldsymbol{\sigma}) = 0$, $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$ and $F(2\mu\,\boldsymbol{\sigma}, \mathbf{X}_{cp}, R_0, R) \leq 0$. The idea to tackle this problem is to use solution methods for solving parabolic variational inequalities, cf. e.g. [Nau84]. Let $\chi_{\mathbf{K}} : [L^2(\Omega)]^9 \to \mathbb{R} \cup \{+\infty\}$ be the indicator function on $\mathbf{K}$, i.e. $\chi_{\mathbf{K}}(\mathbf{u}) = 0$ if $\mathbf{u} \in \mathbf{K}$ and $\chi_{\mathbf{K}}(\mathbf{u}) = +\infty$ if $\mathbf{u} \notin \mathbf{K}$. The variational inequality (52) can be rewritten as a differential inclusion $\frac{\partial \boldsymbol{\varepsilon}_{cp}}{\partial t} \in \partial\chi_{\mathbf{K}}(\boldsymbol{\sigma})$, cf. [Zei85] for details. Using (56) and this differential inclusion (2μ is a positive multiplier), (47) – (48) and (17) are equivalent to find the stress deviator $\boldsymbol{\sigma}^* : \Omega \times [0,T[\to \mathbb{R}^{3\times 3}_{\mathrm{sym}}$, s.t.

$$\frac{\partial \boldsymbol{\sigma}^*}{\partial t}(t) + \partial\chi_{\mathbf{K}}(\boldsymbol{\sigma}^*(t)) \ni 2\mu\left(\boldsymbol{\varepsilon}^*\left(\frac{\partial \mathbf{u}}{\partial t}(t)\right) - \frac{\partial \boldsymbol{\varepsilon}_{trip}}{\partial t}(t)\right) \text{ f.a.a. } t \in]0,T[\tag{58}$$

$$\boldsymbol{\sigma}^*(0) = \boldsymbol{\sigma}_0^* := 2\mu\boldsymbol{\varepsilon}^*(\mathbf{u}_0). \tag{59}$$

This leads to the theory of differential inclusions and/or evolution equations of subgradient type, cf. e.g. [Wat73, Ken75, Bar76, Ken77, Pap90, Ahm92, Pap95].

3 Numerical Examples

In this section some numerical simulations with realistic material data are presented to demonstrate the distortion effect of metallurgical phase transitions in the context of small deformations (for large deformations cf. e.g. [MWSB12]).

3.1 Description of the setting

In order to show phase induced thermo-mechanical effects, we implement the presented model in COMSOL Multiphysics®, cf. e.g. [Zim06] and simulate the Jominy-End-Quench-Test. The Jominy-End-Quench-Test is a standard test to determine the hardenability of steels. Moreover, it is useful for simulation testing. Here, it is used to test the thermo-mechanical model with phase transitions and TRIP and to illustrate the results (cf. e.g. [Höm96, Höm97, HLHM04, NKSF05]). The heat treatment process for most steels involves heating the alloy until austenite forms, then cooling it so rapidly that the transformation into martensite occurs almost immediately. The presence of two (or more) phases leads to plastic deformation due to the volume differences in the phases. There are situations, where classical plasticity is negligible and TRIP is the decisive factor, cf. e.g. [WBS09]. For a sufficiently high cooling rate, i.e. close to the quenched boundary

parts, where the temperature descends very quickly, austenite is transformed into the hard phase martensite, whereas a slower temperature change, e.g. in the interior of a big workpiece, causes usually softer phases like ferrite, pearlite or bainite to grow. A correlation of the temperature change and the phase transformation can be obtained from the time-temperature-transformation diagram. Due to the fact that the product phases (e.g. pearlite and martensite) have different thermal expansion (different (lower) densities in comparison with austenite), their formation influences the deformation of the workpiece.
In order to avoid technicalities, we consider only the cooling of a steel specimen from high temperature phase austenite with fraction p_A to one product phase (martensite) with phase fraction p_M. This applies for instance in martensitic hardening of eutectoid carbon steel.

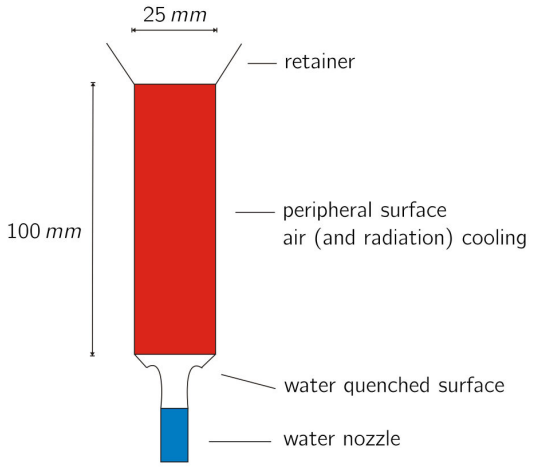
3.2 Literature review: Numerical simulation for thermo-mechanical models

In this section some references connected with the problem of interest are collected. For the implementation of algorithms in elasto-plasticity there exist some literature, cf. e.g. [SH98, Mah99]. Simulation of steel quenching process using a multi-phase transformation model is discussed in [RFF01] and a finite element analysis of coupled thermo-inelastic problem with phase transformation is given in [IW82]. A adaptive finite element simulation of a model for TRIP in steel are presented in [SWB03, SSM$^+$06].
Adaptive finite element methods with ALBERTA (cf. e.g. [SS05]) are investigated in the work of [Suh10] for numerical simulations, concerning analysis of distortion for workpieces with and without phase changes. Throughout the thesis a mathematical model for steel quenching is introduced, a numerical scheme is developed and in simulations for conical rings it is shown that the model is in accordance with the reality. Numerical treatment of models including phase transitions, transformation-induced and classical plasticity is rarely found in the literature so far. A semi-implicit numerical scheme is derived for both models. In order to identify the model parameters for the more complex hardening model an optimization procedure is developed.
The papers [CHK07, HK09] and the thesis [Ker11] are concerned with thermo-mechanical modeling and numerical treatment of metallurgical phase transitions in steel during quenching. Their quasi-static model is similar to the presented model without the inertia term, without classical plasticity and with pure zero boundary conditions, but it still captures the effect of TRIP. The implementation is done within the finite element framework provided by the WIAS-toolbox p∂elib (cf. [FKL98]) using a semi-implicit approach for time-stepping. The resulting code is applied to investigate the effect of inhomogeneous quenching strategies of roller bearing rings. Moreover, a strategy for distortion compensation by means of a gradient method obtained from optimal control theory is introduced.
A semi-implicit algorithm (predictor-corrector approach based on [SH98]) for incorporating the interaction between (classical) plasticity and TRIP in steel is developed in [WBMS11]. Contrary to the usual elasto-plasticity, the underlying model of material behavior of steel is far more complex. A special application of this approach for small and large deformations in SIMULIA Abaqus FEA® is provided in [MWSB12].

3.3 Numerical Implementation

The objective is to simulate the quenching process of a steel specimen. We consider a two-dimensional cross-section (due to rotation symmetry) of a steel cylinder made of the eutectoid carbon steel 100Cr6 of dimension 100mm $\times$ 25mm and infer specific cooling to obtain corresponding phase distribution. We assume the specimen to be the closure of a Lipschitz domain Ω. As mentioned above, we consider only the cooling and not the preliminary heating process.

(a) Photo from [Lie05].



(b) Scheme from [HLHM04].

Figure 1: Jominy-End-Quench-Test.

Therefore we assume a sufficiently high, homogeneous initial temperature and complete austenitization. Moreover, we distinguish between the reference and the initial geometry. Using the initial value $\mathbf{u}_0(\mathbf{x}) = \alpha_A\,(\theta_0 - \theta_{\text{air}})\,\mathbf{x}$ for the displacement, we take this initial thermal expansion into account. Creep effects and TRIP during the austenitization are not considered.
In the model the workpiece is quenched at the bottom (this corresponds to nonzero Robin boundary conditions) and it is assumed to be fixed on top. Furthermore, we suppose that the whole upper boundary part may only shrink horizontally. Moreover, it is assumed to be thermally insulated. The left and the right edges fulfill Robin boundary conditions as well, but the cooling rate is considerably lower. The following initial conditions f.a. $\mathbf{x}$ in Ω:

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \qquad \mathbf{u}'(\mathbf{x},0) = \mathbf{0}, \qquad \theta(\mathbf{x},0) = \theta_0, \tag{60}$$

$$\mathbf{p}(\mathbf{x},0) = \mathbf{p}_0(\mathbf{x}), \qquad \boldsymbol{\varepsilon}_{trip}(\mathbf{x},0) = \mathbf{0}, \qquad \boldsymbol{\varepsilon}_{cp}(\mathbf{x},0) = \mathbf{0} \tag{61}$$

and the mixed boundary conditions for $\mathbf{u}$ and for θ

$$\boldsymbol{\sigma}\cdot\boldsymbol{\nu}_{\Gamma_{left}} = \mathbf{0} \quad \text{and} \quad -\lambda_\theta \nabla\theta\cdot\boldsymbol{\nu}_{\Gamma_{left}} = \delta_{\text{air}}\big(\theta - \theta_{\text{air}}\big) \quad \text{on} \quad \Gamma_{left} \tag{62}$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{\nu}_{\Gamma_{bottom}} = \mathbf{0} \quad \text{and} \quad -\lambda_\theta \nabla\theta\cdot\boldsymbol{\nu}_{\Gamma_{bottom}} = \delta_{\text{water}}\big(\theta - \theta_{\text{water}}\big) \quad \text{on} \quad \Gamma_{bottom} \tag{63}$$

$$\mathbf{u} = \mathbf{0} \quad \text{and} \quad -\lambda_\theta \nabla\theta\cdot\boldsymbol{\nu}_{\Gamma_{top}} = 0 \quad \text{on} \quad \Gamma_{top} \tag{64}$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{\nu}_{\Gamma_{right}} = \mathbf{0} \quad \text{and} \quad -\lambda_\theta \nabla\theta\cdot\boldsymbol{\nu}_{\Gamma_{right}} = \delta_{\text{air}}\big(\theta - \theta_{\text{air}}\big) \quad \text{on} \quad \Gamma_{right} \tag{65}$$

are included. We consider only two phases, a parent phase, austenite and a forming phase, martensite (cf. [DSB83, GZWD00, GTJS01, BHL$^+$06]). This behavior is given by the Leblond-Devaux model, cf. rem. 4:

$$p_A'(\mathbf{x},t) = -p_M'(\mathbf{x},t), \qquad p_A(\mathbf{x},0) = 1,$$
$$p_M'(\mathbf{x},t) = \mu\left(\bar{p}_M(\theta(\mathbf{x},t)) - p_M(\mathbf{x},t)\right), \qquad p_M(\mathbf{x},0) = 0$$

for $\mathbf{x}\in\Omega$, where $p_1 = p_A$ – austinite phase fraction, $p_2 = p_M$ – martensite phase fraction, $\mathbf{p}_0 = (p_A(0), p_M(0))^T$, θ – given temperature and $\bar{p}_M$ represents the maximal martensitic phase fraction that can be attained. We use the following Koistinen-Marburger ansatz (cf. (42)):

$$\bar{p}_M(\theta) = 1 - \exp\left(\frac{\theta - \theta_{ms}}{\theta_{m0}}\right) \text{ for } \theta\in[\theta_{mf},\theta_{ms}] \text{ and } \bar{p}_M(\theta) = 0 \text{ for } \theta\in[\theta_{ms},\theta_0].$$

Moreover, we assume $\mathbf{f} = (0, \rho_0 g)^T$ and $r = 0$. Furthermore, we assume a linear mixture rule between both phases f.a. material parameters, i.e. the value of a material parameter is calculated by $\pi = \pi_A p_A + \pi_M p_M$, where p_A, p_M are the austenitic and martensitic phase fraction and π_A, π_M are the corresponding material parameters, which are taken from data table 1 for eutectoid carbon steel 100Cr6. The parameter μ is calculated via the measured data from dilatometer or Gleeble™ experiments (cf. [HTY09, WBLS05, WBS04]).

	Property	**Unit**	**Phase**	
			Austenite	*Martensite*
λ	Thermal Conductivity	$\frac{\mathrm{W}}{\mathrm{mm}\,^\circ\mathrm{C}}$	0.02012	0.04273
c_e	Specific Heat Capacity	$\frac{\mathrm{J}}{\mathrm{kg}\,^\circ\mathrm{C}}$	560.7	501.3
ρ	Density	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	7798	7741
E	Elastic Modulus	MPa	170665	204671
ν	Poisson Ratio	–	0.3318	0.3556
R_0	Initial Yield Strength	MPa	173.3	1278.4
α	Thermal Expansion Coefficient	$\frac{10^{-6}}{^\circ\mathrm{C}}$	23.8	10.9
ρ_0	Initial Density	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	8041.4	
ΔH_{a-m}	Transformation Enthalpy	$\frac{\mathrm{J}}{\mathrm{kg}}$	78520	
θ_0	Initial Temperature	°C	850	
θ_{air}	Air Temperature	°C	22	
θ_{water}	Water Temperature	°C	18	
θ_{ms}	Martensite Start Temperature	°C	211	
θ_{mf}	Martensite Finish Temperature	°C	−174	
θ_{m0}	Koistinen-Marburger Temperature	°C	93.4	
δ_{air}	Heat Transfer Coefficient (Air)	$\frac{\mathrm{W}}{\mathrm{m}^2\mathrm{K}}$	150	
δ_{water}	Heat Transfer Coefficient (Water)	$\frac{\mathrm{W}}{\mathrm{m}^2\mathrm{K}}$	3200	
κ	Greenwood-Johnson Parameter	$\frac{1}{\mathrm{MPa}}$	$7 \cdot 10^{-5}$	
μ	Leblond-Devaux Parameter	–	5.95	
g	Gravitational Acceleration	$\frac{\mathrm{m}}{\mathrm{s}^2}$	9.81	

Table 1: Average material properties and their units and dimensions, cf. [ADF+08a, ADF+08b, ŞLH+09, Suh10].

3.4 Simulation results and conclusion

Fig. 2 and fig. 3 demonstrate the process at a sample of time steps. The workpiece is shown at times $t = 0$s, 0.2s, 2s, 5s, 10s, 20s, 30s, 40s, 50s and 100s. Colors indicate the temperature in fig. 2 and the martensite fraction in fig. 3, where blue corresponds to low values and red to high values of temperature or phase fraction. The background rectangle gives the initial geometry. The deformation of the workpiece is magnified by a factor of 10.

At time $t = 0$s, the initially rectangular specimen is completely heated and stress-free, cf. fig. 2a and fig. 3a. A strong cooling is applied to the bottom, the left and right side is cooled moderately and there is no heat transfer at the top of the sample. When quenching sets in, we can observe the shrinking of the quenched area in fig. 2c and fig. 3c. Because of the strong cooling, the sample contracts more at the left and right bottom vertexes in vertical direction. After a while, thermoelastic effects may be observed first, i.e. the shrinking due to classical thermo-elasticity can be observed. After some time, the austenite-martensite-transformation sets in (cf. fig. 2d and fig. 3d), beginning at the left and right bottom vertexes, where the temperature has already dropped below the martensite start temperature, i.e. the rapid cooling

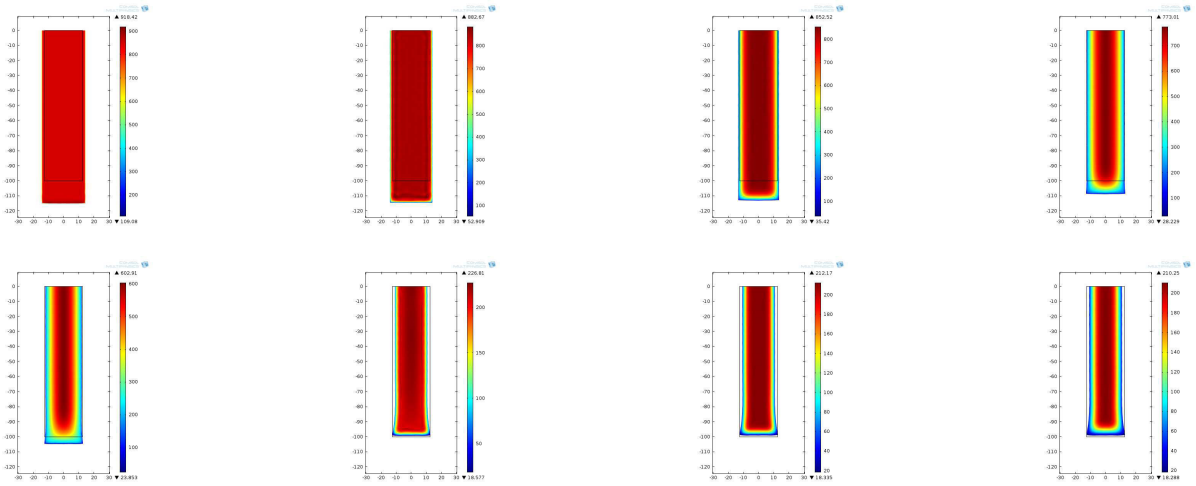


Figure 2: Surface plot: Temperature

effected the growth of martensite in the lower part of the specimen. Martensite has a lower density and thereby a larger volume and higher expansion than austenite. Therefore the sample starts to expand in this area. Thus, the transformation pushes the material outward, which causes a huge bulge in the specimen (cf. fig. 2e – g and fig. 3e – g) and remains until the heat treatment is completed, cf. fig. 2h and fig. 3h. This corresponds to the observed behavior in experiments, cf. [HLHM04, NKSF05] for instance.

Fig. 4 shows the influence of different effects of the fully coupled model. Fig. 4a corresponds with fig. 2h in order to compare the following different scenarios. Fig. 4b (without intrinsic dissipation), fig. 4c (without inertia term in the momentum balance) and fig. 4e (without TRIP) show a similar result. The importance of considering the phase transitions and the plastic effects is shown in fig. 4d (without classical plasticity), fig. 4f (without plasticity) and fig. 4g (without phases), where the deviation from the fully coupled model in fig. 4a is very big. The simple thermo-elastic model shown in fig. 4h is even worse.

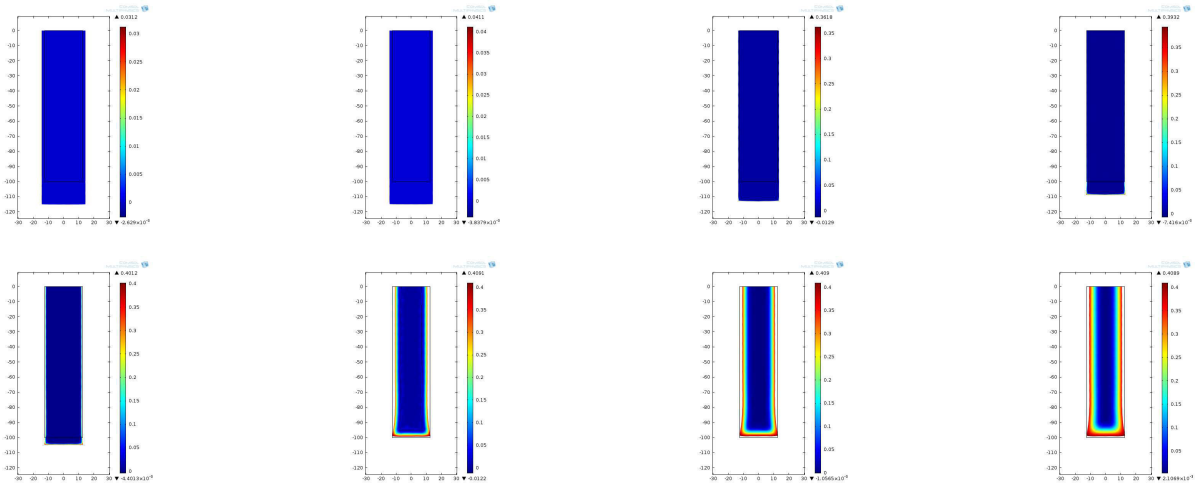


Figure 3: Surface plot: Martensitic phase fraction

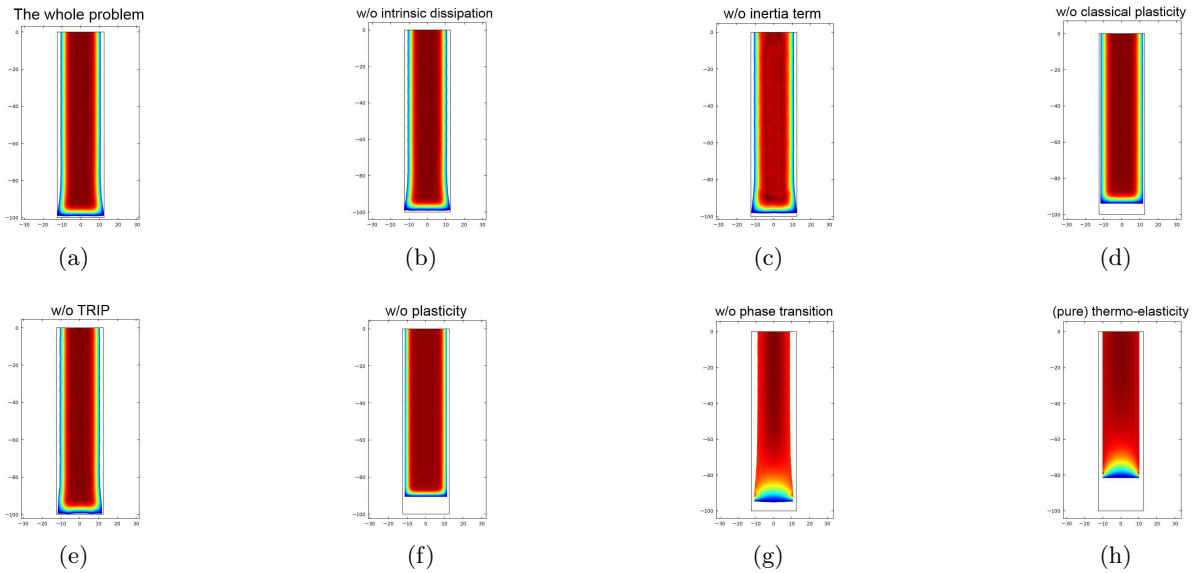


Figure 4: Surface plot: Temperature for different scenarios

4 Discussion and outlook

In this work we introduced and investigated a mathematical model for steel quenching.

Modeling: A further continuation at the level of mathematical modeling would be the connection of this problem with micro- and meso-investigations (cf. e.g. [Fis90, DSB95] for micro-models for TRIP), in particular of phase transformations, transformation-induced plastic behavior and the interaction with classical plasticity, which leads to the method of mathematical homogenization (cf. [OSY92, Vis06, Vis08, Sch09, SV10] for homogenization approaches).
Moreover, dimensional analysis could be helpful to reduce the number of key parameters in order to accomplish qualitative investigations or to prepare approximate calculations (cf. [WBF08]).
In order to investigate special heat treatment processes, like carbonization, the description of the carbon diffusion would be interesting (cf. ansatz in [WBM06, Hüß07]).
More complex phenomena, like additional inelastic dissipation or non-constant material parameters could be taken into account. The investigation of more general saturation functions (cf. rem. 1) or more general evolution equations for the phase fractions could also be discussed. Finally, in the context of heat treatment, (kinematic) hardening, creep (cf. [NA07, BWD$^+$11]) and damage (e.g. fatigue, ratcheting, friction (cf. [Ell97, ASS99, HSS01, LD05, Cha06, AMM07])) may be relevant and need to be investigated (cf. [WBBD12]). To describe phase transformations during the complete heating and cooling process cf. e.g. the ansatz in [SKHZ08]. Moreover, considering small and large deformations would be interesting as well.

Simulation: The numerical simulation should be extended in order to incorporate additional forming phases like ferrite and bainite. Moreover, the simulation of other geometries should be taken into account. Therefore, an complex implementation with real data and the comparison of the simulation results with experimental data could follow up this work as a larger project (cf. [Suh10, Ker11]).

Application: The effect of inhomogeneous quenching strategies could be investigated and the numerical computations should be compared with the experimental results in order to follow up

the work [CHK07, HK09, Ker11, Boe12a] to some extent. Therefore, a strategy for distortion compensation by means of a optimization method obtained from optimal control theory has to be introduced.
Possible extensions are also testing and evaluating models for phase transformations, TRIP and stress-dependent transformation behavior for under-eutectoid steels with different carbon content as well as the evaluation of relevant creep models based on measured data (cf. [BWD+11, WBBD12]).

In summary, the results give a theoretical basis for further mathematical investigation or the efficient implementation of numerical algorithms suitable for real-world applications.

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