Phase transformation in steel

austenite & cementite to ferrite & cementite

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Introduction

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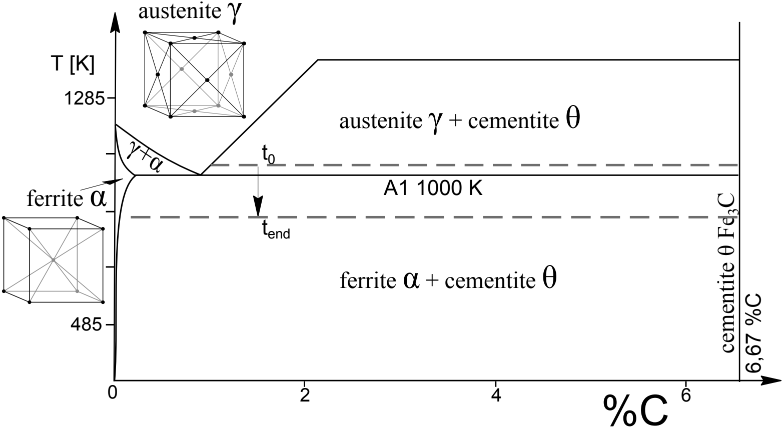
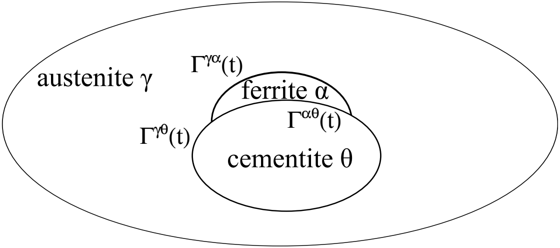
Steel

Steel



austenite γ
T [K]
1285
485
γ+α
ferrite α
t0
A1 1000 K
tend
austenite γ + cementite θ
ferrite α + cementite θ
cementite θ Fe3C
6,67 %C
0
2
4
6
%C

Model



$$
\begin{cases}
\frac{\partial c_{\gamma/\alpha}}{\partial t}(\mathbf{x},t) = \nabla \cdot \left(D_{\gamma/\alpha}(\mathbf{x},t) \nabla \frac{\partial c_{\gamma/\alpha}}{\partial n}(\mathbf{x},t) \right) & , \mathbf{x} \in \Omega_{\gamma/\alpha}(t) \\
c_\theta(\mathbf{x},t) = c_\theta & , \mathbf{x} \in \Omega_\theta(t) \\
\frac{\partial c}{\partial n}(\mathbf{x},t) = 0 & , \mathbf{x} \in \partial\Omega \\
\text{BC} \quad \Gamma^{\gamma\alpha}(t), \Gamma^{\gamma\theta}(t), \Gamma^{\alpha\gamma}(t), \Gamma^{\alpha\theta}(t), t > t_0 \\
\text{Initial conditions } c_\gamma(\mathbf{x},t_0), c_\alpha(\mathbf{x},t_0), \Gamma^{\gamma\alpha}(t_0), \Gamma^{\gamma\theta}(t_0), \Gamma^{\alpha\theta}(t_0)
\end{cases}
$$

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BC $\Gamma^{\gamma\alpha}, \Gamma^{\gamma\theta}, \Gamma^{\alpha\gamma}, \Gamma^{\alpha\theta}$

Stefan condition from mass conservation, for $\Gamma^{\gamma/\alpha\theta}$:

$$(c_{\gamma/\alpha} - c_\theta)\frac{d\Gamma^{\gamma/\alpha\theta}}{dt} = D_{\gamma/\alpha}\frac{\partial c_{\gamma/\alpha}}{\partial n} - \cancel{D_\theta\frac{\partial c_\theta}{\partial n}}$$

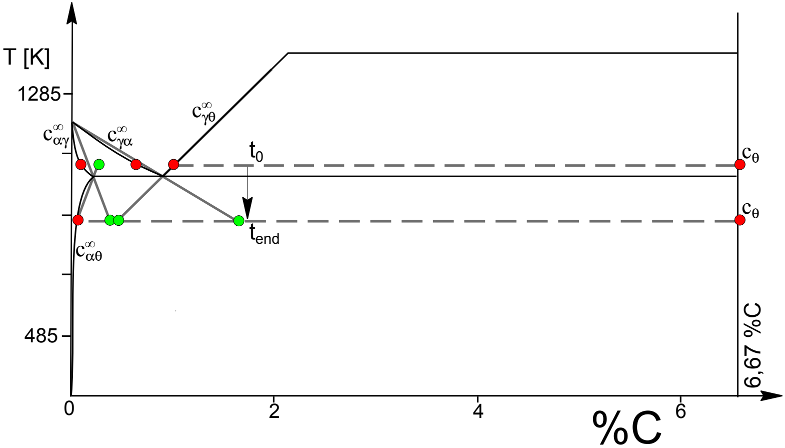
- $\frac{d\Gamma^{\gamma/\alpha\theta}}{dt}$ described by first-order reaction flux.

for $\Gamma^{\gamma\alpha}$:

$$(c_\gamma - c_\alpha)\frac{d\Gamma^{\gamma\alpha}}{dt} = D_\gamma\frac{\partial c_\gamma}{\partial n} - D_\alpha\frac{\partial c_\alpha}{\partial n}$$

- para-equilibrium: c_α is at equilibrium $c^\infty_{\alpha\gamma}$,
- $\frac{d\Gamma^{\gamma\alpha}}{dt}$ described by first-order reaction flux.

Equilibrium parameters c^{∞}



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Solving the motion of the interfaces

Level-set method uses signed-distance function $\phi(\mathbf{x}, t)$

$$\phi^{kl}(\mathbf{x}, t) = \begin{cases} +\min\limits_{\mathbf{y}\in\Omega(t)} ||\mathbf{y}-\mathbf{x}||_2 & \text{if } \mathbf{x} \in \overline{\Omega_k}(t)\backslash\Gamma^{kl}(t), \\ 0 & \text{if } \mathbf{x} \in \Gamma^{kl}(t), \\ -\min\limits_{\mathbf{y}\in\Omega(t)} ||\mathbf{y}-\mathbf{x}||_2 & \text{if } \mathbf{x} \in \overline{\Omega_l}(t)\backslash\Gamma^{kl}(t). \end{cases}$$

ϕ^{kl} is updated by convection equation with convection coefficient $v_n^{\text{ex},kl}(\mathbf{x}, t)$ obtained from

$$\begin{cases} \Delta v_n^{\text{ex},kl} = 0 & , \mathbf{x} \in \Omega_k\backslash\Gamma^{kl}, \\ v_n^{\text{ex},kl} = \frac{d\Gamma^{kl}}{dt} & , \mathbf{x} \in \Gamma^{kl}. \end{cases}$$

Solving the diffusion equation

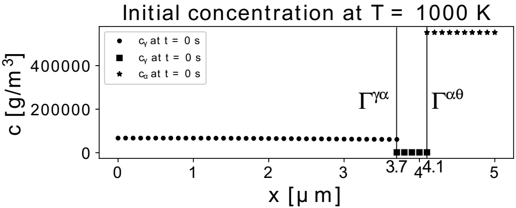
Space discretisation by Galerkin FEM

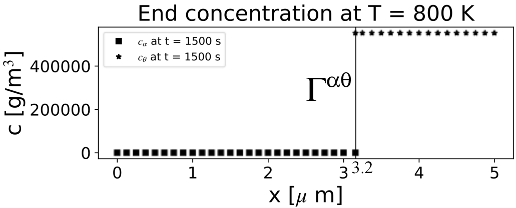
$$M_{\gamma/\alpha}(t)\frac{d\mathbf{c}_{\gamma/\alpha}}{dt}(t) = S_{\gamma/\alpha}\left(t, \mathbf{c}_{\gamma/\alpha}(t)\right)\mathbf{c}_{\gamma/\alpha}(t) + \mathbf{f}_{\gamma/\alpha}\left(t, \mathbf{c}_{\gamma/\alpha}(t)\right).$$

Time discretisation with backward Euler

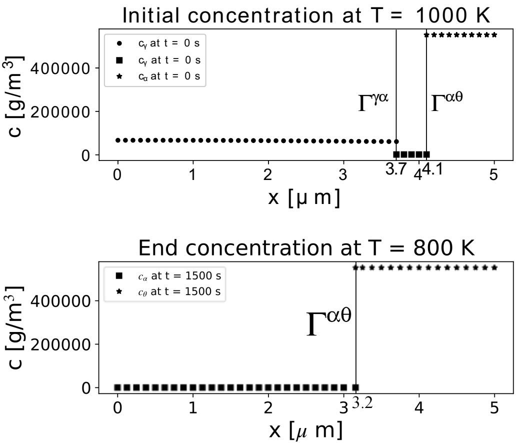
$$\left(M^{n+1}_{\gamma/\alpha} - \Delta t S^{n+1}_{\gamma/\alpha}\right)\mathbf{c}^{n+1}_{\gamma/\alpha} = M^{n+1}_{\gamma/\alpha}\mathbf{c}^{n}_{\gamma/\alpha} + \Delta t \mathbf{f}^{n+1}_{\gamma/\alpha}.$$

1D implementation





1D implementation



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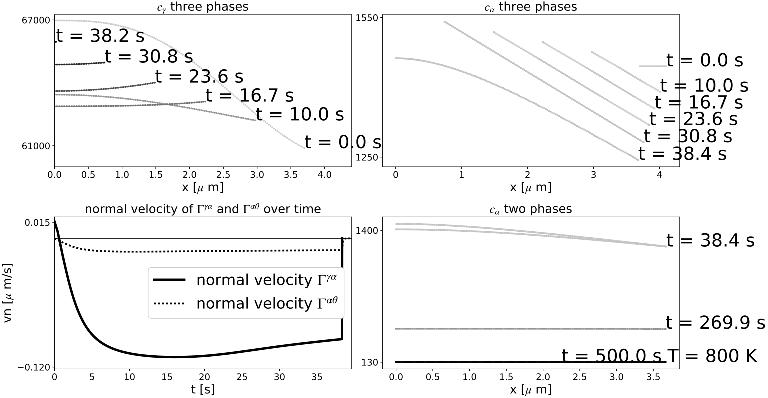
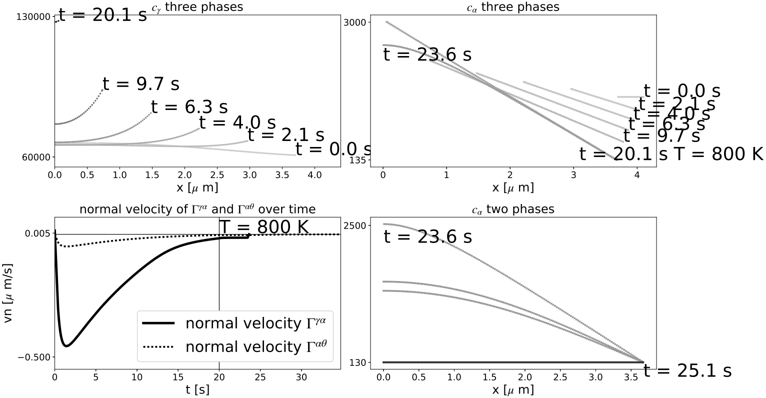
1D implementation medium cooling



1D implementation fast cooling



1D convergence

Constant $T = 800K$

Start with	end with	approximated order
3 phases	2 phases	0.68
3 phases	3 phases	1.15
2 phases*	2 phases	0.83

*Interface $\Gamma^{\alpha\theta}$ position as 3 phase-model ended.

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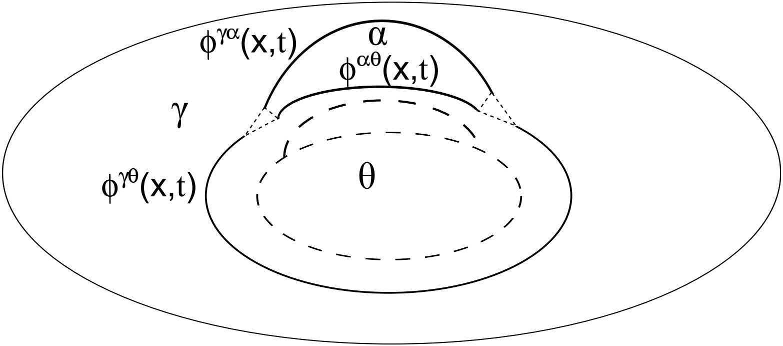
Future work: 2D level-set



Future work: accuracy

- Handling the (open) problem of jump in BC.
- More accurate time integration (Theta-method, RK, ...).

Questions, suggestions, remarks, ... ?