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On a thermomechanical model of phase transitions in steel

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Abstract

We investigate a thermomechanical model of phase transitions in steel. The strain is assumed to be additively decomposed into an elastic and a thermal part as well as a contribution from transformation induced plasticity. The resulting model can be viewed as an extension of quasistatic linear thermoelasticity. We prove existence of a unique solution and conclude with some numerical simulations.

1 Introduction

Every heat treatment is accompanied by distortion, i.e. alterations in size and shape of the respective workpiece. In earlier investigations we have considered the relationship between phase transition kinetics and temperature evolution with respect to modelling and simulation [4, 5, 6] as well as with respect to process control [8, 9, 10].

To understand the distortion phenomena it is necessary to study the thermomechanical evolution of a workpiece subject to a heat treatment. A first step in this direction including a number of simplifications has been made in [7].

The goal of this paper is to derive and analyse a fairly complete thermomechanical phase transition model. In the next section we will derive the thermomechanical model. Even in the special case of materials without phase transitions the resulting nonlinear system seems to be new. In Section 3 we will prove the existence of a unique weak solution. To demonstrate the distortion effect of phase transitions the last section is devoted to presenting some numerical simulations.

There is a vast literature on the mathematical analysis of thermomechanical models. Besides classical works as the monograph [14] we would especially like to mention recent results on thermo-viscoelasticity and thermoplasticity [1].

2 The mathematical model

To avoid technicalities, in contrast to [7], we consider only the cooling of a steel specimen from high temperature phase austenite with phase fraction z_0 to two different product phases with fractions z_1 and z_2. This applies for instance to a plain carbon steel of eutectoid composition, where two phase transitions may occur: one from austenite to pearlite governed by carbon diffusion and another one from austenite to martensite. While the first one admits a growth of the product phase pearlite also in isothermal situations,

the latter one only admits a growth of the product phase martensite in the case of cooling. A simple rate law to describe the behaviour is given by

$$\dot{z}_1 = f_1(\theta, z, \sigma) = (1 - z_1 - z_2) g_{11}(\theta) g_{12}(\sigma) \tag{2.1a}$$

$$\dot{z}_2 = f_2(\theta, z, \sigma) = [\min\{\bar{m}(\theta), 1 - z_1\} - z_2]_+ g_{21}(\theta) g_{22}(\sigma) \tag{2.1b}$$

$$z(0) = 0\,. \tag{2.1c}$$

Here, z_1 and z_2 are the phase fractions of pearlite and martensite, respectively. The bracket $[x]_+$ denotes the positive part function $[x]_+ = \max\{x, 0\}$, $\bar{m}(\theta)$ is the fraction of martensite which can be attained at temperature θ. The term $\min\{\bar{m}(\theta), 1-z_1\}$ represents the maximal fraction that can be transformed to martensite.

The functions g_{12} and g_{22} describe the influence of stresses σ on the phase transition kinetics. It has been found experimentally [2] that the growth rate decreases with increasing hydrostatic pressure.

The displacement u (or velocity $v = u_t$, respectively), the stress σ and temperature θ are governed by the quasistatic momentum balance and the balance law of internal energy e, which we formulate in the undeformed domain assuming that only small deformations occur,

$$-\operatorname{div}\sigma = F \tag{2.2a}$$

$$\varrho e_t + \operatorname{div}\mu = \sigma : \varepsilon(v) + h\,. \tag{2.2b}$$

Here, ϱ is the mass density, F an external force, h a heat source, μ the heat flux, and

$$\varepsilon(v) = \frac{1}{2}\left(\mathcal{D}v + \mathcal{D}^T v\right) \tag{2.3}$$

the symmetric part of the strain rate tensor. The scalar product in $\mathbb{R}^{3,3}$ is denoted by ':' and the corresponding norm by $|.|$.

We employ the laws of Fourier and Hooke, respectively,

$$\mu = -k \operatorname{grad}\theta \tag{2.4}$$

$$\sigma = K\varepsilon^{el}\,, \tag{2.5}$$

with thermal conductivity k and the elastic strain ε^{el}. Moreover, K is the stiffness tensor, assumed to be isotropic, i.e.

$$K_{ijke} = \lambda\delta_{ij}\delta_{ke} + 2\mu\delta_{ik}\delta_{je} \tag{2.6}$$

with the Lamé coefficients λ and μ. We assume that the strain

$$\varepsilon(u) = \varepsilon^{el} + \varepsilon^{th} + \varepsilon^{trip} \tag{2.7}$$

can be decomposed additively into an elastic part ε^{el}, a thermal one ε^{th}, and one describing additional plastic effects caused by the phase transitions.

Figure 1 shows the result of a dilatometer cooling experiment, where temperature is plotted against length change of the specimen.

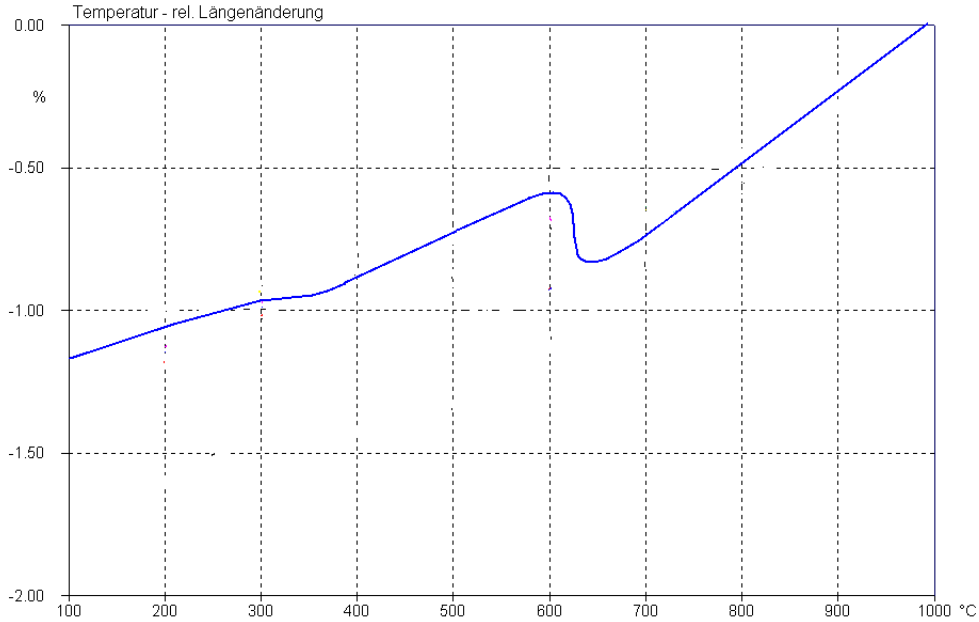


Figure 1: Dilatometer curve with 2 product phases (Courtesy of IEHK, Aachen).

The straight parts of the curve represent the thermal expansion in the different phases which is almost linear. Hence, an appropriate model for the thermal expansion in each phase is

$$\varepsilon_i^{th} = q_i(\theta - \theta_{ref}^i)$$

with a constant reference temperature θ_{ref}^i. The expansion coefficients q_0, q_1, q_2, correspond to austenite, pearlite and martensite, respectively. The overall strain is computed from the mixture ansatz

$$\varepsilon^{th} = z_1\varepsilon_1^{th} + z_2\varepsilon_2^{th} + (1 - z_1 - z_2)\varepsilon_0^{th}\,.$$

Without loss of generality, in the sequel we assume

$$\theta_{ref}^0 = \theta_{ref}^1 = \theta_{ref}^2 = 0\,.$$

Then we obtain

$$\varepsilon^{th} = q(z)\theta$$

where $q(z)$ is given by

$$q(z) = q_1 z_1 + q_2 z_2 + q_0(1 - z_1 - z_2)\,.$$

The fact that the product phases pearlite and martensite have different expansion coefficients leads to high internal stresses around phase boundaries. This is one of the main reasons for distortions, i.e. undesired alterations of workpiece size and shape, during heat treatments (see Section 5).

It is well-known that phase transition experiments with steel specimens under loading exhibit an additional irreversible deformation even when the equivalent stress corresponding to the load is far below the yield stress.

A standard model to describe the *transformation induced plasticity* contribution of the product phase z_i is given by the following formula

$$\varepsilon_{i,t}^{trip} = \lambda_{i1}(\theta)\,\frac{\partial \lambda_{i2}(z_i)}{\partial z_i}\,z_{i,t}S\,. \tag{2.8}$$

From this we can infer that indeed the flow as in standard plasticity is in direction of the deviator S, i.e. the trace free part of the stress tensor. It is volume preserving and grows proportionally to the growth rate $z_{i,t}$ of phase z_i. In [3] a review of various models for λ_{ij} can be found, as well as some micromechanical considerations to motivate the specific form as given in (2.8). In the sequel, we will write the *trip* contributions as

$$\varepsilon_t^{trip} = \gamma(\theta, z, z_t)S\,. \tag{2.9}$$

Now our goal is to derive a constitutive relation for the internal energy. To this end we introduce the *Helmholtz free energy* ψ and entropy s, related by the thermodynamic identity

$$e = \psi + \theta s\,, \tag{2.10}$$

and proceed in the spirit of [12, Section 2.4.2]. We assume the existence of a twice continuously differentiable material function $\hat{\psi}$ such that

$$\psi = \hat{\psi}(\varepsilon^{el}, \theta, z)\,, \tag{2.11}$$

where the phase fractions z_i turn up as internal variables.

Taking the derivative with respect to t in (2.11) we obtain

$$\psi_t = \frac{\partial \hat{\psi}}{\partial \varepsilon^{el}} : \varepsilon_t^{el} + \frac{\partial \hat{\psi}}{\partial \theta}\theta_t + \frac{\partial \hat{\psi}}{\partial z}\cdot z_t \tag{2.12}$$

where $'\cdot'$ denotes the scalar product in $\mathbb{R}^3$. A thermodynamically consistent model has to satisfy the Clausius-Duhem inequality, which in the case of small deformations reads as follows:

$$\sigma : \varepsilon(v) - \varrho(\psi_t + s\theta) - \frac{1}{\theta}\,q\cdot \operatorname{grad}\theta \geq 0\,. \tag{2.13}$$

Inserting (2.4), (2.7), and (2.12), we obtain

$$\begin{aligned}\left(\sigma - \varrho\,\frac{\partial \hat{\psi}}{\partial \varepsilon^{el}}\right) : \varepsilon_t^{el} - \varrho\left(s + \frac{\partial \hat{\psi}}{\partial \theta}\right)\theta_t \\ + \sigma : \left(\varepsilon_t^{th} + \varepsilon_t^{trip}\right) - \varrho\frac{\partial \hat{\psi}}{\partial z}\cdot z_t + \frac{1}{\theta}\,k|\nabla\theta|^2 \geq 0\,.\end{aligned} \tag{2.14}$$

To exploit this inequality which holds for all solutions to the field equations, we first consider a purely elastic deformation at constant and uniform temperature without change of inelastic strains or phase fractions. Since (2.14) has to be valid for all elastic strain rates, we obtain

$$\sigma = \varrho\frac{\partial \hat{\psi}}{\partial \varepsilon^{el}}\,. \tag{2.15}$$

Similar reasoning yields

$$s = -\frac{\partial \hat{\psi}}{\partial \theta}\,. \tag{2.16}$$

Moreover, we define the thermodynamic force associated with the internal variable z_i as

$$L_i = -\frac{\partial \psi}{\partial z_i} \tag{2.17}$$

and call $L_i > 0$ the latent heat of phase z_i. Since $z_{i,t} \geq 0$, (2.14) finally reduces to

$$\sigma : (\varepsilon_t^{th} + \varepsilon_t^{trip}) \geq 0 \tag{2.18}$$

reflecting the fact that the intrinsic dissipation is necessarily positive.

Coming back to our goal of computing a constitutive relation for the internal energy e, we differentiate (2.10) with respect to time, as well as (2.16), to obtain

$$\varrho e_t = \varrho \psi_t + \varrho \theta_t s + \varrho \theta s_t \tag{2.19}$$

and

$$s_t = -\frac{\partial}{\partial \theta}\left(\frac{1}{\varrho}\right) : \varepsilon_t^{el} + \frac{\partial s}{\partial \theta}\,\theta_t + \frac{\partial L}{\partial \theta} \cdot z_t\,. \tag{2.20}$$

Assuming tacitly $\frac{\partial L}{\partial \theta} = 0$ and defining the specific heat capacity at constant strain as

$$c_\varepsilon = \theta\,\frac{\partial s}{\partial \theta}\,, \tag{2.21}$$

we can use (2.10), (2.12), and (2.20) to end up with

$$\varrho e_t = \sigma : \varepsilon_t^{el} - \varrho L \cdot z_t - \varrho \theta\,\frac{\partial}{\partial \theta}\left(\frac{1}{\varrho}\,\sigma\right) : \varepsilon_t^{el} + \varrho c_\varepsilon \theta_t\,. \tag{2.22}$$

Remark 2.1 *To simplify the further derivations, let us assume that the temperature dependency of ε^{trip} can be neglected, i.e. $\varepsilon_\theta^{trip} \approx 0$.*

Then we can use Hooke's law (2.5) and (2.7) to infer

$$\frac{\partial}{\partial \theta}\left(\frac{1}{\varrho}\,\sigma\right) = \frac{1}{\varrho}\,\sigma_\theta = -\frac{1}{\varrho}\,K q(z) I = -\frac{3\kappa}{\varrho}\,q(z) I \tag{2.23}$$

with the bulk modulus

$$\kappa = \frac{1}{3}(3\lambda + 2\mu)\,.$$

Substituting (2.22) and (2.23) in the energy balance (2.2b), we finally obtain the following nonlinear parabolic equation:

$$\begin{aligned} \alpha(\theta, \sigma, z)\theta_t - &\operatorname{div}(k \operatorname{grad} \theta) + 3\kappa q(z)\theta \operatorname{div} v \\ &= (\varrho L + tr\sigma\theta\bar{q} + 9\kappa\theta^2 q(z)\bar{q}) \cdot z_t + \gamma(\theta, z, z_t)|S|^2 + h\,, \end{aligned} \tag{2.24}$$

where α is defined as

$$\alpha(\theta, \sigma, z) = \varrho c_\varepsilon - tr\sigma q(z) - 9\kappa q(z)^2\theta\,. \tag{2.25}$$

Here we define $\bar{q} = \nabla q = (q_1 - q_0,\, q_2 - q_0)^T$ such that $\beta_z(\theta, z) = \theta\bar{q}$.

3 Assumptions and main result

Let $\Omega \subset \mathbb{R}^3$ with smooth boundary $\partial\Omega$ and $Q = \Omega \times (0,T)$ the corresponding time cylinder. Throughout the paper we will assume

(A1) k, κ, c_ε, L are positive constants

(A2) γ is bounded and Lipschitz-continuous

(A3) q_1, q_2, q_3 are positive constants

(A4) $\bar{m}$ is Lipschitz-continuous satisfying $\bar{m}(\vartheta) \in [0,1]$ for all $\vartheta \in \mathbb{R}$

(A5) g_{ij} are bounded and Lipschitz-continuous.

Summarizing the model equations of Section 2, we consider the following boundary value problem.

$$\operatorname{div}\sigma = -F \quad \text{in } Q \tag{3.1a}$$

$$\sigma = K\Big(\varepsilon(u) - \beta(\theta,z)I - \int_0^t \gamma(\theta,z,z_\tau)S d\tau\Big) \quad \text{in } Q \tag{3.1b}$$

$$u = 0 \quad \text{on } \partial\Omega \times (0,T)$$

$$z_t = f(\theta,z,\sigma) \quad \text{in } Q \tag{3.1c}$$

$$z(0) = 0 \quad \text{in } \Omega \tag{3.1d}$$

$$\alpha(\theta,\sigma,z)\theta_t - k\Delta\theta + 3\kappa q(z)\theta \operatorname{div} u_t = h + (\varrho L + tr\sigma\theta\bar{q} + 9\kappa\theta^2 q(z)\bar{q})z_t \tag{3.1e}$$

$$+ \gamma(\theta,z,z_t)|S|^2 \quad \text{in } Q \tag{3.1f}$$

$$\frac{\partial\theta}{\partial n} = 0 \quad \text{on } \partial\Omega \times (0,T) \tag{3.1g}$$

$$\theta(0) = \theta_0 \quad \text{in } \Omega\,. \tag{3.1h}$$

The function α is given by the formula

$$\alpha(\theta,\sigma,z) = \varrho c_\varepsilon - tr\sigma q(z) - 9\kappa q(z)^2\theta\,. \tag{3.2}$$

and $f = (f_1, f_2)^T$ denotes the right-hand side of (2.1a), (2.1b).

We are going to prove that under regularity assumptions for given data and smallness of the derivative of β the considered problem possesses a unique weak solution. More precisely, our main result is

Theorem 3.1 *Suppose that $F \in W^{1,p}(0,T;L^p(\Omega)) \cap L^{2p}(Q)$, $\theta_0 \in W^{1,p}(\Omega)$ and $h \in L^p(Q)$, $p > 4$. If $\delta := \max\{q_1,q_2,q_3\}$ is sufficiently small then the problem* (3.1a)–(3.1h) *possesses a unique solution (u,θ,z) such that*

$$u \in L^p(0,T;W^{2,p}(\Omega))\,,\ u_t \in L^p(0,T;W^{1,p}(\Omega))\,,$$

$\theta \in W^{2,1}_p(Q)$, $z_i \in W^{1,p}(0,T;W^{1,p}(\Omega))$, $i = 1,2$ and $z_1 + z_2 \in [0,1]$ a.e. in Q.

4 Proof of Theorem 3.1

The main idea of the proof is a fixed point argument. To do this we start with the following auxiliary lemmas

Lemma 4.1 *a) Assume that $\theta, \sigma_{ij} \in L^p(Q)$ with $p \in [1, \infty]$ for $i, j \in \{1, 2, 3\}$ then the ordinary differential equation* (3.1c), (3.1d) *has a unique solution satisfying*

$$\| \, |z| \, \|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \leq C \tag{4.1}$$

where the constant C does not depend on θ and σ. Moreover, $z_1 + z_2 \in [0, 1]$ for a.e. $(x, t) \in Q$. If additionally $\nabla\theta, \nabla\sigma_{ij} \in L^p(Q)$ then $\nabla z \in L^\infty(0, T; L^p(\Omega))$.

b) Let z^i be the solution from a) corresponding to σ^i, θ^i, $i = 1, 2$, then

$$\| \, |z^1 - z^2| \, \|_{W^{1,p}(0,T;L^p(\Omega))} \leq \Lambda_1 \|\theta^1 - \theta^2\|_{L^p(Q)} + \Lambda_2 \|\sigma^1 - \sigma^2\|_{L^p(Q)} \, . \tag{4.2}$$

Proof: Existence and uniqueness of solutions to the considered problem follow from the theorem of Carathéodory [16]. The estimate for z is a consequence of the differential inequality

$$\bar{z}_t \leq (1 - \bar{z})\phi(t) \, , \qquad z(0) = 0 \, ,$$

where $\bar{z} = z_1 + z_2$ and $\phi(t) = g_{11}(\theta)g_{12}(\sigma) + g_{21}(\theta)g_{22}(\sigma)$. The estimate for the gradient will be obtained from the system of ordinary differential equations for $i = 1, 2$,

$$\begin{aligned} \nabla z_{i,t} &= f_{i,\theta}(\theta, z, \sigma)\nabla\theta + \sum_{k,l=1}^{3} f_{i,\sigma_{kl}}(\theta, z, \sigma)\nabla\sigma_{kl} + \sum_{l=1}^{2} f_{i,z_l}(\theta, z\sigma)\nabla z_l \\ \nabla z_i(0) &= 0 \, . \end{aligned}$$

According to the global Lipschitz continuity of f the result follows immediately. To prove the last estimate we consider the difference

$$z_t^1 - z_t^2 = f(\theta^1, z^1, \sigma^1) - f(\theta^2, z^2, \sigma^2) \, , \; (z^1 - z^2)(0) = 0 \, .$$

Multiplying by $z^1 - z^2$ and using the Lipschitz continuity of f we have

$$|z^1 - z^2|_t \leq \Lambda_1 |\theta^1 - \theta^2| + \Lambda_2 |\sigma^1 - \sigma^2| + \Lambda_3 |z^1 - z^2| \, .$$

The Gronwall inequality completes the proof. ∎

Remark 4.1 *Let $\delta := \max\{q_1, q_2, q_3\}$. Then*

$$|q(z)| \leq \delta$$

and $|\bar{q}| = \sqrt{(q_1 - q_0)^2 + (q_2 - q_0)^2} \leq \delta\sqrt{2}$. Moreover, it is convenient to write

$$q(z) = q_0 + \bar{q} \cdot z \, .$$

For $k = 1, 2$, let us denote by $W_p^{k,1}(Q)$ the space $L^p(0,T;W^{k,p}(\Omega)) \cap W^{1,p}(0,T;L^p(\Omega))$. If $p > \frac{5}{2}$ then $W_p^{2,1}(Q) \hookrightarrow L^\infty(Q)$ (see for example [11]). In the next lemma we are going to study the coupling of the elliptic equation for the displacement with the ordinary differential equation for z assuming that the temperature is known and belongs to the space $W_p^{2,1}(Q)$.

Lemma 4.2 *Let $\hat{\theta} \in W_p^{2,1}(Q)$, $p > 4$ and $F \in W^{1,p}(0,T;L^p(\Omega))$. Then the system of equations*

$$-\operatorname{div}\sigma = F \quad \text{in } Q \tag{4.3a}$$

$$\sigma = K\left(\varepsilon(u) - \beta(\hat{\theta}, z)I - \int_0^t \gamma(\hat{\theta}, z, z_\tau) S d\tau\right) \quad \text{in } Q \tag{4.3b}$$

$$u = 0 \quad \text{on } \partial\Omega \times (0,T) \tag{4.3c}$$

$$z_t = f(\hat{\theta}, z, \sigma) \quad \text{in } Q \tag{4.3d}$$

$$z(0) = 0 \quad \text{in } \Omega \tag{4.3e}$$

has a unique solution satisfying

$$\|u\|_{L^p(0,T;W^{2,p}(\Omega))} + \|u_t\|_{L^p(0,T;W^{1,p}(\Omega))} \leq C_1 + C_2\|\hat{\theta}\|_{W_p^{2,1}(Q)}\,. \tag{4.4}$$

Proof: We are going to use a standard fixed point argument. Before we start with the proof let us give the following regularity result for the elasticity system:

Let $F \in L^q(0,T;L^p(\Omega))$ and $\tau \in L^q(0,T;W^{1,p}(\Omega))$ for $p, q \in (1,\infty)$. Denote by u the weak solution of the problem

$$\int_\Omega K\varepsilon(u) : \varepsilon(w)dx = \int_\Omega \tau : \varepsilon(w)dx + \int_\Omega f w dx \quad \forall w \in W_0^{1,p'}(\Omega) \tag{4.5}$$

then u satisfies the estimate

$$\|u\|_{L^q(0,T;W^{2,p}(\Omega))} \leq C_1\|f\|_{L^q(0,T;L^p(\Omega))} + C_2\|\tau\|_{L^q(0,T;W^{1,p}(\Omega))} \tag{4.6}$$

where the positive constants C_1, C_2 do not depend on u, f and τ. This regularity result can be found in [13, Theorem 3.1.1] or in [15]. Let us define the set

$$K_T = \left\{\varsigma \in W_p^{1,1}(Q) : \|\varsigma\|_{W_p^{1,1}(Q)} \leq M\right\}$$

with a positive constant M. Then we define an operator

$$\mathcal{P} : K_T \longrightarrow L^p(0,T;W^{1,p}(\Omega))\,, \quad \hat{\sigma} \mapsto \sigma = \mathcal{P}(\hat{\sigma})\,, \tag{4.7}$$

where σ is the weak solution of the problem

$$\operatorname{div}\sigma = -F \quad \text{in } Q \tag{4.8a}$$

$$\sigma = K\left(\varepsilon(u) - \beta(\hat{\theta}, z)I - \int_0^t \gamma(\hat{\theta}, z, z_\tau)\hat{S} d\tau\right) \quad \text{in } Q \tag{4.8b}$$

$$u = 0 \quad \text{on } \partial\Omega \times (0,T)\,. \tag{4.8c}$$

The function z is the solution of the ODE

$$z_t = f(\hat{\theta}, z, \hat{\sigma}) \quad \text{in } Q\,, \qquad z(0) = 0 \quad \text{in } \Omega \tag{4.9}$$

and $\hat{S}$ is the deviatoric part of $\hat{\sigma}$. The goal is to show that for sufficiently small $T > 0$ and large M, $\mathcal{P}(\hat{\sigma}) \in K_T$. By definition of σ we have

$$\begin{aligned}\int_\Omega K\varepsilon(u) : \varepsilon(w)dx = \int_\Omega Fwdx + 3\kappa \int_\Omega \beta(\hat{\theta}, z) \operatorname{div} wdx \\ + \int_\Omega \int_0^t \gamma(\hat{\theta}, z, z_\tau)\hat{S}d\tau : \varepsilon(w)dx\,.\end{aligned} \tag{4.10}$$

Using the $W^{2,p}$-estimate (4.6) for solutions to the elasticity system we obtain

$$\begin{aligned}\|u\|_{L^p(0,T;W^{2,p}(\Omega))} \le C_1\|F\|_{L^p(0,T;L^p(\Omega))} + C_2\Big(\|\beta(\hat{\theta}, z)\|_{L^p(0,T;W^{1,p}(\Omega))} \\ + \Big\|\int_0^t \gamma(\hat{\theta}, z, z_\tau)\hat{S}d\tau\Big\|_{L^p(0,T;W^{1,p}(\Omega))}\Big)\,.\end{aligned} \tag{4.11}$$

Regularity of $\hat{\theta}, z$ and the continuous embedding $K_T \subset L^\infty(Q)$ for $p > 4$ yield

$$\|\beta(\hat{\theta}, z)\|_{L^p(0,T;W^{1,p}(\Omega))} \le \delta\|\hat{\theta}\|_{L^p(0,T;W^{1,p}(\Omega))} \tag{4.12}$$

as well as

$$\begin{aligned}\Big\|\int_0^t \gamma(\hat{\theta}, z, z_\tau)\hat{S}d\tau\Big\|_{L^p(0,T;W^{1,p}(\Omega))} \le T\Big(\|\gamma(\hat{\theta}, z, z_t)\hat{S}\|_{L^p(Q)} \\ + \|\gamma_\theta\nabla\hat{\theta} + \gamma_z\nabla z + \gamma_{z_t}\nabla z_t\|_{L^p(Q)}\|\hat{S}\|_{L^\infty(Q)} \\ + \|\gamma(\hat{\theta}, z, z_t)\|_{L^\infty(Q)} \cdot \|\operatorname{div}\hat{S}\|_{L^p(Q)}\Big) \le C_1TM + C_2TM^2\end{aligned} \tag{4.13}$$

where the constants C_1, $C_2 > 0$ do not depend on M.

Inserting the two last estimates into (4.11) we arrive at the inequality

$$\|u\|_{L^p(0,T;W^{2,p}(\Omega))} \le \tilde{C}_1 + \tilde{C}_2T^{1/p}M + \tilde{C}_3TM + \tilde{C}_4M^2T\,. \tag{4.14}$$

According to the constitutive relation (4.8b) between stress and strain we obtain a similar inequality for σ, i.e.

$$\|\sigma\|_{L^p(0,T;W^{1,p}(\Omega))} \le C_1 + C_2T^{1/p}M + C_3TM + C_4TM^2\,. \tag{4.15}$$

Next, we are going to prove an estimate for the time derivative of u. Hence, we have to consider

$$\begin{aligned}\int_\Omega K\varepsilon(u_t) : \varepsilon(w)dx = \int_\Omega F_twdx + 3\kappa \int_\Omega \beta_t(\hat{\theta}, z) \operatorname{div} wdx \\ + \int_\Omega \gamma(\hat{\theta}, z, z_t)\hat{S} : \varepsilon(w)dx \quad \forall w \in W_0^{1,q}(\Omega)\,.\end{aligned}$$

By (4.6) we have

$$\|u_t\|_{L^p(0,T;W^{1,p}(\Omega))} \leq C_1\|F_t\|_{L^p(Q)} + C_2\big(\|\beta_t(\hat{\theta},z)\|_{L^p(Q)} + \|\gamma(\hat{\theta},z,z_t)\hat{S}\|_{L^p(Q)}\big)\,. \tag{4.16}$$

Regarding the regularity of β we obtain

$$\begin{aligned}\|\beta_t(\hat{\theta},z)\|_{L^p(Q)} &\leq \delta\|\hat{\theta}_t\|_{L^p(Q)} + \sqrt{2}\delta\|z_t\hat{\theta}\|_{L^p(Q)}\\ &\leq C_1 + C_2T^{1/p}\|\hat{\sigma}\|_{L^p(Q)}\,.\end{aligned} \tag{4.17}$$

To estimate the last term we see that

$$\|\gamma(\hat{\theta},z,z_t)\hat{S}\|_{L^p(W)} \leq C\|\hat{S}\|_{L^p(Q)}\,. \tag{4.18}$$

Unfortunately, we cannot estimate $\|\hat{S}\|_{L^p(Q)}$ by M only, because the constant C in front may not be small. We are going to prove that the operator $\mathcal{P}$ maps the set

$$R_T = \{\varsigma \in L^p(Q) : \|\varsigma\|_{L^p(Q)} \leq R\}$$

into R_T for sufficiently large R and sufficiently small T. To do this we again utilize (4.6) to obtain

$$\begin{aligned}\|u\|_{L^p(0,T;W^{1,p}(\Omega))} &\leq C_1\|F\|_{L^p(Q)} + C_2\left(\|\beta(\hat{\theta},z)\|_{L^p(Q)} + \left\|\int_0^t \gamma(\hat{\theta},z,z_\tau)\hat{S}d\tau\right\|_{L^p(Q)}\right)\\ &\leq \tilde{C}_1 + \tilde{C}_2TR\end{aligned} \tag{4.19}$$

where $\tilde{C}_1$ and $\tilde{C}_2$ do not depend on R. This result and Hooke's law yield that a similar inequality holds for σ, i.e.

$$\|\sigma\|_{L^p(Q)} \leq \tilde{C}_1 + \tilde{C}_2TR\,. \tag{4.20}$$

Choosing T sufficiently small and R sufficiently large we obtain that $\mathcal{P}(\hat{\sigma}) = \sigma \in R_T$. Next we return to the estimate (4.16). Invoking (4.17), (4.18) and (4.20) yields

$$\|u_t\|_{L^p(0,T;W^{1,p}(\Omega))} \leq C_1 + C_2T^{1/p}M + CR \tag{4.21}$$

where R is chosen such that $\mathcal{P} : R_T \to R_T$. The last estimate implies that

$$\|\sigma\|_{L^p(0,T;W^{1,p}(\Omega))} + \|\sigma_t\|_{L^p(Q)} \leq C_1 + C_2T^{1/p}M + C_3TM + C_4TM^2 + CR\,. \tag{4.22}$$

Hence, choosing T sufficiently small and M sufficiently large we have that

$$\mathcal{P} : K_T \cap R_T \longrightarrow K_T \cap R_T\,.$$

To prove that the map $\mathcal{P}$ has a fixed point we want to use the Schauder theorem. Observe that the set $K_T \cap R_T$ is compact and convex in the space $L^p(Q)$. To end the proof we have to show that $\mathcal{P} : L^p(Q) \to L^p(Q)$ is continuous. Let $\hat{\sigma}^n \to \hat{\sigma}$ in $L^p(Q)$, we are going to prove that $\mathcal{P}(\hat{\sigma}^n) = \sigma^n$ converges to $\mathcal{P}(\hat{\sigma}) = \sigma$ in $L^p(Q)$. First we see that from Lemma 4.1 we immediately have that the sequence $\{z^n\}$ defined by $z_t^n = f(\hat{\theta}, z^n, \hat{\sigma}^n)$ in Q, $z^n(0) = 0$ in Ω, converges in the space $W^{1,p}(0,T;L^p(\Omega))$ to the solution of the ODE $z_t = f(\hat{\theta}, z, \hat{\sigma})$ in Q, $z(0) = 0$ in Ω.

Moreover, the Lipschitz continuity of β and γ gives that

$$\beta(\hat{\theta}, z^n) \longrightarrow \beta(\hat{\theta}, z) \quad \text{in } L^p(Q)\,,$$
$$\gamma(\hat{\theta}, z^n, z_t^n) \longrightarrow \gamma(\hat{\theta}, z, z_t) \quad \text{in } L^p(Q)\,.$$

Passing eventually to a subsequence we can assume that $\gamma(\hat{\theta}, z^n, z_t^n) \to \gamma(\hat{\theta}, z, z_t)$ pointwise a.e. in Q.

Owing to Lebesgue's theorem we infer

$$\Big\| \big(\gamma(\hat{\theta}, z^n, z_t^n) - \gamma(\hat{\theta}, z, z_t)\big)\hat{S} \Big\|_{L^p(Q)} \longrightarrow 0$$

and hence,

$$\begin{aligned} &\|\gamma(\hat{\theta}, z^n, z_t^n)\hat{S}^n - \gamma(\hat{\theta}, z, z_t)\hat{S}\|_{L^p(Q)} \\ &\qquad \le C_1\|\hat{S}^n - \hat{S}\|_{L^p(Q)} + \|(\gamma(\hat{\theta}, z^n, z_t^n) - \gamma(\hat{\theta}, z, z_t))S\| \underset{n\to\infty}{\longrightarrow} 0\,. \end{aligned}$$

Invoking (4.6) once again we obtain that $u^n \to u$ in $L^p(0,T;W^{1,p}(\Omega))$ and $\mathcal{P}(\hat{\sigma}^n) \to \mathcal{P}(\hat{\sigma})$ in $L^p(Q)$. The Schauder fixed point theorem completes the proof of existence.

We see that T does not depend on the value of $\sigma(0)$ and therefore the solution can be extended on a finite time interval. To end the proof of the lemma we have to show uniqueness of solutions. To this end, we denote by (σ^1, z^1), (σ^2, z^2) two solutions of the considered problem and use the abbreviations $\beta^i(t) = \beta(\hat{\theta}(t), z^i(t))$, $\gamma^i(t) = \gamma^i(\hat{\theta}(t), z^i(t), z_t^i(t))$ and estimate

$$\begin{aligned} \|\sigma^1(t) - \sigma^2(t)\|^2_{L^2(\Omega)} \le C\Big(\|u^1(t) - u^2(t)\|^2_{W^{1,2}(\Omega)} + \|\beta^1(t) - \beta^2(t)\|^2_{L^2(\Omega)}\Big) \\ + \int_0^t \Big(\|\gamma^1(t)S^1(\tau) - \gamma^2(t)S^2(\tau)\|^2_{L^2(\Omega)}\Big)d\tau\,. \end{aligned} \tag{4.23}$$

Using (4.2) we obtain

$$\|z^1(t) - z^2(t)\|_{L^2(\Omega)} \le C\int_0^t \|\sigma^1(\tau) - \sigma^2(\tau)\|_{L^2(\Omega)}d\tau$$

and consequently

$$\begin{aligned} \|\beta^1(t) - \beta^2(t)\|^2_{L^2(\Omega)} &= \|\beta(\hat{\theta}, z^1) - \beta(\hat{\theta}, z^2)\|^2_{L^2(\Omega)} \\ &\le C\int_0^t \|\sigma^1(\tau) - \sigma^2(\tau)\|^2_{L^2(\Omega)}d\tau\,. \end{aligned} \tag{4.24}$$

Moreover, according to the estimate $\|\sigma^i\|_{L^\infty(Q)} \le M$ where M depends on $\hat{\theta}$, we conclude that

$$\begin{aligned} &\int_0^t \|\gamma^1(\tau)S^1(\tau) - \gamma^2(\tau)S^2(\tau)\|^2_{L^2(\Omega)}d\tau \le C\Big(\int_0^t \|\gamma^1(\tau) - \gamma^2(\tau)\|^2_{L^2(\Omega)}\|S^1(\tau)\|^2_{L^\infty(\Omega)}d\tau \\ &+ \int_0^t \|\gamma^2(\tau)\|^2_{L^\infty(\Omega)}\|S^1(\tau) - S^2(\tau)\|^2_{L^2(\Omega)}d\tau\Big) \le \tilde{C}\Big(\int_0^t \|\sigma^1(\tau) - \sigma^2(\tau)\|^2_{L^2(\Omega)}d\tau\Big)\,. \end{aligned}$$

Finally using the weak formulation of the elasticity system we have

$$\int_\Omega K\varepsilon(u^1(t)-u^2(t)):\varepsilon(u^1(t)-u^2(t))dx = \int_\Omega (\beta^1(t)-\beta^2(t))\operatorname{div}(u^1(t)-u^2(t))dx$$
$$+\int_\Omega\int_0^t (\gamma^1(\tau)|S^1(\tau)|^2-\gamma^2(\tau)|S^2(\tau)|^2)d\tau:\varepsilon(u^1(t)-u^2(t))dx\,.$$

Hence, we obtain

$$\begin{aligned}\|u^1(t)-u^2(t)\|_{W^{1,2}(\Omega)} &\le C\Big(\|\beta^1(t)-\beta^2(t)\|_{L^2}^2\\ &\quad+\int_0^t \|\gamma^1(\tau)S^1(\tau)-\gamma^2(\tau)S^2(\tau)\|_{L^2}^2 d\tau\Big)\\ &\le C\int_0^t \|\sigma^1-\sigma^2\|_{L^2}^2 d\tau\,.\end{aligned} \tag{4.25}$$

Inserting this into (4.23) we have

$$\|\sigma^1(t)-\sigma^2(t)\|_{L^2(\Omega)}^2 \le C\int_0^t \|\sigma^1(\tau)-\sigma^2(\tau)\|_{L^2(\Omega)}^2 d\tau\,. \tag{4.26}$$

Since $\sigma^1(0)=\sigma^2(0)$ we obtain $\sigma^1(t)=\sigma^2(t)$ and consequently $z^1(t)=z^2(t)$.

Now we are in position to study the complete nonlinear system (3.1a)–(3.1h).

Proof of Theorem 3.1: Let us first observe that for $\hat\theta\in W_p^{2,1}(Q)$ the solution from Lemma 4.2 satisfies $H(\sigma,z,\hat\theta)=\gamma(\hat\theta,z,z_t)|S|^2\in L^p(Q)$ and $\|H\|_{L^p(Q)}$ does not depend on $\hat\theta$. This follows from the additional assumption $F\in L^{2p}(Q)$. Let us define the set

$$\begin{aligned}\mathcal{M}=\Big\{&\theta\in W_p^{2,1}(Q):\|\theta\|_{L^p(0,T;W^{2,p}(\Omega))}+\|\theta_t\|_{L^p(Q)}\le R\,,\\ &\frac{\partial\theta}{\partial n}=0\quad\text{on }\partial\Omega\times(0,T)\quad\text{and }\theta(0)=\theta_0\Big\}\,.\end{aligned}$$

For the moment we assume that an arbitary function $H\in L^p(Q)$ and $\|H\|_{L^p(Q)}\le K$ is given. Let us select $\hat\theta\in\mathcal{M}$ and consider the following initial-boundary value problem

$$\begin{aligned}\varrho c_\varepsilon\theta_t-k\Delta\theta &= (q(z)tr\sigma+9k\beta q(z)^2\hat\theta)\hat\theta_t-3\kappa q(z)\hat\theta\operatorname{div}u_t+h \qquad (4.27a)\\ &\quad+(\varrho L+tr\sigma\hat\theta\bar q+9\kappa\hat\theta^2 q(z)\bar q)z_t+H\\ \frac{\partial\theta}{\partial n} &= 0\quad\text{on }\partial\Omega\times(0,T) \qquad (4.27b)\\ \theta(0) &= \theta_0 \qquad (4.27c)\end{aligned}$$

where (u,σ,z) depend on $\hat\theta$ according to Lemma 4.2. This means that the right-hand side in the last equation is known. We are going to prove that for δ sufficiently small $\theta\in\mathcal{M}$. Using the maximal regularity estimate for solutions to linear parabolic problems we obtain that

$$\|\theta_t\|_{L^p(Q)}+\|\theta\|_{L^p(0,T;W^{2,p}(\Omega))}\le C\|P\|_{L^p(Q)} \tag{4.28}$$

where P denotes the right-hand side of the considered equation.

$$\begin{aligned}\|P\|_{L^p(Q)} \le C_1\Big(&\delta\|\sigma\|_{L^\infty(Q)} + \delta^2\|\hat\theta\|_{L^\infty(Q)}\|\hat\theta_t\|_{L^p(Q)} + \delta\|\hat\theta\|_{L^\infty(Q)}\|\operatorname{div} u_t\|_{L^p(Q)}\\ &+ \delta\|\sigma\|_{L^\infty(Q)}\|\hat\theta\|_{L^\infty(Q)}\|z_t\|_{L^p(Q)}\\ &+ \delta\|\hat\theta\|^2_{L^\infty(Q)}\|z_t\|_{L^p(Q)}\Big) + \|H\|_{L^p(Q)} + C_2\,,\end{aligned} \tag{4.29}$$

where C_2 only depends on h, g, and L.

According to the estimate from Lemma 4.2 we conclude that for δ sufficiently small and R sufficiently large $\theta \in \mathcal{M}$. Hence, we have defined an operator

$$\mathcal{M} \ni \hat\theta \mapsto \mathcal{R}(\hat\theta) = \theta \in \mathcal{M}\,.$$

Next we prove that for δ small $\mathcal{R}$ is a contraction. Let us denote

$$\theta^i = \mathcal{R}(\hat\theta^i) \quad \text{for } i = 1, 2\,.$$

Then we have

$$\begin{aligned}\varrho c_2(\theta^1_t - \theta^2_t) - k(\Delta\theta^1 - \Delta\theta^2) &= q(z^1)tr\sigma^1\hat\theta^1_t - q(z^2)tr\sigma^2\hat\theta^2_t + 9\kappa q(z^1)^2\hat\theta^1\hat\theta^1_t\\ &\quad - 9\kappa q(z^2)^2\hat\theta^2\hat\theta^2_t - 3\kappa q(z^1)\hat\theta^1\operatorname{div} u^1_t \qquad (4.30a)\\ &\quad + 3\kappa q(z_2)\hat\theta^2\operatorname{div} u^2_t + tr\sigma^1\hat\theta^1\bar q z^1_t - tr\sigma^2\hat\theta^2\bar q z^2_t\\ &\quad + 9\kappa(\hat\theta^1)^2 q(z^1)\bar q z^1_t - 9\kappa(\hat\theta^2)^2 q(z^2)\bar q z^2_t + \varrho L(z^1_t - z^2_t)\\ \frac{\partial(\theta^1-\theta^2)}{\partial n} &= 0 \quad \text{on } \partial\Omega\times(0,T) \qquad (4.30b)\\ (\theta^1-\theta^2)(0) &= 0\,. \qquad (4.30c)\end{aligned}$$

Hence, we have to estimate the L^p-norm of the right-hand side of equation (4.30a). Let us denote the six differences on the right-hand side by $I_1, .., I_6$. Then

$$\begin{aligned}\|I_1\|_{L^p(Q)} \le &\|q(z^1)tr\sigma^1 - q(z^2)tr\sigma^2\|_{L^\infty(Q)}\|\hat\theta^1_t\|_{L^p(Q)}\\ &+ \|q(z^2)tr\sigma^2\|_{L^\infty(Q)}\|\hat\theta^1_t - \hat\theta^2_t\|_{L^p(Q)}\,.\end{aligned}$$

To estimate the first term we see that

$$\|q(z^1)tr\sigma^1 - q(z^2)tr\sigma^2\|_{L^\infty(Q)} \le \delta\|\sigma^1 - \sigma^2\|_{L^\infty(Q)} + \sqrt{2}\delta\|\sigma^2\|_{L^\infty(Q)}\|z^1 - z^2\|_{L^\infty(Q)}\,.$$

According to the embedding $W^{1,1}_p(Q) \subset C(Q)$ for $p > 4$ we can invoke Lemma 4.1 b) and an estimate for $\sigma^1 - \sigma^2$ along the lines of estimates (4.11) and (4.13) to obtain

$$\|I_1\|_{L^p(Q)} \le C\delta\|\hat\theta^1 - \hat\theta^2\|_{W^{2,1}_p(Q)} \tag{4.31}$$

and C does not depend on δ and $\hat\theta$.

In the same manner we estimate $I_2, .., I_6$:

$$\begin{aligned}\|I_2\|_{L^p(Q)} \le C\Big(&\|q(z^1)^2\hat\theta^1 - q(z^2)^2\hat\theta^2\|_{L^\infty(Q)}\|\hat\theta^1_t\|_{L^p(Q)}\\ &+ \|q(z^2)^2\hat\theta^2\|_{L^\infty(Q)}\|\hat\theta^1_t - \hat\theta^2_t\|_{L^p(Q)}\Big) \le C\delta\|\hat\theta_1 - \hat\theta_2\|_{W^{2,1}_p(Q)}\,,\end{aligned} \tag{4.32}$$

$$\|I_3\|_{L^p(Q)} \leq C\Big(\|q(z^1)\hat{\theta}^1 - q(z^2)\hat{\theta}^2\|_{L^\infty(Q)}\|\operatorname{div} u_t^1\|_{L^p(Q)} + \|q(z^2)\hat{\theta}^2\|_{L^\infty(Q)}\|\operatorname{div} u_t^1 - \operatorname{div} u_t^2\|_{L^p(Q)}\Big)\,.$$

Using (4.4) we arrive at the inequality

$$\|I_3\|_{L^p(Q)} \leq C\delta\|\hat{\theta}^1 - \hat{\theta}^2\|_{W_p^{2,1}(Q)} \tag{4.33}$$

where C does not depend on δ and $\hat{\theta}$. Reasoning as before, we obtain

$$\begin{aligned}
\|I_4\|_{L^p(Q)} &\leq C_1\delta\|\sigma^1\|_{L^\infty(Q)}\|\hat{\theta}^1\|_{L^\infty(Q)}\|z_t^1 - z_t^2\|_{L^p(Q)} \\
&\quad + C_2\delta\|z_t^2\|_{L^\infty(Q)}\|\sigma^1\hat{\theta}^1 - \sigma^2\hat{\theta}^2\|_{L^p(Q)} \\
&\leq C\delta\|\hat{\theta}_1 - \hat{\theta}_2\|_{W_p^{2,1}(Q)} \\
\|I_5\|_{L^p(Q)} &\leq C\|(\hat{\theta}^1)^2 q(z^1)\bar{q}z_t^1 - (\hat{\theta}^2)^2 q(z^2)\bar{q}z_t^2\|_{L^p(Q)} \\
&\leq C\delta\|\hat{\theta}_1 - \hat{\theta}_2\|_{W_p^{2,1}(Q)}\,.
\end{aligned}$$

Owing to Lemma 4.1 we obtain for I_6

$$\|I_6\|_{L^p(Q)} \leq CT\|\hat{\theta}_1 - \hat{\theta}_2\|_{W_p^{2,1}(Q)}\,. \tag{4.34}$$

Hence, we conclude that for δ sufficiently small and $T^+ \leq T$ small enough,

$$\|\mathcal{R}(\hat{\theta}^1) - \mathcal{R}(\hat{\theta}^2)\|_{W_p^{2,1}(Q_{T+})} \leq \Lambda\|\hat{\theta}^1 - \hat{\theta}^2\|_{W^{2,1}(Q_{T+})} \quad \text{and } \Lambda < 1 \tag{4.35}$$

where $Q_{T^+} = \Omega \times (0, T^+)$.

Using the Banach fixed point theorem we have that there exists $\theta \in \mathcal{M}$ such that $\mathcal{R}(\theta) = \theta$ and again the solution can be extended to any finite time interval.

The last step in the proof is a study of the following problem

$$\begin{aligned}
\varrho c_\varepsilon\theta_t - k\Delta\theta &= q(z)tr\sigma + 9\kappa q(z)^2\theta)\theta_t - 3\kappa q(z)\theta\operatorname{div} u_t + h \qquad (4.36a)\\
&\quad + (\varrho L + tr\sigma\theta\bar{q} + 9\kappa\theta^2 q(z)\bar{q})z_t + \tilde{\gamma}|\tilde{S}|^2 \\
\frac{\partial\theta}{\partial n} &= 0 \quad \text{on } \partial\Omega \times (0,T)\,, \qquad (4.36b)\\
\theta(0) &= \theta_0 \qquad (4.36c)
\end{aligned}$$

where $(\tilde{\sigma}, \tilde{z})$ is a solution according to Lemma 4.2 for $\tilde{\theta} \in \mathcal{M}$, $\tilde{\gamma} = \gamma(\tilde{\theta}, \tilde{z}, \tilde{z}_t)$. Hence, we have an operator

$$\mathcal{M} \ni \tilde{\theta} \mapsto \tilde{\mathcal{R}}(\tilde{\theta}) = \theta \in \mathcal{M}\,.$$

Note that $\tilde{\gamma}|\tilde{S}|^2 \in L^p(Q)$ and from the above step of the proof we have that $\tilde{\mathcal{R}}(\tilde{\theta}) = \theta \in \mathcal{M}$. Moreover note that for $\tilde{\theta} \in L^p(Q)$ the operator $\tilde{\mathcal{R}}$ is also well-defined and $\tilde{\mathcal{R}}(\tilde{\theta}) \in W_p^{2,1}(Q) \subset L^p(Q)$.

We are going to prove that $\tilde{\mathcal{R}}$ is a continuous map from $L^p(Q)$ into $L^p(Q)$. Let $\tilde{\theta}^n \to \tilde{\theta}$ in $L^p(Q)$ then we have that $\tilde{z}^n \to \tilde{z}$ in $W^{1,p}(0,T; L^p(\Omega))$, $\beta(\tilde{\theta}^n, \tilde{z}^n) \to \beta(\tilde{\theta}, \tilde{z})$ in $L^p(Q)$ and pointwise a.e. in Q (eventually passing to a subsequence), $\gamma(\tilde{\theta}^n, \tilde{z}^n, \tilde{z}_t^n) \to \gamma(\tilde{\theta}, \tilde{z}, \tilde{z}_t)$ in

$L^p(Q)$ and pointwise a.e. in Q and $\beta_z(\tilde{\theta}^n, \tilde{z}^n) \to \beta_z(\tilde{\theta}, \tilde{z})$ in $L^p(Q)$ and pointwise a.e. in Q. Moreover, $\tilde{\sigma}^n \to \tilde{\sigma}$ in $L^{2p}(Q)$ because $F \in L^{2p}(Q)$ and $\beta(\tilde{\theta}^n, z^n) \to \beta(\tilde{\theta}, \tilde{z})$ in $L^{2p}(Q)$ also. Hence, in the same manner as at the end of Lemma 4.2 we prove that $\tilde{\gamma}^n|\tilde{S}^n|^2 \to \tilde{\gamma}|\tilde{S}|^2$ in $L^p(Q)$. Consequently, using the main estimate from the first step of the proof we deduce that $\tilde{\mathcal{R}}$ is continuous from $L^p(Q)$ into $L^p(Q)$. The Schauder fixed point theorem completes the proof. ∎

To prove uniqueness we only have to show that in the last step the solution is unique. From the derivation of (4.35) in the previous step we can also infer

$$\|\theta^1 - \theta^2\|_{W_p^{1,2}(Q)} \leq \|H^1 - H^2\|_{L^p(Q)} \tag{4.37}$$

where H^1, H^2 are given functions from $L^p(Q)$. To end the proof we have to estimate

$$\|\gamma^1|S^1|^2 - \gamma^2|S^2|^2\|_{L^p(Q)} = J \tag{4.38}$$

where $\gamma^i = \gamma(\theta^i, z^i, \gamma^i)$, $i = 1, 2$.

In the same manner as in the proof of Lemma 4.2 we show that

$$\|z^1(t) - z^2(t)\|_{L^p(\Omega)} \leq C\bigg(\int_0^T \|\sigma^1 - \sigma^2\|_{L^p(\Omega)}dt + \int_0^T \|\theta^1 - \theta^2\|_{L^p(\Omega)}dt\bigg) \tag{4.39}$$

and

$$\|\sigma^1(t) - \sigma^2(t)\|_{L^p(\Omega)} \leq C\int_0^T \|\theta^1 - \theta^2\|_{L^p(\Omega)}dt\,. \tag{4.40}$$

Next, we estimate

$$\begin{aligned} J \leq \|\gamma^1\|_{L^\infty(Q)}\|\,|S^1| + |S^2|\,\|_{L^\infty(Q)}\|S^1 - S^2\|_{L^p(Q)} \\ + \|\gamma^1 - \gamma^2\|_{L^p(Q)}\|\,|S^2|^2\|_{L^\infty(Q)}\,. \end{aligned} \tag{4.41}$$

Using (4.39), (4.40), and (A2) we conclude that

$$\|\theta^1 - \theta^2\|_{W_p^{1,2}(Q)} \leq C\bigg(\|\theta^1 - \theta^2\|_{L^p(Q)} + \int_0^T \|\theta^1 - \theta^2\|_{L^p(Q)}d\tau\bigg)\,.$$

According to the fact that $\theta^1(0) = \theta^2(0)$ we have

$$\|\theta^1 - \theta^2\|_{L^p(Q)} \leq \bigg\|\int_0^t (\theta^1_\tau - \theta^2_\tau)d\tau\bigg\|_{L^p(Q)} \leq T\|\theta^1_t - \theta^2_t\|_{L^p(Q)}\,. \tag{4.42}$$

Hence, for small T we obtain

$$\|\theta^1 - \theta^2\|_{W_p^{1,2}(Q)} \leq 0 \Rightarrow \theta^1 = \theta^2\,.$$

Next, we observe that the length of the time interval do not depend on the initial data θ^0. Hence, we conclude the uniqueness result for all bounded time intervals. ∎

5 Numerical Results

In this section we present some numerical simulations to demonstrate the distortion effect of metallurgical phase transitions. We assume that the workpiece has already been heated up to the high temperature phase austenite and consider only the cooling stage of a heat treatment. For a sufficiently high cooling rate, i.e. close to the quenched boundary parts where temperature descends very quickly, austenite is transformed into the hard phase martensite (z_2), whereas a slower temperature change, e.g. in the interior of a big workpiece, causes the softer phase pearlite (z_1) to grow. The correlation of temperature change and phase transformation can be obtained by isothermal and non-isothermal time-temperature-transformation (ttt) diagrams which are attained by measurements. In particular, one can find which time-temperature evolutions are feasible for sufficient martensite formation. Due to the fact that the product phases pearlite and martensite exhibit different thermal expansion their formation influences the deformation of the workpiece as described in Section 2. This leads to the afore-mentioned distortion, for which we will give concrete examples in the following simulations. The underlying model is based on the equations (3.1a)–(3.1h). To achieve easily visible effects we consider a simple 2-dimensional geometry, i.e. a steel slab of dimension 100mm $\times$ 20mm, and infer specific cooling to obtain a corresponding phase distribution. As mentioned before we consider only the cooling, not the prior heating process. Therefore we assume a sufficiently high, homogeneous initial temperature and complete austenization.

In the model the workpiece is assumed to be fixed in only one single point to avoid additional stress caused by mere thermoelastic effects. The fixation point is the upper right corner, that is, the displacement in this point is set to be zero. We suppose further that the workpiece is aligned at its right side such that the whole right boundary part may only shrink vertically.

Material parameters are taken from data tables for the eutectoid carbon steel C 1080. For simplicity and lack of precise data we have assumed $g_{12}(\sigma) = g_{22}(\sigma) \equiv 1$.

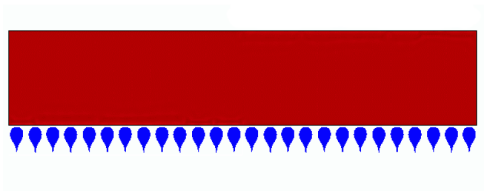


Figure 2: One-sided cooling of a hot slab.

To give a first impression of the phase induced thermomechanical effects, we consider a steel slab which is quenched from the bottom, which corresponds to nonzero Neumann conditions in (3.1g), the other three edges are assumed to be thermally insulated, see Figure 2. The rapid cooling causes the austenite close to the quenched boundary parts to transform to the hard and brittle steel phase martensite whereas the remaining austenite cools down more slowly and therefore transforms to the softer phase pearlite. Figure 3 demonstrates the process at a sample of time steps. At time $t = 0s$, the specimen is completely heated and stress-free. When quenching sets in, thermoelastic effects may be observed at first. The picture for time $t = 5s$ shows the shrinking of the quenched area.

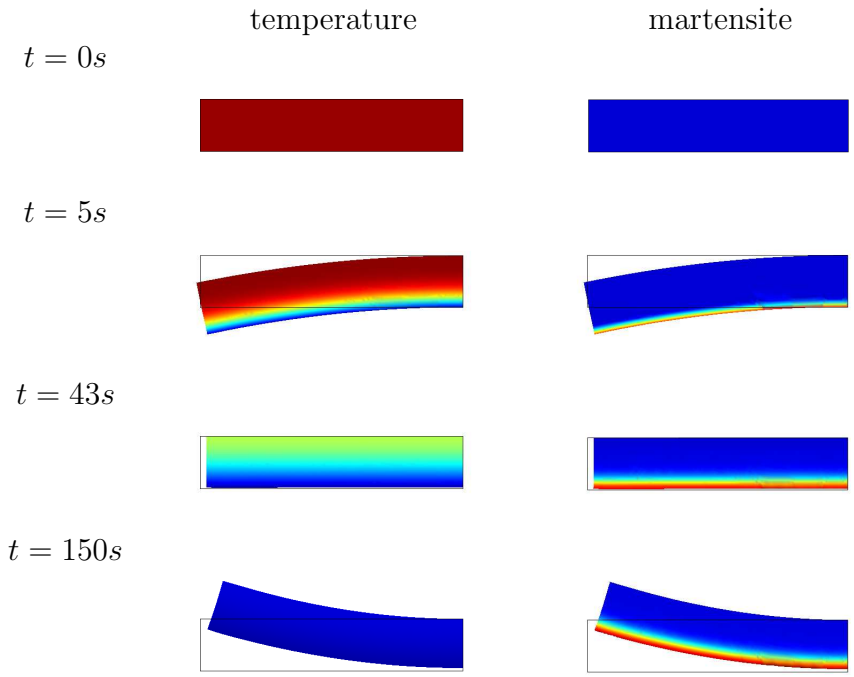


Figure 3: Workpiece at times $t = 0s$, $5s$, $43s$, and $150s$. Colours indicate temperature in the left column, martensite fraction in the right column where blue corresponds to 0 % and red to 100 % martensite, respectively. The background rectangle gives the initial geometry, the deformation of the workpiece is magnified by factor 10.

As we assume that yield stress is not exceeded and no plastic deformation occurs, this state of shape is only temporary and will be superseded by phase transformation induced deformation. This can be seen in the third picture for $t = 150s$ where the bulge points exactly in the opposite direction. As the picture for the martensite fraction at $t = 150s$ in Figure 3 shows, the rapid cooling effected the growth of martensite in the lower part of the specimen. The remaining part consists of the softer phase pearlite. Martensite has a lower density and a higher expansion coefficient than pearlite. Hence, martensite takes a bigger volume than pearlite and thus pushes the material outward which causes the bulge in the fourth picture.

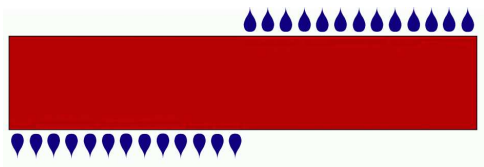
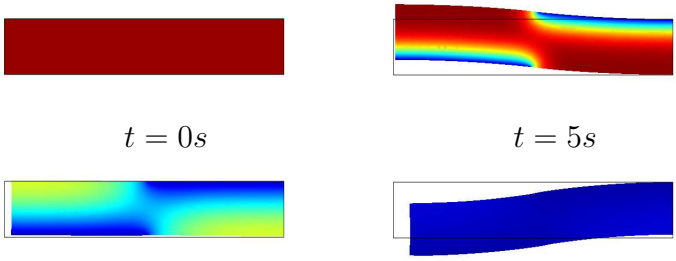


Figure 4: Inhomogeneous cooling of a hot slab.

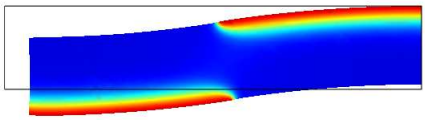
Figure 4 depicts the second investigated configuration: the drops in the lower left and the upper right indicate boundary sections where quenching is applied. The remaining parts of the boundary are thermally insulated. Figure 5 shows the process at four time steps. Again, the specimen is completely heated and stress-free at time $t = 0s$.



$t = 0s$ $t = 5s$

$t = 40s$ $t = 150s$

Figure 5: Workpiece at times $t = 0s$, $5s$, $40s$, and $150s$. Colours indicate temperature, the background rectangle gives the initial geometry, the deformation of the workpiece is magnified by factor 10.



$t = 150s$

Figure 6: Distribution of phase martensite at time $t = 150s$. Blue corresponds to 0 % and red to 100 %, respectively.

The picture for time $t = 5s$ shows that the quenched areas shrink and cause an antisymmetric contraction, which results in a reverse S-shaped (antisigmoidal) geometry. As we assume that yield stress is not exceeded and no plastic deformation occurs, this state of shape is only temporary and will level out after a sufficiently long time, when a stationary, homogeneous temperature distribution is achieved. Accordingly, the picture for $t = 40s$ shows a shrunk, but rectangular shape like the initial geometry. Finally, phase transformation induced deformation prevails as demonstrated in the fourth picture for $t = 150s$. The inhomogeneous phase distribution and their different densities induce a completely reversed situation compared to the thermoelastic effect. In the lower left and upper right martensite is formed (see Figure 6) which pushes the material outward by its smaller density and higher volume respectively. A lasting S-shaped (sigmoidal) deformation is generated when workpiece temperature has adjusted to the ambient medium.

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