Adaptive FEM for mesoscopic models of phase transformations in steel

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Work in progress

Phase transitions in steel

Motivation: Special research project in Bremen:
SFB 570 “Distortion Engineering”
(engineering project, joint with applied math)

Study (both experimentally and numerically)
mechanisms which lead to distortions (= unwanted deformations)
during production of steel workpieces
(steeels 100Cr6 and 20MnCr5)

Final goal: minimize distortions

Various steps of production: forming, cutting, ..., heat treatment.
Phase transitions in steel

Here: **solid-solid phase transitions during heat treatment**
expecially: Cooling of a hot steel workpiece

Transformation between solid phases:
Austenite $\rightarrow$ Pearlite - Bainite (-Martensite)

Here: consider diffusive transformations ($A\rightarrow P,B$)

Different phases have different densities and thermal expansion parameters: leads to thermoelastic stresses and deformations

**Macroscopic models** wanted for simulation of complete workpiece (like a cogwheel, e.g.)
Phase transitions in steel

Macroscopic variables:

- temperature,
- phase fractions,
- elastic and plastic deformations,
- (concentrations of carbon and additional ingredients)

Interactions:
Macroscopically observable effects:

<table>
<thead>
<tr>
<th>Temp → PT</th>
<th>dependence of PT on temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>PT → Temp</td>
<td>latent heat, release or consumption</td>
</tr>
<tr>
<td>Temp → Def</td>
<td>thermal expansion, density depends on T</td>
</tr>
<tr>
<td>Def → Temp</td>
<td>dissipation of mechanical energy to heat</td>
</tr>
<tr>
<td>PT → Def</td>
<td>density depends on phase, TRIP</td>
</tr>
<tr>
<td>Def → PT</td>
<td>stress dependent PT</td>
</tr>
</tbody>
</table>
Multi-scale phenomenon
Various time/space scales:

- Temperature diffusion: fast, long-range
- Chemical diffusion in solids: slow, short-range
- Diffusion of C in transition layer: very short range, relatively fast
- Phase transition $A \rightarrow P$: several (many) seconds for macroscopic transition, temperature may vary substantially meanwhile
Selection of scale – selection of model

**Macro:** work piece (1-100 cm),
continuum mechanics, no grain structure,
temperature diffusion,
phase fraction (mean value over reference volume)

**Meso 1:** multiple grains (10-100 µm)
continuum mechanics, grain structure, resolve austenite-pearlite PT,
non-conservative, nearly no diffusion of C

**Meso 2:** one or few grains (0.1-10 µm)
continuum mechanics, grain structure,
resolve structure of pearlite (lamella of ferrite and carbide),
diffusion of C in transition layer, Fe and C conserved

**Micro:** scale of atoms / clusters (nm),
plastic deformation by relocation of atoms, MD/MC simulations,
energy potentials for Fe/C/Cr/Mn mixtures? temperature? time-scale?
Macroscopically observable behaviour (dilatometer experiments)

Measure temperature and length changes of a small cylinder (assumed homogeneous)

Temperature, measured change in length (%), length change over $T$

Compute experimental phase fraction:
Phase transitions in steel

Classical macroscopic model describing diffusive phase transitions:

**Johnson-Mehl-Avrami (JMA) equation**

\[ p(t) = 1 - \exp \left( -\left(\frac{t}{\tau}\right)^n \right) \]

or its differential form

\[ p'(t) = \left(1 - p(t)\right) \frac{n}{\tau} \left(-\ln(1 - p(t))\right)^{\frac{n-1}{n}} \]

\(n, \tau\): material parameters, depending on temperature, stress, ...

Derivation based on mesoscopic model with constant nucleation rate and growth rate of pearlite grains

OK for isothermal phase transitions

Other, extended models for macroscopic phase transitions, for example by D. Hömberg
Mesoscopic behaviour:

Picture from experiment: Pearlite transition

Sketch of mesoscopic phase transition (grain size approx. 10-50 \( \mu \text{m} \))
Phase transitions in steel

3d model for mesoscopic phase transition [Hunkel]
Stress dependent phase transition:
Phase transformation is faster when external force is applied!
Transformation induced plasticity (TRIP):
During phase transformations, even relatively small applied stresses (below the yield stress) lead to permanent (plastic) deformations.

Macroscopic model:
during restructuring of the crystal structure, plastic deformations can easily take place.
Simple model: ODE for the TRIP strain component, for example

\[ \varepsilon'_{TRIP}(t) = a(t)\left( \varepsilon^*(t) - \varepsilon_{TRIP}(t) \right) \]

(plastic deformation is non-deviatoric)

Mesoscopic model:
Effects are due to classical plasticity on the mesoscopic scale, where the yield stress may be reached.
Phase transitions in steel

Some modifications of JMA equation are available, but not satisfying (for example only applicable for a narrow range of cooling rates, or constant stress)

Heat treatment of a complicated work piece (cogwheel, e.g.): varying cooling conditions over the geometry, varying stresses due to temperature and phase distribution, or generated by previous production steps

Need better models! ⇒ mesoscale models and simulations
Mesoscale modelling

**Meso 1:** multiple grains (10-100 µm) 
continuum mechanics, grain structure, resolve austenite-pearlite PT, 
non-conservative, nearly no diffusion of C

Phase boundaries in grains change topology:

- new pearlite regions nucleate,
- union of initially separate regions,
- no boundaries left in case of full transformation
Due to topology changes (especially in 3D!), *phase field models* are more appropriate than sharp interface models for phase boundary motion.

Finite element simulations $\Rightarrow$ **Adaptivity** is needed (especially in 3D)

For example:
Error estimators and adaptive methods for temperature-driven phase field problem with Allen-Cahn equation
[Chen, Nochetto, S.], [Kessler, Nochetto, S.]
Mesoscale modelling

Appropriate phase field models in the literature?

- many liquid-solid, not solid-solid,
- martensitic transformations (these are different, instantaneous)
- phase separation (conserved order parameter) (including elasticity) [Garcke, Garcke/Rumpf/Weickart, e.g.]
- solid-solid transitions including crystal orientations (shape memory alloys)
- surface diffusion (including elasticity), [John Barrett’s talk, ...]
- ...
- only few for diffusive phase transitions in steel!
Example of a model from literature:

Jérôme Paret (2001):
Phase field model of stressed incoherent solid-solid interfaces

Free energy functional:

$$ F = \int_{\Omega} \gamma \varepsilon^2 |\nabla \phi|^2 + g(\phi) + f_{el}(\phi, \Sigma) $$

with stress-dependent term

$$ f_{el}(\phi, \Sigma) = \frac{1 + \nu(\phi)}{2E(\phi)} \Sigma : \Sigma - \frac{\nu(\phi)}{2E(\phi)} \text{tr} \Sigma^2 $$

with appropriate stress coefficients $E(\phi), \nu(\phi)$ varying smoothly between the corresponding values for the pure phases.

(remember John Barrett’s talk: $\cdots + d\gamma(\phi)C\mathcal{E} : \mathcal{E}$)
Asymptotic analysis leads to the sharp interface limit

\[ V = -c \left( \frac{E_\beta - E_\alpha}{2E_\beta^2} \left( \Sigma_{tt} - \Sigma_{nn} \right)^2 + \gamma \kappa \right) \]

where \( \alpha, \beta \) denote the two pure phases, \( n, t \) normal and tangential directions to the interface, \( \kappa \) its curvature.

Difference of elastic moduli, combined with stresses at the interface determine the interface velocity.

Model has severe restrictions (purely stress-driven phase transition, no temperature or concentration fields, ...) but can give hints in which direction to proceed
**Phase field model** with double obstacle potential for temperature $\theta$ and phase variable $\varphi$

\[
\partial_t (\theta + \lambda \varphi) - \Delta \theta = f
\]

\[
\varepsilon \partial_t \varphi - \varepsilon \text{div}(a(\nabla \varphi)) + \Lambda(\varphi) - \frac{1}{\varepsilon} \beta \varphi \ni \gamma \theta
\]

in $\Omega \times (0, T')$ plus B.C. and I.C.

$\Lambda$ is a maximal monotone graph (set valued), subdifferential of the double obstacle potential,

\[
\Lambda(s) = \begin{cases} 
(-\infty, 0] & \text{if } s = -1 \\
0 & \text{if } s \in (-1, 1) \\
[0, +\infty) & \text{if } s = +1
\end{cases}
\]

with the effect that values of $\varphi$ are in the interval $[-1, +1]$. 

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Mesoscale modelling
Augment this model with stress dependent terms and couple with (quasi-static) elasticity equation, for example:

\[
\partial_t (\theta + \lambda \varphi) - \text{div}(\kappa \nabla \theta) = f
\]

\[
\varepsilon \partial_t \varphi - \varepsilon \text{div}(a(\nabla \varphi)) + \Lambda(\varphi) - \frac{1}{\varepsilon T} \beta \varphi \geq \gamma \theta - c \Sigma : \Sigma
\]

\[
\text{div}(2 \mu \varepsilon + \lambda \text{tr} \varepsilon I) = -\text{div}(3K \alpha (\theta - \theta_0) I)
\]

\[
-\text{div}(K(\frac{\sum p_i / \rho_i}{\sum \rho_0 / \rho_0} - 1) I)
\]

plus B.C. and I.C.,

where \( \varepsilon = 0.5(\nabla u + (\nabla u)^T) \) linearized strain tensor.

Rhs of elasticity equation models dependence of density on temperature and phase fractions.

Remember: Transformation should be faster when stress is applied!
\[ \Rightarrow \text{Minus-sign in front of } \Sigma : \Sigma \]
This is just a first test to see the influence of stress on the transformation.

Concentration-driven transformation would be more appropriate, as heat diffusion is very fast on the scale of grains.

Isothermal model! ?

But additional temperature-dependence of coefficients / energy is needed for modelling non-isothermal situations.
(VERY preliminary) results of some numerical tests:

Single grain-like geometry, no external force, cooling from left, nucleation of new phase in left corner.

Simulation without stress term in energy:
phase variable after 100, 120, 140, 200 steps
Simulation with stress term:

Phase variable, temperature, stress, deformation after 100 steps
Simulation with stress term:

Phase variable and stress after 100 steps

Phase variable and stress after 120 steps
Comparison of phase fractions with / without elasticity.