On the Modeling and Homogenization of Bainitic Phase Transformations in Steel

Michael Eden

University of Bremen

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WG Modeling and PDEs

- Group Leader: Prof. Michael Böhm
- Scientific Staff: Dr. Michael Wolff, Martin Höpker, Simon Grützner, Michael Eden

- Principles of field theory (M. Böhm)
- Multi-scale modeling/thermodynamics on interfaces (M. Wolff)
- Extension operators for Sobolev functions on periodic domains (M. Höpker)
- Damage models and parameter identification for damaged continua (S. Grützner)

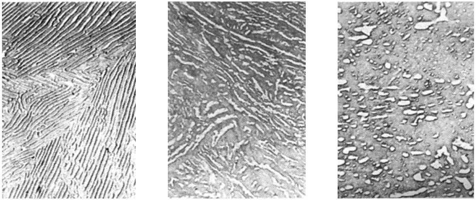
Contents

Overview

Motivation

- **Steel**: alloy of *Iron*, *Carbon* (and other elements)
- Characterized by a complex multiscale material behaviour

Standard steel coil



Different steel microstructures

Motivation behind my Research

- Macroscopic mechanical properties of materials like steal are often influenced/caused by microscale effects.
- Prominent examples for
  - **microscale** phenomenons: *phase transformations*, *dislocations*, *crystal orientation*,
  - **macroscale** phenomenons: *crystal plasticity*, *transformation induced plasticity (TRIP)*,

$\leadsto$ (very general) **Goal/Idea**: Investigate connections of those phenomenons via homogenization, especially:

  - *(Bainitic) phase transformations* $\leftrightarrow$ *TRIP*

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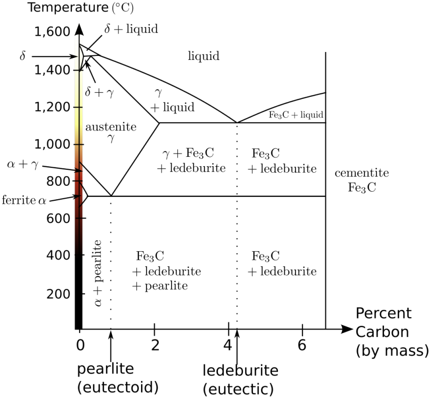
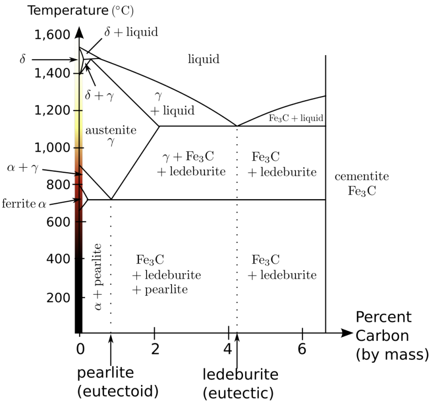
Overview

Microstructures/Phases



Microstructures/Phases



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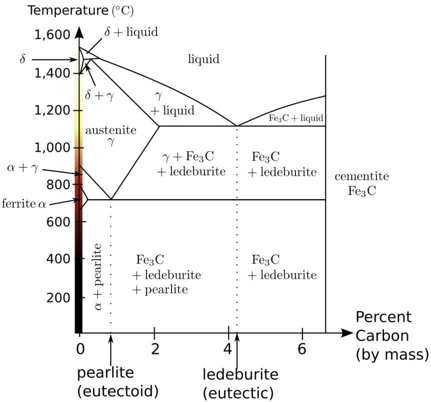

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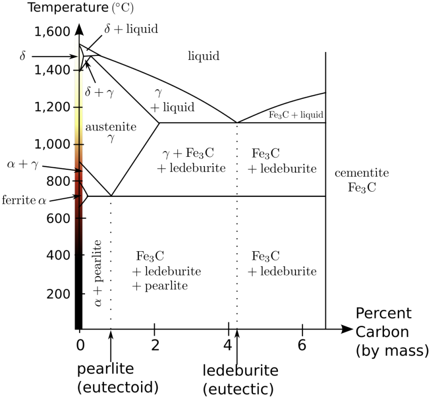

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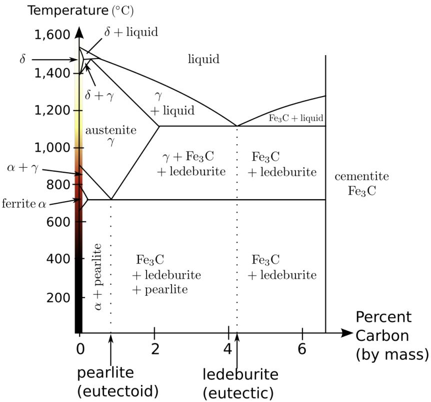

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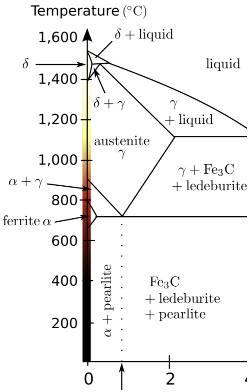
$\rightsquigarrow$ Non-equilibrium micro structures!

Bainite



- Non-equilibrium micro structure,
- consits of *cementite* (Fe_3C) and *ferrite*,
- forms from undercooled (range 250-550°C) *austenite* when (significant) diffusion of iron is not possible anymore,

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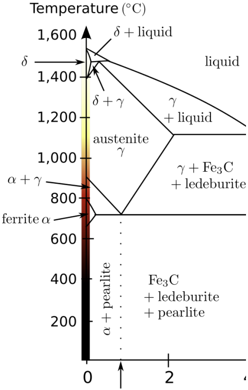

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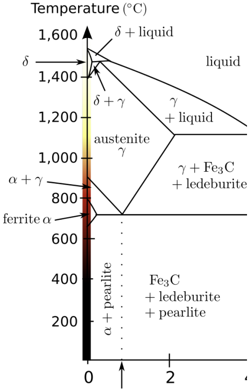

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  ⇝? Cause/contributor to macroscale effects like TRIP

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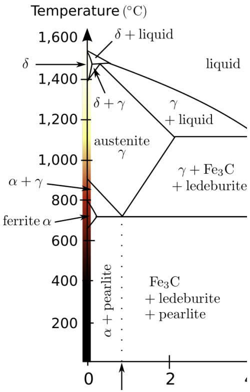

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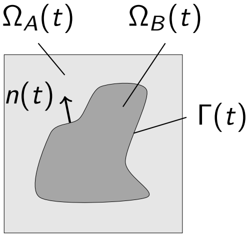
General Setting

- Two phases present, Austenite, $\Omega_A(t)$, and Bainite, $\Omega_B(t)$
- $\Gamma(t)$ is a sharp (free moving) interface,

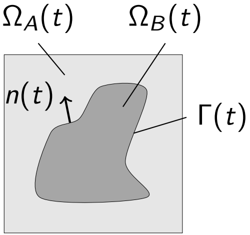


Geometry at time t.

General Setting

- Two phases present, Austenite, $\Omega_A(t)$, and Bainite, $\Omega_B(t)$
- $\Gamma(t)$ is a sharp (free moving) interface,
- Notations:

$$n(t) = \text{outer normal vector of } \Omega_B(t),$$
$$W_\Gamma(t) = \text{velocity of } \Gamma(t) \text{ in } n(t) \text{ direction},$$
$$H_\Gamma(t) = \text{mean curvature of } \Gamma(t),$$
$$Q_i = \bigcup_{t\in(0,T)} (\{t\} \times \Omega_i(t)),$$
$$\Sigma = \bigcup_{t\in(0,T)} (\{t\} \times \Gamma(t)).$$



Geometry at time t.

General Scenario

We need to consider the following effects

- Mechanic: Deformations, stresses
- Energy: Internal energy, heat flux, dissipation
- Carbon content: concentration, diffusion, precipitation
- Phase transformation $\rightsquigarrow$ Interface movement
- Transmission conditions at interface $\rightsquigarrow$ Jump conditions

Mechanic

u_i - deformation vectors, P_i - Piola-Kirchhoff stress tensors, θ_i - temperatures ($i \in \{A, B\}$)

$$\begin{aligned} \rho_A \partial_{tt} u_A - \operatorname{div} P_A &= f_{u_A} && \text{in} \quad Q_A, \\ \rho_B \partial_{tt} u_B - \operatorname{div} P_B &= f_{u_B} && \text{in} \quad Q_B, \end{aligned}$$

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Assumptions:

1. Quasi-stationary mechanics

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Assumptions:

1. Quasi-stationary mechanics
2. Linear Thermoelasticity: $P_i = C_i e(u_i) - \alpha_i \theta_i \mathbb{I}_3$, $e(u) = \frac{1}{2}\left(\nabla u + \nabla u^T\right)$

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[\![u]\!] &= 0 && \text{on} \quad \Sigma, \\
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Energy balance

e_i - internal energies, Q_i - heat fluxes

$$\rho_A \partial_t e_A + \operatorname{div} Q_A = f_{\theta_A} + P_A : \nabla \partial_t u_A \quad \text{in} \quad Q_A,$$
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Assumptions:

1. Internal energy is given as $e_i = c_{di} \theta_i$
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Mass balance (carbon)

c_i - carbon concentration, Φ_i - carbon fluxes

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Assumptions:

1. Fick's law of diffusion: $\Phi_i = -D_i(\theta_i)\nabla c_i$

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Assumptions:

1. Fick's law of diffusion: $\Phi_i = -D_i(\theta_i)\nabla c_i$
2. $f_{c\Gamma}$: carbon well due to the precipitation of $\mathrm{Fe_3C}$ (*cementite*)

Interface movement

- Common approaches (often scaled to $\theta_{crit} = 0$):

$$\begin{aligned} \theta &= \theta_{crit} && \textit{(classical condition)}, \\ \theta &= \theta_{crit} + \sigma_0 H_\Gamma && \textit{(Gibbs-Thomson law)} \end{aligned}$$

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  - In the following: W_Γ *a priori* known!

Summary of the Model Equations

Model equations for *deformations* u_i, *temperatures* θ_i, and *carbon concentrations* c_i:

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\begin{aligned}
-\operatorname{div}\left(C_i e(u_i) - \alpha_i \theta_i \mathbb{I}_3\right) &= f_{u_i} \quad &(\textbf{Momentum bal.}),\\
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Periodic Setting

- Periodic domains $\Omega_A^\varepsilon(0)$, $\Omega_B^\varepsilon(0)$ and periodic interface $\Gamma^\varepsilon(0)$,
- $\Omega_A^\varepsilon(t) \cap \Omega_B^\varepsilon(t) = \emptyset$,
- $\Gamma^\varepsilon(t) = \partial\Omega_B^\varepsilon(t)$,
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- $\Omega = \Omega_A^\varepsilon(t) \cup \Omega_B^\varepsilon(t) \cup \Gamma^\varepsilon(t)$ time independent,
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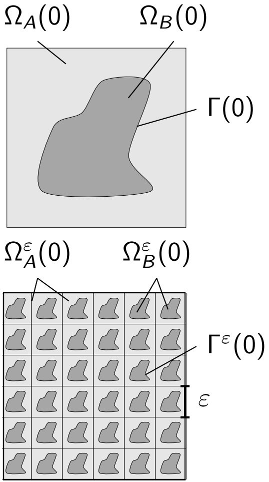

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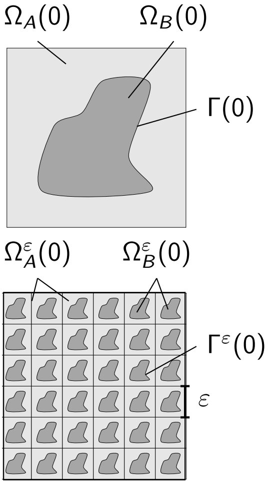

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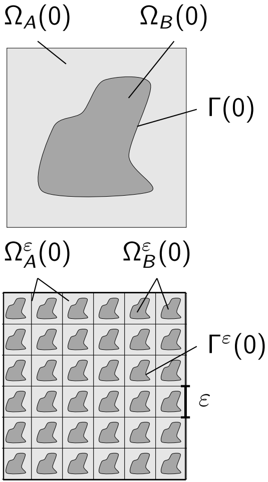

Interface movement

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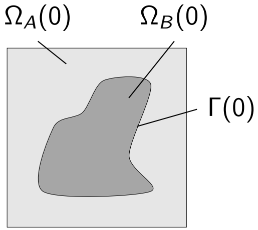

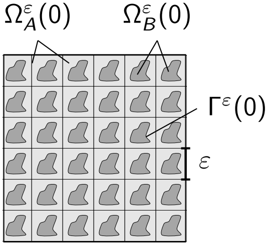

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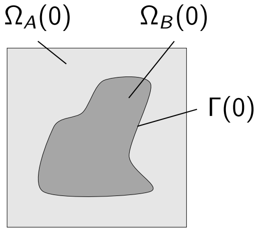

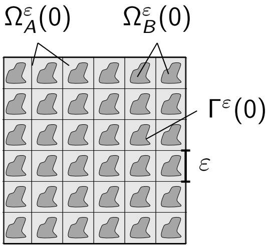

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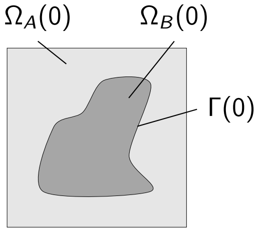

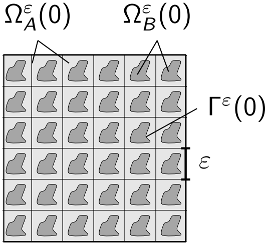

ε-scaling

Balance equations:

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\begin{aligned}
-\operatorname{div}\big(C_A e(u_A^\varepsilon) - \alpha_A\theta_A\mathbb{I}_3\big) &= f_{u_A}^\varepsilon,\\
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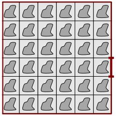

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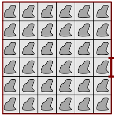

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Overview

Analysis of the model

1. Transform the system to the initial configuration ($u^\varepsilon = U^\varepsilon(s^\varepsilon)$)

$$-\operatorname{div}(C_i^{ref} e(U_i^\varepsilon) - \Theta_i^\varepsilon \alpha_i^{ref}) = f_{u_i}^{ref} \quad \text{in} \quad \Omega_i^\varepsilon, \ t \in S,$$

$$\partial_t(c_i^{ref}\Theta^\varepsilon + \gamma_i^{ref} : \nabla U_A^\varepsilon) + \operatorname{div}((\gamma_i^{ref} : \nabla U_A) b^{ref})$$

$$-\operatorname{div}(K_i^{ref}\nabla\Theta^\varepsilon + \Theta^\varepsilon b^{ref}) = f_{\theta_i}^{ref} \quad \text{in} \quad S \times \Omega_i^\varepsilon.$$

2. Corresponding operator formulation

$$E_C^\varepsilon(t)U^\varepsilon - e_{te}^\varepsilon(t)\Theta^\varepsilon = \mathcal{F}_u^\varepsilon(t) \quad \text{in } H^{-1}(\Omega)^3,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(B_\theta^\varepsilon(t)\Theta^\varepsilon + B_u^\varepsilon(t)U^\varepsilon) + A_\theta^\varepsilon(t)\Theta^\varepsilon + A_u^\varepsilon(t)U^\varepsilon = \mathcal{F}_\theta^\varepsilon(t) \quad \text{in } H^1(\Omega)^*.$$

3. Existence of a unique solution in $L^2(S; H_0^1(\Omega)^3 \times H^1(\Omega))$.

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Analysis of the model

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3. Existence of a unique solution in $L^2(S; H_0^1(\Omega)^3 \times H^1(\Omega))$.
4. Establishing a priori estimates:

$$\|\Theta^\varepsilon\|_{L^\infty(S;L^2(\Omega))} + \|\nabla\Theta_A^\varepsilon\|_{L^2(S\times\Omega_A^\varepsilon)^3} + \varepsilon\|\nabla\Theta_B^\varepsilon\|_{L^2(S\times\Omega_B^\varepsilon)^3} \leq C,$$
$$\operatorname*{ess\,sup}_{t\in S}\left(\|U^\varepsilon\|_{L^2(\Omega)^3} + \|e(U_A^\varepsilon)\|_{L^2(\Omega_A^\varepsilon)^{3\times3}} + \varepsilon\|e(U_B^\varepsilon)\|_{L^2(\Omega_B^\varepsilon)^{3\times3}}\right) \leq C.$$

Analysis of the model

1. Transforming the system to the referential configuration
2. Corresponding operator formulation

$$E_C^\varepsilon(t)U^\varepsilon - e_{te}^\varepsilon(t)\Theta^\varepsilon = \mathcal{F}_u^\varepsilon(t) \quad \text{in } H^{-1}(\Omega)^3,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(B^\varepsilon(t)\Theta^\varepsilon\right) + A^\varepsilon(t)\Theta^\varepsilon = \mathcal{F}^\varepsilon(t) \quad \text{in } H^1(\Omega)^*.$$

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Overview

Two-scale convergence

Definition

A sequence v^ε in $L^2(S \times \Omega)$ two-scale converges to $v_0 \in L^2(S \times \Omega \times Y)$, $(v^\varepsilon \overset{2}{\to} v_0)$, if, for all $\varphi \in L^2(S \times \Omega; C_\#(Y))$, we have that

$$\lim_{\varepsilon \to 0} \int_Q v^\varepsilon(t,x)\varphi(t,x,\frac{x}{\varepsilon})\,\mathrm{d}x\,\mathrm{d}t = \int_Q \int_Y v(t,x,y)\varphi(t,x,y)\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}y.$$

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Theorem (Nguetseng 1989, Allaire 1992)

Let v^ε be a bounded sequence in $L^2(S \times \Omega)$. Then, there exists a function $v \in L^2(S \times \Omega \times Y)$ such that, at least up to a subsequence, $v^\varepsilon \overset{2}{\to} v_0$.

Theorem (Existence of two-scale limit functions)

There are

$$\begin{aligned}
u_A &\in L^2(S; H_0^1(\Omega))^3 && \textit{such that} \;\; \partial_t u_A \in L^2(S \times \Omega)^3, \\
U_B &\in L^2(S \times \Omega; H^1_\#(Y))^3 && \textit{such that} \;\; \partial_t U_B \in L^2(S \times \Omega \times Y)^3, \\
\theta_A &\in L^2(S; H^1(\Omega)) && \textit{such that} \;\; \partial_t \theta_A \in L^2(S \times \Omega), \\
\Theta_B &\in L^2(S \times \Omega; H^1_\#(Y)) && \textit{such that} \;\; \partial_t \Theta_B \in L^2(S \times \Omega \times Y), \\
\widehat{U}_A &\in L^2(S \times \Omega; H^1_\#(Y))^3, && \textit{and} \;\; \widehat{\Theta}_A \in L^2(S \times \Omega; H^1_\#(Y))
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\end{aligned}
$$

such that for a subsequence of $(U_A^\varepsilon, U_B^\varepsilon, \Theta_A^\varepsilon, \Theta_B^\varepsilon)$

$$
\begin{aligned}
U_A^\varepsilon &\overset{2}{\to} u_A, & e(U_A^\varepsilon) &\overset{2}{\to} e(u_A) + e_Y(\widehat{U}_A),\\
U_B^\varepsilon &\overset{2}{\to} U_B, & e(U_B^\varepsilon) &\overset{2}{\to} e_Y(U_B),\\
\chi_A^\varepsilon\Theta_A^\varepsilon &\overset{2}{\to} \chi_A\theta_A, & \chi_A^\varepsilon\nabla\Theta_A^\varepsilon &\overset{2}{\to} \chi_A(\nabla\theta_A + \nabla_Y\widehat{\Theta}_A),\\
\chi_B^\varepsilon\Theta_B^\varepsilon &\overset{2}{\to} \chi_B\Theta_B, & \varepsilon\chi_B^\varepsilon\nabla\Theta_B^\varepsilon &\overset{2}{\to} \chi_B\nabla_Y\Theta_B.
\end{aligned}
$$

Homogenized problem

- The macroscopic equations for the austenite:

$$-\operatorname{div}\left(C_A^{eff} e(u_A) - \alpha_A^{eff}\theta_A\right) = f_u^{eff} + H_\Gamma^{eff} \quad \text{in} \quad S \times \Omega,$$

$$\partial_t\left(c^{eff}\theta_A + \rho_B c_{dB}\int_{Y_B(t,x)}\theta_B \,\mathrm{d}y + \gamma_A^{eff} : \nabla u_A\right)$$

$$-\operatorname{div}\left(K_A^{eff}\nabla\theta_A\right) = W_\Gamma^{eff} + f_\theta^{eff} \quad \text{in} \quad S \times \Omega.$$

Homogenized problem

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$$-\operatorname{div}\left(C_A^{eff}e(u_A)-\alpha_A^{eff}\theta_A\right)=f_u^{eff}+H_\Gamma^{eff}\quad \text{in}\quad S\times\Omega,$$

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$$\partial_t\left(c^{eff}\theta_A + \rho_B c_{dB}\int_{Y_B(t,x)} \theta_B \,\mathrm{d}y + \gamma_A^{eff} : \nabla u_A\right)$$

$$-\operatorname{div}\left(K_A^{eff}\nabla\theta_A\right) = W_\Gamma^{eff} + f_\theta^{eff} \quad \text{in} \quad S \times \Omega.$$

- The microscopic equations for the bainite ($t \in S$, $x \in \Omega$)

$$-\operatorname{div}_Y\left(C_B e_Y(u_B) - \alpha_B\theta_B\mathbb{I}_3\right) = f_{Bu} \quad \text{in} \quad Y_B(t,x),$$

$$\rho_B c_{dB}\partial_t\theta_B + \gamma_B\partial_t \operatorname{div}_Y u_B - \operatorname{div}_Y\left(K_B\nabla_Y\theta_B\right) = f_{\theta_B} \quad \text{in} \quad Y_B(t,x),$$

$$u_B = u_A, \quad \theta_B = \theta_A \quad \text{on} \quad \partial Y_B(t,x).$$

Overview

- Simplified problem:
  - Corrector estimates
  - Properties of the homogenized problem
- Full problem: (with unknown interface movement)
  - highly nonlinear, but there are results (Escher et al., 2003, Prüss et al., 2013)
    - Local in time solution: What happens when $\varepsilon \to 0$?
    - Also a problem: establishing ε estimates

Thank you for listening.

Tack så mycket för er uppmärksamhet!

Danke für die Aufmerksamkeit!