

## Outcomes of the diploma thesis

# Analysis of the mathematical problem of linear thermo-elasticity taking into account phase transitions and transformation-induced plasticity

Sören Boettcher

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Analysis of the  
mathematical  
problem

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Boettcher

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and objective

Modeling of  
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behaviour of  
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  - Linear thermo-elasticity with phase transitions
  - Linear thermo-elasticity with phase transitions and transformation-induced plasticity
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## Unrequested distortion of steel workpieces during heat treatment

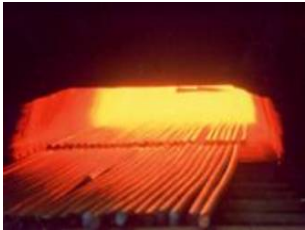


Figure: entering the furnace



Figure: after hardening

**source:** Krupp Edelstahl Profile, Siegen

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## General purpose

- Systematic analysis of the causes of distortion
- Prediction of distortion and required counteractions for compensation of distortion via simulations
- Minimization of distortion at the end of the production process

## Aim of this work

- Mathematical modeling of the complex material behaviour of steel
  - ⇒ Coupled system of ordinary and partial differential equations
  - ⇒ Existence and uniqueness of solutions???

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## Basics

- Mostly used metallic material in various areas of application
  - High demands on quality
  - High complexity of the material behaviour
- Alloy consisting mostly of iron, with a carbon content between 0.2% and 2.14% by weight
- Significance of carbon:
  - Steel properties
  - Phase transitions in dependence of
    - surrounding temperature
    - carbon concentration

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## Formation of different crystal structures in steel

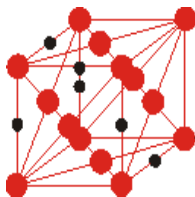


Figure: austenite

- $\gamma$ -iron
- face-centered cubic (FCC) structure
- $\theta \geq 723^\circ\text{C}$
- $a = 0.26\text{ nm}$

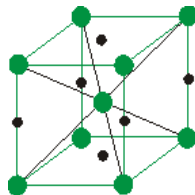


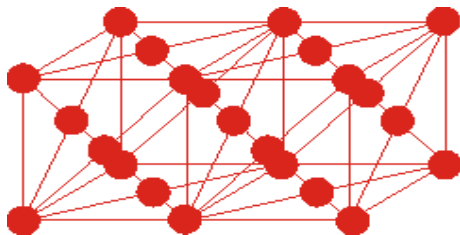
Figure: martensite

- $\alpha$ -iron
- body-centered cubic (BCC) structure
- $\theta \leq \theta_{M_S}$
- $a = 0.29\text{ nm}$

**source:** Frylunds Fagteori, Denmark



The heat treatment process for most steels involves heating the alloy until austenite forms, then cooling it so rapidly that the transformation of martensite occurs almost immediately



**source:** Frylunds Fagteori, Denmark

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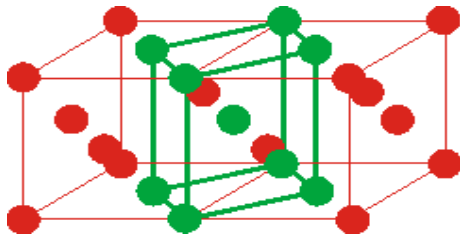
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## The presence of two phases due to the volume differences in the phases leads to plastic deformation

### ■ Temperature

- ⇒ phase transitions
- ⇒ change of volume and shape of a crystal
- ⇒ complex distribution of stress and deformation
- ⇒ plasticity

### ■ Occurance at

- no stress
- relatively low stress below yield stress
- isothermal and continuous transformation in all phase transition levels

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- Great challenge of modeling and simulation of material behaviour in order to predict
  - stress
  - deformation
  - phase transitions
- Little investigation of coupled models for the material behaviour which describe in addition to the temperature and the deformation as well the phase transitions
  - integration of the material behaviour in general models of thermo-elasticity

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## Momentum equation:

$$\rho_0 \frac{\partial^2 u}{\partial t^2} - \operatorname{div}(S) = \rho_0 f \quad \text{in } \Omega_T$$

## Energy equation:

$$\rho_0 \frac{\partial e}{\partial t} - \operatorname{div}(q) = S : \frac{\partial \varepsilon}{\partial t} + R \quad \text{in } \Omega_T$$

## Equations for the evolution of the phase fractions:

$$\frac{\partial p_i}{\partial t} = \gamma_i(\theta, p), \quad i = 1, \dots, N \quad \text{in } \Omega_T$$

## Momentum equation:

$$\rho_0 \frac{\partial^2 u}{\partial t^2} - \operatorname{div} (S(u, \theta, p)) = \rho_0 f \quad \text{in } \Omega_T$$

## Heat equation:

$$\rho_0 c_e \frac{\partial \theta}{\partial t} - \operatorname{div}(\kappa \nabla \theta) = -3 K_\alpha \theta_0 \operatorname{div} \left( \frac{\partial u}{\partial t} \right) + R(\theta, p) \quad \text{in } \Omega_T$$

## Equations for the evolution of the phase fractions:

$$\frac{\partial p_i}{\partial t} = \gamma_i(\theta, p), \quad i = 1, \dots, N \quad \text{in } \Omega_T$$

**Strain tensor:**

$$\varepsilon := \frac{1}{2} (\nabla u + \nabla u^T)$$

**Stress tensor:**

$$S := 2\mu\varepsilon^* + \lambda \operatorname{tr}(\varepsilon) \operatorname{Id} - 3K_\alpha (\theta - \theta_0) \operatorname{Id} + \\ - K \sum_{i=1}^N \left( \frac{\rho_0}{\rho(\theta_0)} - 1 \right) p_i \operatorname{Id}$$

**Right-hand side:**

$$R := \rho_0 \sum_{i=1}^N L_i \gamma_i(\theta, p) + r$$

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## Momentum equation:

$$\rho_0 \frac{\partial^2 u}{\partial t^2} - 2 \operatorname{div}(\mu \varepsilon) - \operatorname{grad}(\lambda \operatorname{div}(u)) +$$
$$+ 3 \operatorname{grad}(K_\alpha (\theta - \theta_0)) + \operatorname{grad} \left( K \sum_{i=1}^N \left( \frac{\rho_0}{\rho(\theta_0)} - 1 \right) p_i \right) = \rho_0 f$$

## Heat equation:

$$\rho_0 c_e \frac{d\theta}{dt} - \operatorname{div}(\kappa \nabla \theta) =$$
$$= -3 K_\alpha \theta_0 \operatorname{div} \left( \frac{\partial u}{\partial t} \right) + \rho_0 \sum_{i=1}^N L_i \gamma_i(\theta, p) + r$$

## Boundary conditions:

$$\begin{aligned}u &= 0 & \text{on } \Gamma_0 \times ]0, T[ \\S\nu &= 0 & \text{on } \Gamma_1 \times ]0, T[ \\-\kappa \nabla \theta \nu &= \delta(\theta - \theta_\Gamma) & \text{on } \partial\Omega_T\end{aligned}$$

## Initial conditions:

$$\begin{aligned}u(x, 0) &= u_0, \quad \frac{\partial u}{\partial t}(x, 0) = u_1, \quad \theta(x, 0) = \theta_0 & \text{in } \Omega \\ \sum_{i=1}^N p_{0i} &= 1, \quad p_{0i} \geq 0, \quad i = 1, \dots, N & \text{in } \Omega\end{aligned}$$

# Linear thermo-elasticity with phase transitions and transformation-induced plasticity



## Strain tensor:

$$\varepsilon = \varepsilon_{te} + \varepsilon_{trip}, \quad \text{tr}(\varepsilon_{trip}) = 0$$

$$\varepsilon_{trip} := -3\mu \sum_{i=1}^N \int_0^t G_i \frac{\partial \Phi_i}{\partial p_i} \max \left\{ \frac{\partial p_i}{\partial s}, 0 \right\} \left( S - \frac{1}{3} \text{tr}(S) \text{Id} \right) ds$$

## Stress tensor:

$$\begin{aligned} S := & 2\mu \varepsilon_{te}^* + \lambda \text{tr}(\varepsilon_{te}) \text{Id} - 3K_\alpha (\theta - \theta_0) \text{Id} + \\ & - K \sum_{i=1}^N \left( \frac{\rho_0}{\rho(\theta_0)} - 1 \right) p_i \text{Id} + \\ & - 3\mu \sum_{i=1}^N \int_0^t G_i \frac{\partial \Phi_i}{\partial p_i} \max \left\{ \frac{\partial p_i}{\partial s}, 0 \right\} \left( S - \frac{1}{3} \text{tr}(S) \text{Id} \right) ds \end{aligned}$$

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# Linear thermo-elasticity with phase transitions and transformation-induced plasticity



## Momentum equation:

$$\begin{aligned} & \rho_0 \frac{\partial^2 u}{\partial t^2} - 2 \operatorname{div} (\mu \varepsilon) - \operatorname{grad} (\lambda \operatorname{div}(u)) + \\ & + 3 \operatorname{grad} (K_\alpha (\theta - \theta_0)) + \operatorname{grad} \left( K \sum_{i=1}^N \left( \frac{\rho_0}{\rho(\theta_0)} - 1 \right) p_i \right) + \\ & + 3 \operatorname{div} \left( \mu \sum_{i=1}^N \int_0^t G_i \frac{\partial \Phi_i}{\partial p_i} \max \left\{ \frac{\partial p_i}{\partial s}, 0 \right\} \left( S - \frac{1}{3} \operatorname{tr}(S) \operatorname{Id} \right) ds \right) = \rho_0 f \end{aligned}$$

## Heat equation:

$$\begin{aligned} & \rho_0 c_e \frac{\partial \theta}{\partial t} - \operatorname{div} (\kappa \nabla \theta) = \\ & = -3 K \alpha \theta_0 \operatorname{div} \left( \frac{\partial u}{\partial t} \right) + \rho_0 \sum_{i=1}^N L_i \gamma_i(\theta, p) + r \end{aligned}$$

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# Particularities in the treatment of evolution equations



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## 1. Idea: dealing with the space variable $x$ and the time variable $t$ in different ways

- For fixed time  $t$ , think of the function  $x \mapsto u(x, t)$  of the space variable  $x$  as an element of the Sobolev space  $V$
- Notation:  $u(t) \in V$
- If we now vary the time  $t$  in the interval  $[0, T]$ , then we obtain a function  $t \mapsto u(t)$
- Thus arises from the real function  $(x, t) \mapsto u(x, t)$  the function  $t \mapsto u(t)$  with values in the Banach space  $V$
- We are looking for the function  $t \mapsto u(t)$  with  $u(t) \in V$  for all  $t \in [0, T]$

# Particularities in the treatment of evolution equations



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## 2. Two spaces $H$ and $V$

- $H$  is obtained in connection with the time derivative, and  $V$  results from the elliptic term and the boundary condition
- Concept of the evolution triple

## 3. We think of the time derivative as the generalized derivative on $]0, T[$ :

$$\int_0^T u(t) \varphi'(t) dt = - \int_0^T w(t) \varphi(t) dt \quad \forall \varphi \in C_0^\infty(0, T)$$

## 4. Choice of the space for the solution: $L^2(0, T; V)$ consists of all those functions such that the following holds:

$$u(\cdot, t) \in V \quad \forall t \in (0, T), \quad F \in L^2(0, T) \text{ with } F(t) := \|u(\cdot, t)\|_V$$

## Definition 1

$$V_u := \left\{ u \in [W^{1,2}(\Omega)]^3 : u = 0 \text{ auf } \Gamma_0 \right\}$$

$$H_u := [L^2(\Omega)]^3$$

$$V_\theta := W^{1,2}(\Omega)$$

$$H_\theta := L^2(\Omega)$$

$$V_p := \left\{ p \in [L^\infty(\Omega \times ]0, T[)]^N : \frac{\partial p}{\partial t} \in [L^\infty(\Omega \times ]0, T[)]^N \right\}$$



# Linear thermo-elasticity with phase transitions



## Definition 2

Under suitable assumptions a triple  $(u, \theta, p) \in L^2(0, T; V_u) \times L^2(0, T; V_\theta) \times \mathcal{V}_p$  with  $u' \in L^2(0, T; V_u)$  is called weak solution if the following holds:

$$\begin{aligned} & - \int_0^T \int_{\Omega} \rho_0 u'(t) \varphi'(t) \, dx \, dt + 2 \int_0^T \int_{\Omega} \mu \varepsilon(u(t)) : \varepsilon(\varphi) \, dx \, dt + \\ & + \int_0^T \int_{\Omega} \lambda(x) \operatorname{div}(u(t)) \operatorname{div}(\varphi) \, dx \, dt + 3 \int_0^T \int_{\Omega} K_\alpha (\theta(t) - \theta_0) \operatorname{div}(\varphi(t)) \, dx \, dt + \\ & + \int_0^T \int_{\Omega} K \sum_{i=1}^N \left( \frac{\rho_0}{\rho_i(\theta_0)} - 1 \right) p_i(t) \operatorname{div}(\varphi(t)) \, dx \, dt = \\ & = \int_0^T \int_{\Omega} f(t) \varphi(t) \, dx \, dt + \int_{\Omega} \rho_0 u_1 \varphi(0) \, dx \\ & - \int_0^T \int_{\Omega} \rho_0 c_e \theta(t) \psi'(t) \, dx \, dt + \int_0^T \int_{\Omega} \kappa \nabla \theta(t) \nabla \psi \, dx \, dt + \int_0^T \int_{\partial\Omega} \delta \theta(t) \psi \, d\sigma \, dt = \\ & = \int_0^T \int_{\partial\Omega} \delta \theta_\Gamma \psi(t) \, d\sigma \, dt + 3 \int_0^T \int_{\Omega} K_\alpha \theta_0 \operatorname{div}(u'(t)) \psi(t) \, dx \, dt + \\ & + \int_0^T \int_{\Omega} \rho_0 \sum_{i=1}^N L_i \gamma_i(t) \psi(t) \, dx \, dt + \int_0^T \int_{\Omega} r(t) \psi(t) \, dx \, dt + \int_{\Omega} \rho_0 c_e \theta_0 \psi(0) \, dx \\ & \rho_i'(t) = \gamma_i(\theta(t), p(t)), \quad i = 1, \dots, N \end{aligned}$$

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# Linear thermo-elasticity with phase transitions and transformation-induced plasticity



## Definition 3

Under suitable assumptions a triple  $(u, \theta, \rho) \in L^2(0, T; V_u) \times L^2(0, T; V_\theta) \times \mathcal{V}_\rho$  with  $u' \in L^2(0, T; V_u)$  is called weak solution if the following holds:

$$\begin{aligned}
 & - \int_0^T \int_\Omega \rho_0 u'(t) \varphi'(t) \, dx \, dt + 2 \int_0^T \int_\Omega \mu \varepsilon(u(t)) : \varepsilon(\varphi) \, dx \, dt + \\
 & \quad + \int_0^T \int_\Omega \lambda(x) \operatorname{div}(u(t)) \operatorname{div}(\varphi) \, dx \, dt + 3 \int_0^T \int_\Omega K_\alpha (\theta(t) - \theta_0) \operatorname{div}(\varphi(t)) \, dx \, dt + \\
 & \quad + \int_0^T \int_\Omega K \sum_{i=1}^N \left( \frac{\rho_0}{\rho_i(\theta_0)} - 1 \right) \rho_i(t) \operatorname{div}(\varphi(t)) \, dx \, dt + \\
 & \quad + 2 \int_0^T \int_\Omega \mu \int_0^t b(s, t) \varepsilon^*(u(s)) \, ds \varepsilon^*(\varphi(t)) \, dx \, dt + \\
 & \quad = \int_0^T \int_\Omega f(t) \varphi(t) \, dx \, dt + \int_\Omega \rho_0 u_1 \varphi(0) \, dx \\
 & - \int_0^T \int_\Omega \rho_0 c_e \theta(t) \psi'(t) \, dx \, dt + \int_0^T \int_\Omega \kappa \nabla \theta(t) \nabla \psi \, dx \, dt + \int_0^T \int_{\partial\Omega} \delta \theta(t) \psi \, d\sigma \, dt = \\
 & \quad = \int_0^T \int_{\partial\Omega} \delta \theta_\Gamma \psi(t) \, d\sigma \, dt + 3 \int_0^T \int_\Omega K_\alpha \theta_0 \operatorname{div}(u'(t)) \psi(t) \, dx \, dt + \\
 & \quad + \int_0^T \int_\Omega \rho_0 \sum_{i=1}^N L_i \gamma_i(t) \psi(t) \, dx \, dt + \int_0^T \int_\Omega r(t) \psi(t) \, dx \, dt + \int_\Omega \rho_0 c_e \theta_0 \psi(0) \, dx \\
 & \quad \rho_i'(t) = \gamma_i(\theta(t), \rho(t)), \quad i = 1, \dots, N
 \end{aligned}$$

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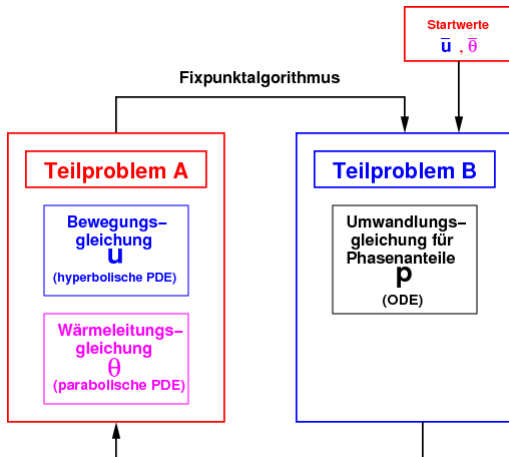
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## Theorem 5.1

*Under suitable assumptions exists a unique weak solution  $(u, \theta) \in L^2(0, T; V_u) \times L^2(0, T; V_\theta)$  of*

<b>Problem A</b>
<i>momentum equation</i>
<i>heat equation</i>
<i>boundary- and initial conditions</i>

*for fixed  $p \in \mathcal{V}_p$ . Furthermore:*

$$u'' \in L^\infty(0, T; H_u), u' \in L^\infty(0, T; V_u), u \in L^\infty(0, T; V_u),$$

$$\text{and } \theta' \in L^\infty(0, T; H_\theta), \theta \in L^\infty(0, T; H_\theta).$$

- Let  $P$  be the exact problem for which we intend to look for the existence of a solution in a space of functions constructed over a separable Hilbert space  $V$
- Existence of the solution
  - Formulation of the approximate problem  $P_m$  in the finite dimensional space  $V_m$  having a unique solution  $u_m$
  - A priori estimates on  $u$  which show that  $\{u_m\}$  belongs to fixed balls of certain normed spaces
  - By using the results of weak compactness of the unit ball in a Banach space, it is possible to extract from  $\{u_m\}$  a subsequence  $\{u'_m\}$  which has a limit in the weak (weak\*) topology of spaces which occur in the estimates
  - $u$  is the solution of problem  $P$

## Sketch of the proof

### Galerkin method

- *A priori estimates provide:*

$$\begin{aligned} \|u'_m\|_{L^\infty(0,T;H_u)} + \|u_m\|_{L^\infty(0,T;V_u)} + \\ + \|\theta_n\|_{L^\infty(0,T;H_\theta)} + \|\theta_n\|_{L^2(0,T;V_\theta)} < \infty \end{aligned}$$

- *A priori estimates **not** satisfactory  
because of coupling terms*

## Sketch of the proof

### Problematical terms:

$$\begin{aligned}
 & \rho_0 \frac{d^2 u}{dt^2} - 2 \operatorname{div}(\mu \varepsilon) - \operatorname{grad}(\lambda \operatorname{div}(u)) + \\
 & + 3 \operatorname{grad}\left(K \alpha (\theta - \theta_0)\right) + \operatorname{grad}\left(K \sum_{i=1}^N \left(\frac{\rho_0}{\rho(\theta_0)} - 1\right) p_i\right) + \\
 & + 3 \operatorname{div}\left(\mu \sum_{i=1}^N \int_0^t G_i \frac{\partial \Phi_i}{\partial p_i} \max\left\{\frac{\partial p_i}{\partial s}, 0\right\} S^* ds\right) = \rho_0 f \\
 & \rho_0 c_e \frac{\partial \theta}{\partial t} - \operatorname{div}(\kappa \nabla \theta) = -3 K \alpha \theta_0 \operatorname{div}\left(\frac{\partial u}{\partial t}\right) + \rho_0 \sum_{i=1}^N L_i \gamma_i + r
 \end{aligned}$$

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## Sketch of the proof

- *A priori estimates because of coupling*  
*not satisfactory*
  - *Integration by parts in the space variable for simple boundary conditions [J. Gawinecki, 1986]*
  - *Differentiation der Galerkin equations with respect to time*
- *Additional a priori estimates provide:*

$$\begin{aligned} \|u_m''\|_{L^\infty(0,T;H_u)} + \|u_m'\|_{L^\infty(0,T;V_u)} + \\ + \|\theta_n'\|_{L^\infty(0,T;H_\theta)} + \|\theta_n'\|_{L^2(0,T;V_\theta)} < \infty \end{aligned}$$



- Linear thermo-elasticity with phase transitions ✓
- Linear thermo-elasticity with phase transitions and transformation-induced plasticity
  - Regularization of the problem
  - Additional assumptions for uniqueness

## Theorem 5.2

*Under suitable assumptions exists a unique solution  $p \in \mathcal{V}_p$  of*

### **Problem B**

*equations for evolution of phase fraction  
initial condition*

*for fixed  $\bar{\theta} \in L^2(0, T; H_\theta)$ .*

## Proof

*I. Hüssler, 2007*



## Theorem 5.3

*Under suitable assumptions exists a unique weak solution  $(u, \theta, p) \in L^2(0, T; V_u) \times L^2(0, T; V_\theta) \times \mathcal{V}_p$  of*

**full problem**

*momentum equation*

*heat equation*

*equations for the evolution of phase fractions*

*boundary- and initial conditions*

## Sketch of the proof

Let  $\mathbf{V} := V_u \times V_\theta$  und  $\mathbf{H} := H_u \times H_\theta$ . Already proved:

- For given  $(\bar{u}, \bar{\theta}) \in L^2(0, T; \mathbf{H})$  exists a unique solution  $p = p(\bar{u}, \bar{\theta}) \in \mathcal{V}_p$  of *problem B*.
- For this given  $p \in \mathcal{V}_p$  exists a unique solution  $(u, \theta) = (u(p(\bar{u}, \bar{\theta})), \theta(p(\bar{u}, \bar{\theta}))) \in L^2(0, T; \mathbf{V})$  of *problem A* with  $\|(u, \theta)\|_{W^{1,2}(0, T; \mathbf{V}, \mathbf{H})} < \infty$ .

Thus defines the following fixed point operator:

$$\begin{aligned} T : L^2(0, T; \mathbf{H}) &\rightarrow V_p \rightarrow L^2(0, T; \mathbf{V}) \hookrightarrow L^2(0, T; \mathbf{H}) \\ (\bar{u}, \bar{\theta}) &\mapsto p \mapsto (u, \theta) \end{aligned}$$

## Sketch of the proof

*Applying the Schauder fixed point theorem, we have to prove:*

$T : \overline{B_R(0)} \subset L^2(0, T; \mathbf{H}) \rightarrow \overline{B_R(0)}$  *is continuous and compact*

- *Mapping of  $\overline{B_R(0)}$  into itself*
  - *A priori estimates*
- *Continuity of the operator:*
  - $p_n \rightarrow p$  in  $\mathcal{V}_p$  for  $(\bar{u}_n, \bar{\theta}_n) \rightarrow (\bar{u}, \bar{\theta})$  in  $L^2(0, T; \mathbf{H})$
  - $(u_n, \theta_n) \rightarrow (u, \theta)$  in  $L^2(0, T; \mathbf{H})$  for  $p_n \rightarrow p$  in  $\mathcal{V}_p$
- *Precompactness of the image*
  - *Lions-Aubin theorem provides the compact imbedding*  
 $W^{1,2}(0, T; \mathbf{V}, \mathbf{H}) \hookrightarrow L^2(0, T; \mathbf{H})$



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  - Preparations
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  - Problem A
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- Presentation of the solution of the coupled system consisting of the heat equation and the equation for the evolution of the phase fractions
- Assumptions:
  - Homogeneous temperature and phase distribution
  - Stress-free phase transition
- Material data from IWT Bremen
- Calculations via MATLAB<sup>®</sup>

Analysis of the  
mathematical  
problem

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Boettcher

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## Heat equation:

$$\theta' = \frac{r}{\rho_0 c_e} + \sum_{i=2}^4 \frac{L_i}{c_e} p_i' - \frac{4 \delta}{D \rho_0 c_e} (\theta - \theta_\Gamma) \quad \text{in } ]0, T[$$

## Equations for the evolution of the phase fractions:

$$p_1' = -p_2' - p_3' - p_4' \quad \text{in } ]0, T[$$

$$p_2' = H_2(\theta, \theta_1, \theta_2) (e_2(\theta) + p_2)^{r_2(\theta)} \max\{\bar{p}_2 - p_2, 0\}^{s_2(\theta)} g_2(\theta) \quad \text{in } ]0, T[$$

$$p_3' = H_3(\theta, \theta_2, \theta_3) (e_3(\theta) + p_3)^{r_3(\theta)} \max\{\bar{p}_3 - p_3, 0\}^{s_3(\theta)} g_3(\theta) \quad \text{in } ]0, T[$$

$$p_4' = H_4(\theta, \theta_3) \max\{\bar{p}_4 - p_4, 0\} \mu \quad \text{in } ]0, T[$$

## Initial conditions:

$$p_1(0) = 1, \quad p_2(0) = 0, \quad p_3(0) = 0, \quad p_4(0) = 0, \quad \theta(0) = \theta_0$$

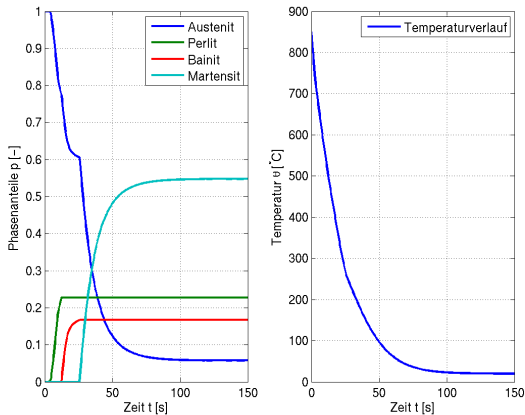


Figure: cooling from the austenitic state

Analysis of the mathematical problem

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- Insight into the problem
- Formulation of the mathematical problem of linear thermo-elasticity taking into account phase transitions and transformation-induced plasticity
- Existence and uniqueness of a weak solution
- Numerical analysis of a coupled system consisting of the heat equation and the equation for the evolution of the phase fractions

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- Further investigation of the uniqueness and the continuity with respect to the data of the full problem
- Application of further proof techniques
  - Regularization methods, e.g. special Galerkin-Bases
  - Time-discrete or fully discrete approximations
- Consideration of
  - Temperature- and phase-dependent parameters
  - Stress-dependent phase transitions
  - Nitriding, nitrocarburization and carbon diffusion
  - Classical plasticity
- Meso-macro-investigations
- Non-dimensionalization
- Numerical analysis

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Thank you for your attention.