Weierstrass Institute for
Applied Analysis and Stochastics

DFG Research Center MATHEON
Mathematics for key technologies

Analysis and simulation of a thermomechanical phase transition model including TrIP

Dietmar Hömberg, Daniela Kern, Wolf Weiss

Content

1 Introduction

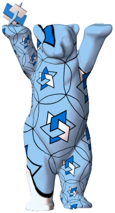
- Institute
- Steel

About MATHEON

- MATHEON: *Mathematics for key technologies*
- research center of the German Research Foundation DFG
- about 100 scientific members
- run by FU, HU, TU (host), Zuse Institute, and WIAS Berlin

DFG Research Center MATHEON
Mathematics for key technologies

- carries out application-driven research in close collaboration with partners from industry, economy, and science
- cooperation with schools, media, and the general public
- application areas are:
  - life sciences
  - networks
  - production
  - electronic and photonic devices
  - finance
  - visualization
  - education, outreach, administration



About WIAS

- *WIAS* (Weierstrass Institute for Applied Analysis and Stochastics)
- institute in *Forschungsverbund Berlin e.V.* , partially funded from the German government
- member of the *Leibniz Association* (umbrella organisation for 87 institutions; topics ranging from humanities and social sciences, economics, and life sciences to mathematics, the natural and engineering sciences and environmental research; *theoria cum praxi: science for the benefit and good of humankind*)

- founded in 1992, follower of *Karl-Weierstraß-Institut für Mathematik* of the former *Akademie der Wissenschaften der DDR*
- about 130 staff members, including more than 100 scientists
- conducts project-oriented research in applied mathematics
- runs research projects in main application areas covering complex problems from economics, science and technology
- hosts the permanent office of the International Mathematical Union (IMU) (since February 2011)

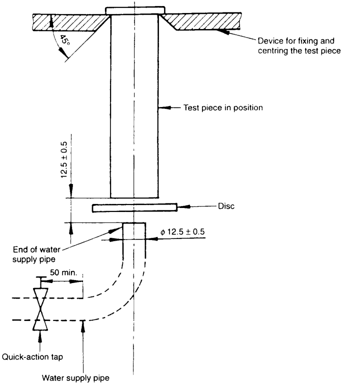
Research Group 4 – Nonlinear Optimization and Inverse Problems

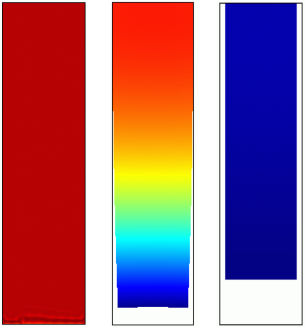
- 18 members
- head: Prof. Dr. Dietmar Hömberg

Topics:

- diffractive optics
- management of electricity portfolios
- simulation and optimal control of production processes
  - automatic reconfiguration of robotic welding cells
  - development of a prognosis tool for the prediction of stable milling processes
  - modeling and optimization of the heat treatment of steel
  - modeling, simulation, and optimization of multifrequency induction hardening
  - simulation and control of phase transitions and mechanical properties during hot-rolling of multiphase steel

Cooling experiment without phase change





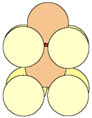
experimental setup:
Jominy end quench test

temperature evolution and corresponding thermoelastic deformation

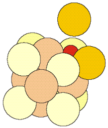
Possible behaviour of more complex materials

... iron:

- rather soft material
- iron atoms are arranged in different lattice structures depending on temperature and pressure



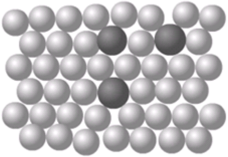
at room temperature: α-iron, bcc (body centered cubic) – few interstices



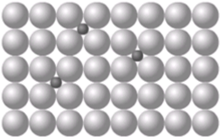
912° - 1394° Celsius: γ-iron, fcc (face centered cubic) – many interstices

... steel:

- iron alloy (with carbon or possibly other additional alloying elements)



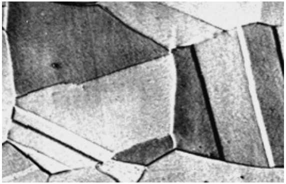
substitutional alloying: replace iron atoms by other similarly large (metal) atoms



interstitional alloying: fill empty spaces in the grid by rather tiny atoms as carbon

- carbon as interstitional alloying component may prevent that iron lattice structure can switch during temperature change
- fast cooling of iron: carbon atoms have no time to diffuse and get stuck, leading to a metastable shifted grid structure and high internal stresses
- moderate cooling: carbon atoms diffuse
- ferrite and cementite form patterns, depending on temperature evolution

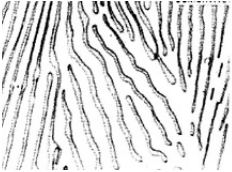
Steel phases



hot steel phase austenite

hard and brittle martensite

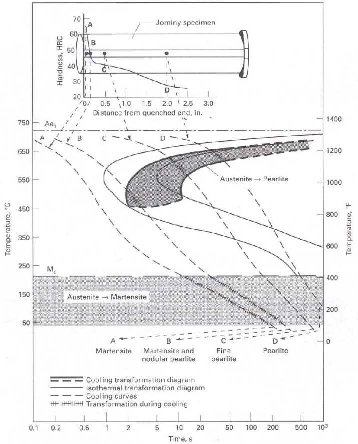
high volume

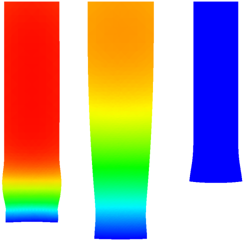


rather soft and ductile pearlite

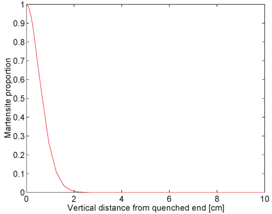
bainite

Cooling experiment with phase change – heat treatment





temperature evolution



hardening curve

Plasticity

- classical plasticity: deformations remain if some critical stress value (yield stress) is exceeded
- creeping: permanent minor loads lead to deformation if applied for a very long time

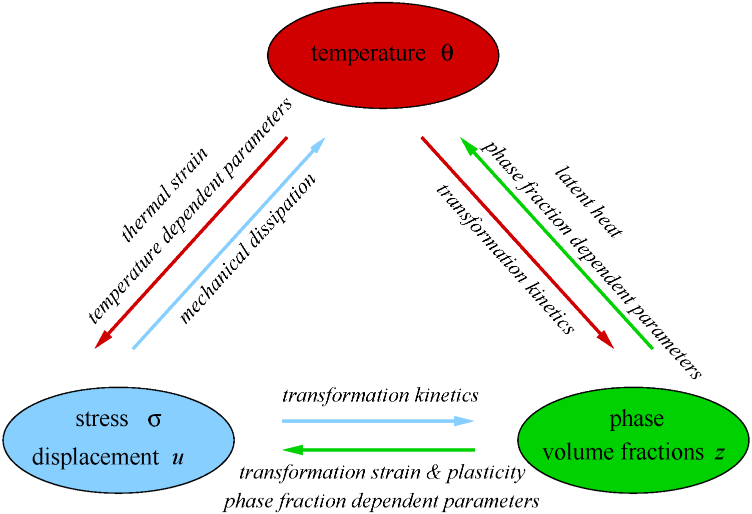
Fig.: Deutsche Edelstahlwerke

- transformation induced plasticity (trip): small stresses lead to lasting deformations when phase transitions occur

2 Model

- Derivation
  - Phase transitions

Interdependencies



Heat treatments:

- consider quenching (cooling) processes
- mostly $\theta_t \leq 0$
- phase transitions considered as irreversible,
  only transitions from austenite to other phases (e.g. martensite) are considered
- initial geometries correspond to the hot state, other reference variables as well

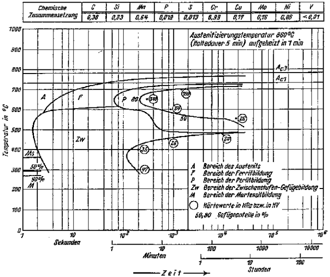
Metallurgical phases:

- mixture approach: at each point phases simultaneously coexist as fractions, $\sum_i z_i = 1$
- phase evolution occurs at each point independently from the neighbouring points and
  phase diffusion is omitted (we do not consider spatial derivatives)

- austenite – pearlite transition:
  - driven by carbon diffusion
  - growth rate influenced by temperature and stress

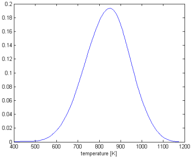
$$\dot{z}_1 = f_1(\theta, z, \sigma) = (1 - z_1 - z_2) g_{11}(\theta) g_{12}(\sigma) \qquad (1)$$
$$z_1(0) = 0.$$

$g_{11}(\theta)$ derived from measurement data: TTT (Time-Temperature-Transformation) diagram:



isothermal diagram $\rightarrow$ fix time θ:

$$g(\theta) = -\frac{1}{t_f - t_s} \ln\left(\frac{0.01}{0.99}\right)$$



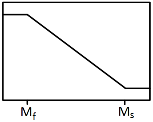
Phase transition model for cooling processes – martensite

- austenite – martensite transition:
  - possible total amount of martensite is limited by a temperature dependent function

$$\dot{z}_2 = f_2(\theta, z, \sigma) = [\min\{\bar{m}(\theta), 1 - z_1\} - z_2]_+ g_{21}(\theta) g_{22}(\sigma) \qquad (2)$$
$$z_2(0) = 0.$$

- $\bar{m}(\theta)$ antisigmoidal (reverse S-shaped) function
  - constantly 0 above martensite start temperature M_s
  - constantly 1 below martensite finish temperature M_f

E.g. simplest choice: piecewise linear function



$u : \mathbb{R}^3 \to \mathbb{R}^3,\ x \mapsto u(x)$: displacement vector

$\varepsilon(u) \in \mathbb{R}^{3\times 3}$: strain tensor of linear(ized) elasticity

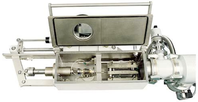
$$\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla^T u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)_{i,j=1,2,3} \tag{3}$$

Additive decomposition of the strain into an elastic, a thermal, and a plastic part:

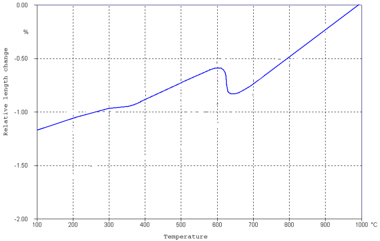
$$\varepsilon = \varepsilon^{el} + \varepsilon^{th} + \varepsilon^{tp}. \tag{4}$$

(We will assume that the plastic effects are merely given by transformation induced plasticity.)

Mechanical quantities – thermal strain



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



- piecewise almost linear correspondence of thermal expansion and temperature
- occurence of phase transitions results in a change of rate

$\Rightarrow$ describe the thermal expansion of each single phase by $\varepsilon_i^{th} = \delta_i(\theta - \theta_{i,ref})I.$ (5)

Overall thermal strain is then computed from the mixture ansatz

$$\varepsilon^{th} = z_1\varepsilon_1^{th} + z_2\varepsilon_2^{th} + (1-z_1-z_2)\varepsilon_0^{th} =: q(z)\theta I + q_{ref}(z)I. \qquad (6)$$

Mechanical quantities – TrIP strain

Transformation induced plasticity

- amounts during phase transitions
- occurs even for small stresses far below yield stress
- accounts for stresses that lead to shear
- volume-preserving

Behaviour modelled by

$$\varepsilon_{i,t}^{tp} = \Phi_{i1}(\theta)\,\frac{\partial \Phi_{i2}(z_i)}{\partial z_i}\,z_{i,t}\sigma^*\,, \qquad \text{short:} \quad \varepsilon_t^{tp} = \gamma(\theta, z, z_t)\sigma^*\,. \tag{7}$$

$$\text{where} \quad \sigma^* = \sigma - \frac{1}{3}tr(\sigma)I \quad \text{deviatoric part of } \sigma.$$

Typical choice of γ:

$$\gamma(\theta, z, z_t) = \frac{3}{2}\zeta \sum_i z_t^i \qquad \text{(Tanaka)} \tag{8}$$

with a Greenwood-Johnson parameter ζ.

Remaining part of the strain $\varepsilon^{el} = \varepsilon(u) - \varepsilon^{th} - \varepsilon^{tp}$; corresponds to $\sigma \in \mathbb{R}^{3\times 3}$.

Stress tensor gained by Hooke's law:

$$\begin{aligned}\sigma &= K\varepsilon^{el} = K(\varepsilon(u) - \varepsilon^{th} - \varepsilon^{tp}) \\ &= 2\mu\varepsilon(u) + \lambda tr(\varepsilon(u))I - b\beta(\theta, z)I - 2\mu\varepsilon^{tp}\end{aligned}$$

with K fourth order tensor,

Lamé parameters λ and μ for steel as a macroscopically homogenous, isotropic material,

$b := (2\mu + 3\lambda)$ (bulk modulus).

Derivation of the model – I

$$-\,div\,\sigma = F \qquad \text{(quasistatic momentum balance)} \tag{9}$$

$$\varrho e_t + div\,\Lambda = \sigma : \varepsilon(v) + h \qquad \text{(balance law of internal energy)} \tag{10}$$

Introduce the Helmholtz free energy ψ and entropy s to derive a constitutive relation.

Thermodynamic identity

$$e = \psi + \theta s \tag{11}$$

Consider ψ as twice differentiable function $\psi(\varepsilon^{el}, \theta, z)$ (see e.g. Petryk).

By the first and second law of thermodynamics, the Clausius-Duhem inequality holds,

$$\sigma : \varepsilon(v) - \varrho(\psi_t + s\theta_t) - \frac{1}{\theta}\,\Lambda \cdot \nabla\theta \geq 0\,. \tag{12}$$

Exploit the law of Fourier,

$$\Lambda = -k\nabla\theta, \tag{13}$$

insert the additive decomposition of ε and apply the chain rule for $\hat{\psi}$, then the inequality delivers

.....

Derivation of the model – II

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

Discussion of different cases:

- purely elastic deformation with θ constant in time and space, z constant in time: then $\varepsilon_t^{th} = 0, \ \varepsilon_t^{tp} = 0,$

  $\rightarrow$ reduced inequality

$$\left(\sigma - \varrho \frac{\partial \hat{\psi}}{\partial \varepsilon^{el}}(\varepsilon^{el}, \theta, z)\right) : \varepsilon_t^{el} \geq 0. \tag{14}$$

  $\rightarrow$ pointwise discussion delivers:

$$\sigma = \varrho \frac{\partial \hat{\psi}}{\partial \varepsilon^{el}}(\varepsilon^{el}, \theta, z) \tag{15}$$

Derivation of the model – III

By similar reasoning:

- set $\nabla\theta = 0$, $z_t = 0$, $\sigma = 0$, vary the sign of θ $\rightarrow$

$$s = -\frac{\partial\hat{\psi}}{\partial\theta}(\varepsilon^{el}, \theta, z), \tag{16}$$

$$\begin{aligned} s_t = (-\frac{\partial\hat{\psi}}{\partial\theta})_t &= -\left(\frac{\partial}{\partial\theta}(\frac{\partial\hat{\psi}}{\partial\varepsilon^{el}} : \varepsilon_t^{el}) + \frac{\partial}{\partial\theta}(\frac{\partial\hat{\psi}}{\partial\theta}\theta_t) + \frac{\partial}{\partial\theta}(\frac{\partial\hat{\psi}}{\partial z}z_t)\right) \\ &= -\frac{1}{\varrho}\frac{\partial\sigma}{\partial\theta} : \varepsilon_t^{el} + \frac{\partial s}{\partial\theta}\theta_t + \frac{\partial L}{\partial\theta}z_t = -\frac{1}{\varrho}\frac{\partial\sigma}{\partial\theta} : \varepsilon_t^{el} + c_\varepsilon\theta_t \geq 0, \end{aligned}$$

where $c_\varepsilon = \frac{\partial s}{\partial\theta}$ gives the specific heat capacity at constant strain and

$$L_i(\varepsilon^{el}, \theta, z) = -\frac{\partial\hat{\psi}}{\partial z_i}(\varepsilon^{el}, \theta, z) \tag{17}$$

the latent heat of the transition from austenite to phase z_i; we assume

$$\frac{\partial L}{\partial\theta} = 0. \tag{18}$$

Derivation of the model – IV

Thereby, differentiation of $e = \psi + \theta s$ with respect to time yields

$$
\begin{aligned}
e_t &= \psi_t + \theta_t s + \theta s_t \\
&= \frac{\partial\hat{\psi}}{\partial\theta}\theta_t + \frac{\partial\hat{\psi}}{\partial\varepsilon^{el}} : \varepsilon_t^{el} + \frac{\partial\hat{\psi}}{\partial z} z_t + \theta_t s + \theta\left(-\frac{1}{\varrho}\frac{\partial\sigma}{\partial\theta} : \varepsilon_t^{el} + \frac{\partial s}{\partial\theta}\theta_t\right) \\
&= -s\theta_t + \frac{1}{\varrho}\sigma : \varepsilon_t^{el} - L z_t + \theta_t s - \frac{1}{\varrho}\theta\frac{\partial\sigma}{\partial\theta} : \varepsilon_t^{el} + c_\varepsilon\theta_t \\
&= \frac{1}{\varrho}\sigma : \varepsilon_t^{el} - L z_t - \frac{1}{\varrho}\theta\frac{\partial\sigma}{\partial\theta} : \varepsilon_t^{el} + c_\varepsilon\theta_t. \qquad (19)
\end{aligned}
$$

Assume $\frac{\partial\varepsilon^{tp}}{\partial\theta} = 0$ and use $\frac{\partial\sigma}{\partial\theta} = -3bq(z)I$, then

$$
e_t = \frac{1}{\varrho}\sigma : \varepsilon_t^{el} - L z_t + \frac{1}{\varrho}\theta 3bq(z)I : \varepsilon_t^{el} + c_\varepsilon\theta_t. \qquad (20)
$$

Inserting these identities into the balance law of internal energy, $\varrho e_t + div\,\Lambda = \sigma : \varepsilon(v) + h$, one obtains ...

$$\alpha^\theta(\theta,\sigma,z)\theta_t - k\Delta\theta + 3bq(z)\theta\,\mathrm{div}\,\mathrm{u_t} = h + \alpha^z(\theta,\sigma,z)\cdot z_t + \gamma(\theta,z,z_t)|\sigma^*|^2 \quad \text{in} \quad Q := \Omega\times[0,T] \tag{21a}$$

$$-k\frac{\partial\theta}{\partial n} = \omega(x,t)(\theta-\theta_a) \quad \text{on} \quad \partial\Omega\times(0,T) \tag{21b}$$

$$\theta(0) = \theta_0 \quad \text{in} \ \Omega\,. \tag{21c}$$

The functions α^θ and α^z are given by

$$\alpha^\theta(\theta,\sigma,z) = \varrho c_\varepsilon - 9b\theta q(z)^2 - q(z)tr(\sigma) \tag{22}$$

$$\alpha_i^z(\theta,\sigma,z) = \varrho L_i + 9bq(z)(q_i-q_0)\theta^2 + 9bq(z)(q_i\theta_{i,ref} - q_0\theta_{0,ref})\theta + ((q_i-q_0)\theta + q_i\theta_{i,ref} - q_0\theta_{0,ref})\,tr(\sigma) \tag{23}$$

ϱ : mass density, c_ε : specific heat capacity. We require the q_i to be sufficiently small

- to have $\alpha^\theta(\theta,\sigma,z)$ positive
- to achieve existence of a solution by the forthcoming fixed point argumentations

$$-\operatorname{div}\sigma = F \quad \text{in} \quad Q \tag{24a}$$

$$\sigma = K\Big(\varepsilon(u) - \beta(\theta, z)I - \int_0^t \gamma(\theta, z, z_s)\sigma^* ds\Big) \quad \text{in} \quad Q \tag{24b}$$

$$u = 0 \quad \text{on} \quad \partial\Omega \times (0, T) \tag{24c}$$

$$z_t = \begin{pmatrix} f_1(\theta, z, \sigma) \\ f_1(\theta, z, \sigma) \end{pmatrix} \quad \text{in} \quad Q \tag{24d}$$

$$z(0) = 0 \quad \text{in} \quad \Omega \tag{24e}$$

$$f_1(\theta, z, \sigma) = (1 - z_1 - z_2)g_{11}(\theta)g_{12}(\sigma)$$

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

3 Analysis

Existence of a solution

$$
\begin{aligned}
\alpha^{\theta}(\theta,\sigma,z)\theta_t - k\Delta\theta + 3bq(z)\theta \operatorname{div} \mathrm{u_t} \\
&= h + \alpha^{z}(\theta,\sigma,z)\cdot z_t + \gamma(\theta,z,z_t)|\sigma^*|^2 \quad \text{in} \;\; Q, \\
-k\frac{\partial\theta}{\partial n} = \omega(x,t)(\theta-\theta^a) \quad \text{on} \;\; \partial\Omega\times(0,T), \qquad \theta(0)=\theta_0 \quad \text{in} \;\; \Omega,
\end{aligned}
$$

$$
\begin{aligned}
&-\operatorname{div}\sigma = F \quad \text{in} \;\; Q, \quad \sigma = K\Big(\varepsilon(u) - \beta(\theta,z)I - \int_0^t \gamma(\theta,z,z_s)\sigma^* ds\Big) \quad \text{in} \;\; Q, \\
&u = 0 \quad \text{on} \;\; \partial\Omega\times(0,T),
\end{aligned}
$$

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

- We require the q_i to be sufficiently small.

Existence of a solution

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

- We require the q_i to be sufficiently small.
- obtain solution the phase equations by Carathéodory's theorem, treat $\theta \in W_p^{2,1}(Q)$ and $\sigma \in W_p^{1,1}(Q)$ as data

$$-\operatorname{div}\sigma = F \quad \text{in} \quad Q, \quad \sigma = K\Big(\varepsilon(u) - \beta(\theta,z)I - \int_0^t \gamma(\theta,z,z_s)\sigma^* ds\Big) \quad \text{in} \quad Q,$$

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

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

- We require the q_i to be sufficiently small.
- obtain solution to the system momentum balance with phase equations by Schauder's fixed point theorem, mapping $M \to M$, $M \subset W_p^{1,1}(Q)$, $\tilde{\sigma} \mapsto z \mapsto \sigma$, treat $\theta \in W_p^{2,1}(Q)$ as data

Existence of a solution

$$\alpha^\theta(\theta,\sigma,z)\theta_t - k\Delta\theta + 3bq(z)\theta\,\mathrm{div}\,\mathrm{u_t}$$
$$= h + \alpha^z(\theta,\sigma,z)\cdot z_t + H \quad \text{in} \quad Q,$$
$$-k\frac{\partial\theta}{\partial n} = \omega(x,t)(\theta-\theta^a) \quad \text{on} \quad \partial\Omega\times(0,T), \qquad \theta(0)=\theta_0 \quad \text{in} \quad \Omega,$$

$$-\,\mathrm{div}\,\sigma = F \quad \text{in} \quad Q, \quad \sigma = K\Big(\varepsilon(u) - \beta(\theta,z)I - \int_0^t \gamma(\theta,z,z_s)\sigma^* ds\Big) \quad \text{in} \quad Q,$$
$$u = 0 \quad \text{on} \quad \partial\Omega\times(0,T),$$

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

- We require the q_i to be sufficiently small.
- obtain solution to the full system without quadratic stress term in the heat equation (replaced by some $H \in L^p(Q)$) by Banach's fixed point theorem, mapping $B \to B$, $B \subset W_p^{2,1}(Q)$, $\tilde\theta \mapsto (\sigma,z) \mapsto \theta$

Existence of a solution

$$\alpha^{\theta}(\theta,\sigma,z)\theta_t - k\Delta\theta + 3bq(z)\theta\,\mathrm{div}\,\mathrm{u_t}$$
$$= h + \alpha^{z}(\theta,\sigma,z)\cdot z_t + \gamma(\theta,z,z_t)|\sigma^*|^2 \quad \text{in} \quad Q,$$
$$-k\frac{\partial\theta}{\partial n} = \omega(x,t)(\theta-\theta^a) \quad \text{on} \quad \partial\Omega\times(0,T), \qquad \theta(0)=\theta_0 \quad \text{in} \quad \Omega,$$

$$-\,\mathrm{div}\,\sigma = F \quad \text{in} \quad Q, \quad \sigma = K\Big(\varepsilon(u) - \beta(\theta,z)I - \int_0^t \gamma(\theta,z,z_s)\sigma^*\,ds\Big) \quad \text{in} \quad Q,$$
$$u = 0 \quad \text{on} \quad \partial\Omega\times(0,T),$$

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

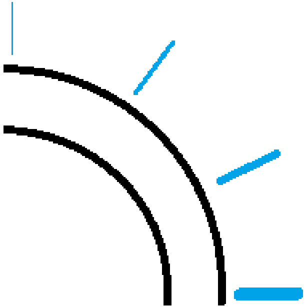
- We require the q_i to be sufficiently small.
- obtain solution to the full system by Schauder's fixed point theorem, mapping $S\to S$, $S\subset W_p^{2,1}(Q)$, $\tilde\theta \mapsto (\sigma,z)\mapsto \gamma(\theta,z,z_t)|\sigma^*|^2 \mapsto \theta$

4 Application

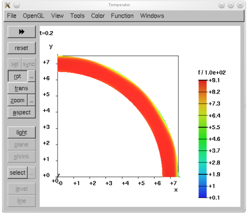
- Numerical results for 100Cr6

Numerical results

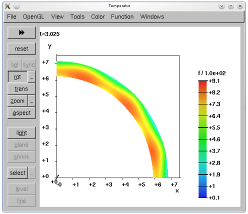
- steel 100Cr6 (one product phase martensite besides remaining austenite)
- inhomogenous cooling of a cylindric ring: cooling ranging from little at 12 o'clock position to much at 3 o'clock position :



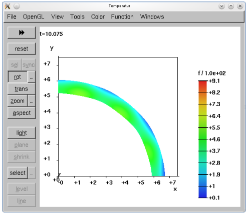
TrIP effect



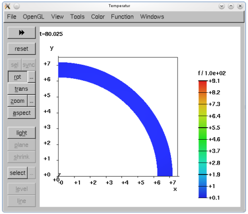
start time



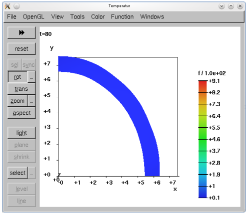
beginning transformation



ongoing transformation



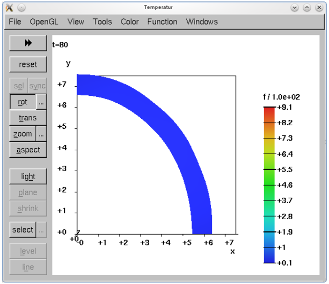
a) end time without TrIP

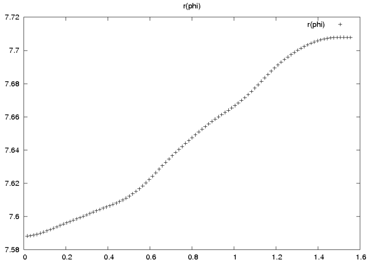


b) end time including TrIP

Initial shrinkage "frozen" by TrIP effect.

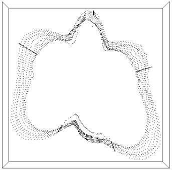
Remaining displacement





- goal: use this effect for distortion compensation
- given start geometries that exhibit "unroundness"
- try to achieve displacement function that annihilates this unroundness and results in a circular ring shape

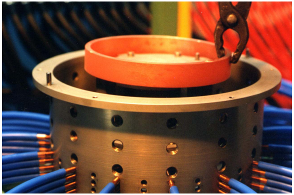
- Problem:
  - accumulation of internal stresses during process chain
  - leads to distortion (undesired alterations in size and shape) of roller bearing rings prior to hardening – “out-of-roundness”



"out-of-roundness"

- Solution: optimal control of phase transitions to compensate distortion

  2 variants:
  - control of phase mixture
  - control of phase growth rates



experiment at Institute for Material Science, IWT Bremen

5 Optimization

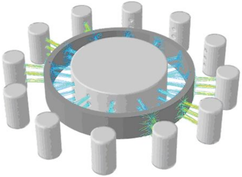
Control problem under investigation

$$\text{Minimize } J(u,\theta,w) = \frac{\alpha_u}{2}\int_0^T\int_\Omega F(u)\,dx\,dt + \frac{\alpha_w}{2}\int_0^T |w|^2 dt$$

s.t.

$$-\,div\,\sigma = f, \qquad u = 0 \quad on\ \Gamma_0, \qquad -\sigma\nu = 0 \quad on\ \Gamma_1$$

$$\sigma = K\left(\varepsilon(u) - q(z,\theta)I - \int_0^t \frac{3}{2}\zeta h(\theta,z) S\,d\tau\right)$$



$$z_t = h(\theta,z), \qquad z(0) = 0$$

$$\theta_t - \Delta\theta = 0, \quad \theta(0) = \theta_0$$

$$-k\partial_\nu\theta = \sum_i \beta_i(x) w_i(t)(\theta - \theta_a)$$

$$w_i \in U_{ad} = \{v \in L^2(0,T)\,;\ 0 \le v(t) \le w_{max}\}$$

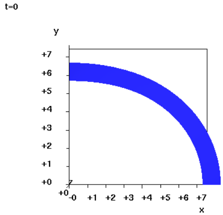
Adjoint equations

$$
\begin{aligned}
\rho c p^{\theta} - k\Delta p^{\theta} &= \partial_\theta h(\theta(T{-}t), z(T{-}t))p^{z} + 3\kappa\partial_\theta q(\theta(T{-}t), z(T{-}t))div(p^{u}) \\
&\quad + 3\zeta\mu(\sum_i \partial_\theta h_i(\theta(T{-}t), z(T{-}t))(\varepsilon^*(u(T{-}t)) - \varepsilon^{trip}(T{-}t)) : p^{trip} \\
-\partial_\nu p^{\theta} &= \frac{1}{k}\beta(x)w(T{-}t)p^{\theta}, \qquad p^{\theta}(0) = 0 \\
p_t^{z} &= \partial_z h(\theta(T{-}t), z(T{-}t))p^{z} + 3\kappa\partial_z q(\theta(T{-}t), z(T{-}t))div(p^{u}) \\
&\quad + 3\zeta\mu(\sum_i \partial_z h_i(\theta(T{-}t), z(T{-}t)))(\varepsilon^*(u(T{-}t)) - \varepsilon^{trip}(T{-}t)) : p^{trip} \\
p^{z}(0) &= 0 \\
-div(p^{\sigma}) &= \alpha_u\partial_u F(u(T{-}t)), \qquad p^{u} = 0 \text{ on } \Gamma_0, \qquad p^{\sigma}n = 0 \text{ on } \Gamma_1 \\
p^{\sigma} &:= K\varepsilon(p^{u})) - 3\zeta\mu(\sum_i h_i(\theta(T{-}t), z(T{-}t)))p^{trip,*} \\
p_t^{trip} &= 2\mu\varepsilon(p^{u}) - 3\zeta\mu(\sum_i h_i(\theta(T{-}t), z(T{-}t)))p^{trip}, \qquad p^{trip}(0) = 0
\end{aligned}
$$

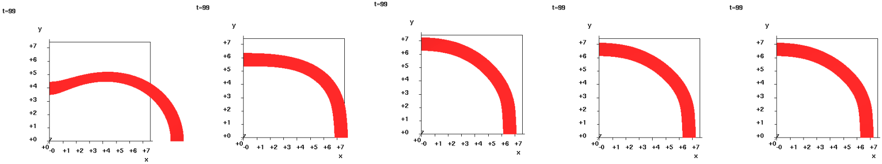
$$
\text{Gradient} \quad \alpha_w w - \int_\Gamma \beta(\theta - \theta^{a})p^{\theta}(T{-}t).
$$

Martensite and deformation

at initial time (same for all gradient steps):



final time of different gradient steps :



The end

Thank you very much!