Modeling three phases of steel

Austenite, ferrite and cementite

Thijs Verbeek
19 April 2018

TUDelft

Introduction

Introduction

1. Physics of phase transformation
2. Mathematical model
3. Discretization
4. Evaluating results

Introduction

1. Physics of phase transformation
2. Mathematical model
3. Discretization
4. Evaluating results

Introduction

1. Physics of phase transformation
2. Mathematical model
3. Discretization
4. Evaluating results

Phase Transformation Ice to Water

Ice to water phase transformation.

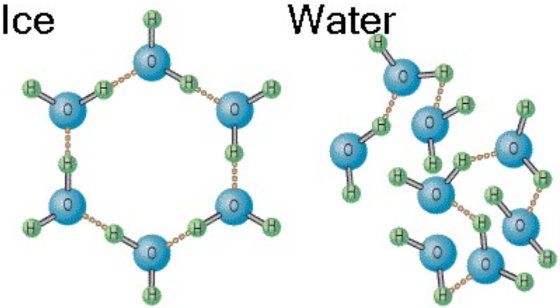


Figure: *https://kids.britannica.com/students/assembly/view/54121*

Phase Transformation Ice

Ice to ice phase transformation.

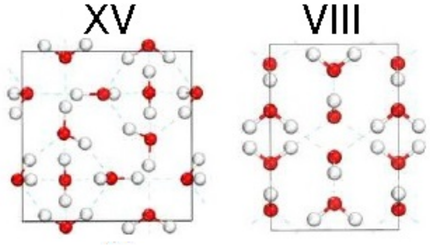
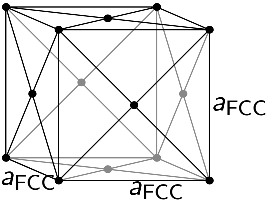
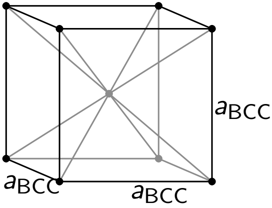


Figure: *The Journal of chemical physics. V 139. 154702. 10.1063/1.4824481.*

Phase Structures Steel



(a) Austenite (γ) crystal structure
Face-Center-Cubic



(b) Ferrite (α) crystal structure
Body-Center-Cubic

Cementite has a fixed ratio of Fe_3C.

TU Delft

Phase Diagram Steel

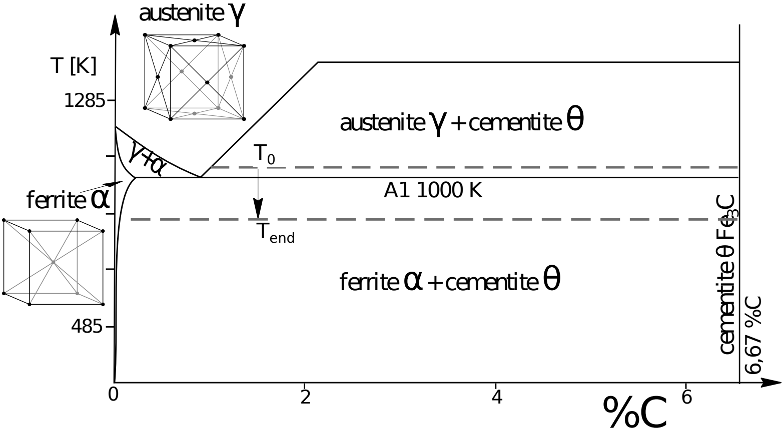
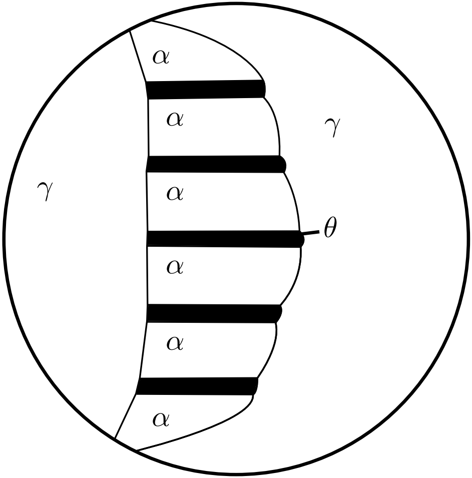
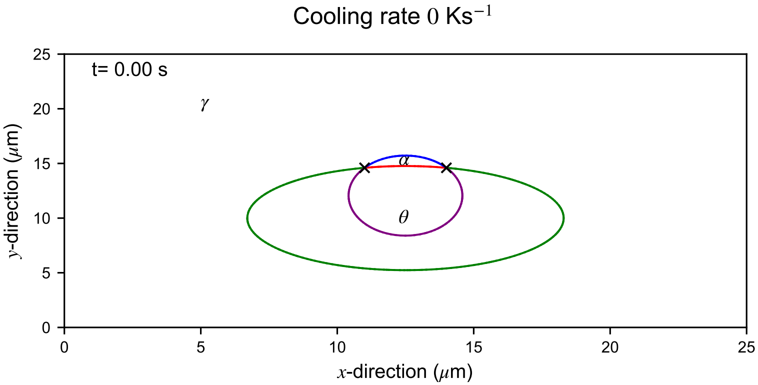


Figure: Part of the steel phase diagram

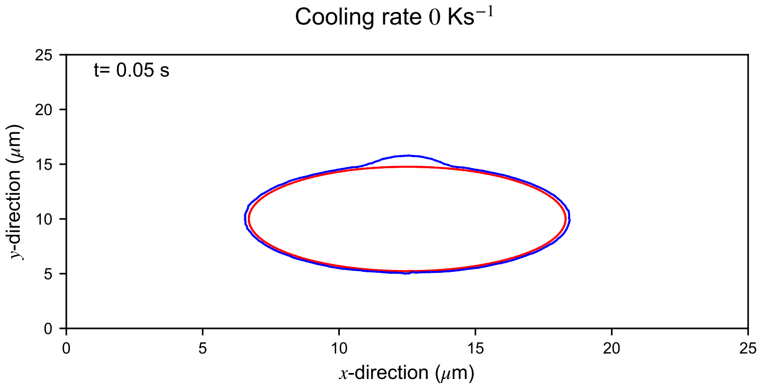
Phase Transformation in Steel



Result Mathematical Model



Result Mathematical Model



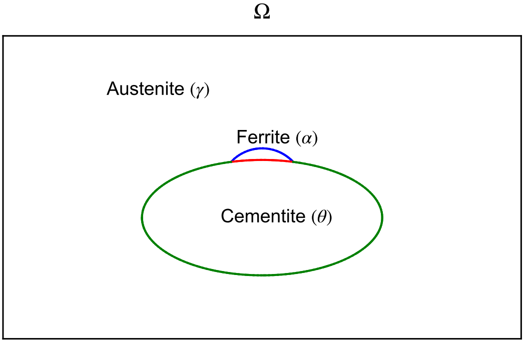
Stefan Problem

$$\begin{cases} \frac{\partial c_\gamma}{\partial t} & = & \nabla \cdot (D_\gamma \nabla c_\gamma) & , \mathbf{x} \in \gamma, \\ \frac{\partial c}{\partial n} & = & 0 & , \mathbf{x} \in \partial\Omega, \\ \text{BC} & \Gamma^{\gamma\alpha}, \Gamma^{\gamma\theta}, & & \\ \multicolumn{4}{l}{\text{Initial conditions for } c_\gamma, c, \Gamma^{\gamma\alpha}, \Gamma^{\gamma\theta}.} \end{cases}$$

$$\begin{cases} \frac{\partial c_\alpha}{\partial t} & = & \nabla \cdot (D_\alpha \nabla c_\alpha) & , \mathbf{x} \in \alpha, \\ \frac{\partial c}{\partial n} & = & 0 & , \mathbf{x} \in \partial\Omega, \\ \text{BC} & \Gamma^{\gamma\alpha}, \Gamma^{\alpha\theta}, & & \\ \multicolumn{4}{l}{\text{Initial conditions for } c_\alpha, \Gamma^{\gamma\alpha}, \Gamma^{\alpha\theta}.} \end{cases}$$

Cementite constant concentration c_θ

Stefan Problem: Domain



Boundary Condition $\Gamma^{\gamma\theta}$

On $\Gamma^{\gamma\theta}$ in γ there are two unknowns c_γ and $v_n^{\gamma\theta}$, so two boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\theta}$.

This gives boundary condition and interface velocity

$$
\begin{aligned}
D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\theta}}{c_\theta}\left(c_\theta - c_\gamma\right)\left(c_{\gamma\theta} - c_\gamma\right), \\
v_n^{\gamma\theta} &= \frac{K^{\gamma}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right).
\end{aligned}
$$

TU Delft

Boundary Condition $\Gamma^{\gamma\theta}$

On $\Gamma^{\gamma\theta}$ in γ there are two unknowns c_γ and $v_n^{\gamma\theta}$, so two boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\theta}$.

This gives boundary condition and interface velocity

$$D_\gamma \frac{\partial c_\gamma}{\partial n} = \frac{K^{\gamma\theta}}{c_\theta}(c_\theta - c_\gamma)(c_{\gamma\theta} - c_\gamma),$$

$$v_n^{\gamma\theta} = \frac{K^\gamma}{c_\theta}(c_{\gamma\theta} - c_\gamma).$$

TUDelft

Boundary Condition $\Gamma^{\gamma\theta}$

On $\Gamma^{\gamma\theta}$ in γ there are two unknowns c_γ and $v_n^{\gamma\theta}$, so two boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\theta}$.

This gives boundary condition and interface velocity

$$
\begin{aligned}
D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\theta}}{c_\theta}\left(c_\theta - c_\gamma\right)\left(c_{\gamma\theta} - c_\gamma\right), \\
v_n^{\gamma\theta} &= \frac{K^{\gamma}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right).
\end{aligned}
$$

TU Delft

Boundary Condition $\Gamma^{\gamma\theta}$

On $\Gamma^{\gamma\theta}$ in γ there are two unknowns c_γ and $v_n^{\gamma\theta}$, so two boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\theta}$.

This gives boundary condition and interface velocity

$$\begin{aligned} D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\theta}}{c_\theta}\left(c_\theta - c_\gamma\right)\left(c_{\gamma\theta} - c_\gamma\right), \\ v_n^{\gamma\theta} &= \frac{K^{\gamma}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right). \end{aligned}$$

Boundary Condition $\Gamma^{\gamma\theta}$

On $\Gamma^{\gamma\theta}$ in γ there are two unknowns c_γ and $v_n^{\gamma\theta}$, so two boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\theta}$.

This gives boundary condition and interface velocity

$$\begin{aligned} D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\theta}}{c_\theta}\left(c_\theta - c_\gamma\right)\left(c_{\gamma\theta} - c_\gamma\right), \\ v_n^{\gamma\theta} &= \frac{K^\gamma}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right). \end{aligned}$$

TUDelft

Boundary Condition $\Gamma^{\alpha\theta}$

Similarly boundary condition and interface velocity on $\Gamma^{\alpha\theta}$

$$
\begin{aligned}
D_\alpha \frac{\partial c_\alpha}{\partial n} &= \frac{K^{\alpha\theta}}{c_\theta}\left(c_\theta - c_\alpha\right)\left(c_{\alpha\theta} - c_\alpha\right), \\
v_n^{\alpha\theta} &= \frac{K^\alpha}{c_\theta}\left(c_{\alpha\theta} - c_\alpha\right).
\end{aligned}
$$

Boundary Condition $\Gamma^{\gamma\alpha}$

On $\Gamma^{\gamma\alpha}$ there are three unknowns c_γ, c_α and $v_n^{\gamma\alpha}$, so three boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\alpha}$,
- c_α at equilibrium concentration $c_{\alpha\gamma}$ in α.

This gives boundary condition and interface velocity

$$\begin{aligned} D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}} (c_{\gamma\alpha} - c_\gamma)(c_{\alpha\gamma} - c_\gamma) + \frac{D_\alpha}{c_{\alpha\gamma}} \frac{\partial c_\alpha}{\partial n} c_\gamma, \\ v_n^{\gamma\alpha} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}} (c_{\gamma\alpha} - c_\gamma) - \frac{D_\alpha}{c_{\alpha\gamma}^{\mathrm{sol}}} \frac{\partial c_\alpha}{\partial n}. \end{aligned}$$

Boundary Condition $\Gamma^{\gamma\alpha}$

On $\Gamma^{\gamma\alpha}$ there are three unknowns c_γ, c_α and $v_n^{\gamma\alpha}$, so three boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\alpha}$,
- c_α at equilibrium concentration $c_{\alpha\gamma}$ in α.

This gives boundary condition and interface velocity

$$
\begin{aligned}
D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}}(c_{\gamma\alpha} - c_\gamma)(c_{\alpha\gamma} - c_\gamma) + \frac{D_\alpha}{c_{\alpha\gamma}} \frac{\partial c_\alpha}{\partial n} c_\gamma, \\
v_n^{\gamma\alpha} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}}(c_{\gamma\alpha} - c_\gamma) - \frac{D_\alpha}{c_{\alpha\gamma}^{\mathrm{sol}}} \frac{\partial c_\alpha}{\partial n}.
\end{aligned}
$$

Boundary Condition $\Gamma^{\gamma\alpha}$

On $\Gamma^{\gamma\alpha}$ there are three unknowns c_γ, c_α and $v_n^{\gamma\alpha}$, so three boundary conditions are needed:

- Mass conservation,
- First-order reaction in flux over $\Gamma^{\gamma\alpha}$,
- c_α at equilibrium concentration $c_{\alpha\gamma}$ in α.

This gives boundary condition and interface velocity

$$
\begin{aligned}
D_\gamma \frac{\partial c_\gamma}{\partial n} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}} (c_{\gamma\alpha} - c_\gamma)(c_{\alpha\gamma} - c_\gamma) + \frac{D_\alpha}{c_{\alpha\gamma}} \frac{\partial c_\alpha}{\partial n} c_\gamma, \\
v_n^{\gamma\alpha} &= \frac{K^{\gamma\alpha}}{c_{\alpha\gamma}} (c_{\gamma\alpha} - c_\gamma) - \frac{D_\alpha}{c_{\alpha\gamma}^{\text{sol}}} \frac{\partial c_\alpha}{\partial n}.
\end{aligned}
$$

TUDelft

Domain Tracking: Level-Set Method

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

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

Domain Tracking: Level-Set Method

$\phi^{kl}(\mathbf{x}, t)$ is updated by convection equation

$$\frac{\partial \phi^{kl}}{\partial t} + v_n^{\mathrm{ex},kl} \|\nabla \phi^{kl}\|_2 = 0,$$

with convection coefficient $v_n^{\mathrm{ex},kl}(\mathbf{x}, t)$ obtained from

$$\begin{cases} \Delta v_n^{\mathrm{ex},kl} = 0 & , \mathbf{x} \in \Omega_k \backslash \Gamma^{kl}, \\ v_n^{\mathrm{ex},kl} = v_n^{kl} & , \mathbf{x} \in \Gamma^{kl}, \\ \frac{\partial v_n^{\mathrm{ex},kl}}{\partial n} = 0 & , \mathbf{x} \in \partial\Omega. \end{cases}$$

TUDelft

Domain Tracking: Level-Set Method

$\phi^{kl}(\mathbf{x}, t)$ is updated by convection equation

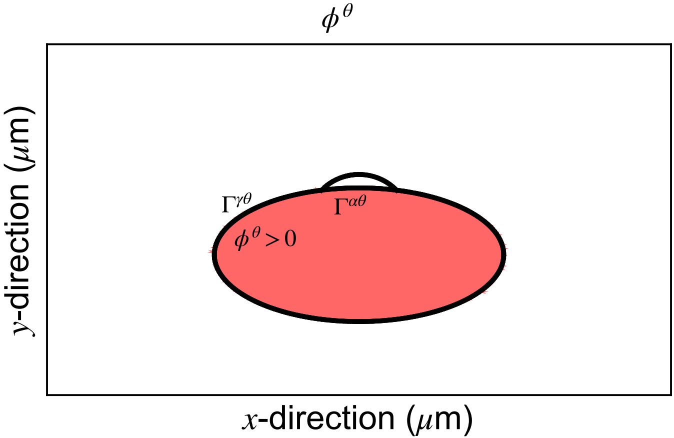
$$\frac{\partial \phi^{kl}}{\partial t} + v_n^{\text{ex},kl} \|\nabla \phi^{kl}\|_2 = 0,$$

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

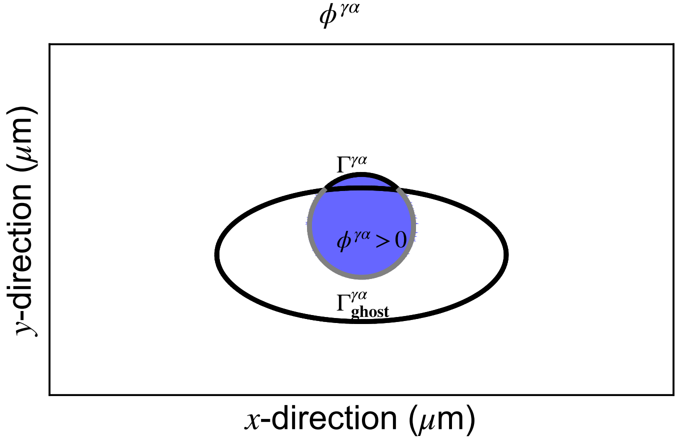
$$\begin{cases} \Delta v_n^{\text{ex},kl} = 0 & , \mathbf{x} \in \Omega_k \backslash \Gamma^{kl}, \\ v_n^{\text{ex},kl} = v_n^{kl} & , \mathbf{x} \in \Gamma^{kl}, \\ \frac{\partial v_n^{\text{ex},kl}}{\partial n} = 0 & , \mathbf{x} \in \partial \Omega. \end{cases}$$

TUDelft

Domain Tracking: Multi Level-Set Method

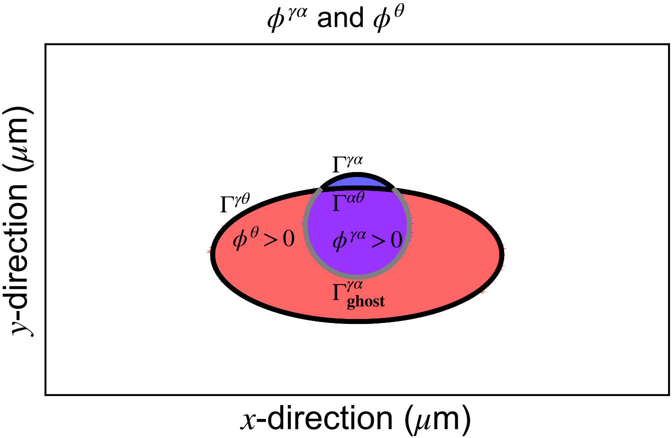


Domain Tracking: Multi Level-Set Method



TUDelft

Domain Tracking: Multi Level-Set Method



Space Discretization and Time Integration

Space discretization

- Galerkins Finite Element Method.

Time integration

- implicit Euler for the Stefan problem,
- Total Variation Diminishing Runge Kutta Third Order (TVD RK3) for the convection equation.

Space Discretization and Time Integration

Space discretization

- Galerkins Finite Element Method.

Time integration

- implicit Euler for the Stefan problem,
- Total Variation Diminishing Runge-Kutta-Third-Order (TVD RK3) for the convection equation.

Space Discretization and Time Integration

Space discretization

- Galerkins Finite Element Method.

Time integration

- implicit Euler for the Stefan problem,
- Total Variation Diminishing Runge-Kutta-Third-Order (TVD RK3) for the convection equation.

TUDelft

Space Discretization and Time Integration

Space discretization

- Galerkins Finite Element Method.

Time integration

- implicit Euler for the Stefan problem,
- Total Variation Diminishing Runge-Kutta-Third-Order (TVD RK3) for the convection equation.

Space Discretization

Define fixed background mesh T, on T is defined

- $\phi^{\gamma\alpha}$,
- ϕ^{θ}.

From $\phi^{\gamma\alpha}, \phi^{\theta}$ we can find the interface points. Adding interface points to T gives enriched mesh T^E. On T^E is defined

- c_γ where $\phi^{\gamma\alpha} \leq 0$ and $\phi^{\theta} \leq 0$,
- c_α where $\phi^{\gamma\alpha} \geq 0$ and $\phi^{\theta} \leq 0$.

Space Discretization

Define fixed background mesh T, on T is defined

- $\phi^{\gamma\alpha}$,
- ϕ^{θ}.

From $\phi^{\gamma\alpha}, \phi^{\theta}$ we can find the interface points. Adding interface points to T gives enriched mesh T^E. On T^E is defined

- c_γ where $\phi^{\gamma\alpha} \leq 0$ and $\phi^{\theta} \leq 0$,
- c_α where $\phi^{\gamma\alpha} \geq 0$ and $\phi^{\theta} \leq 0$.

Space Discretization

Define fixed background mesh T, on T is defined

- $\phi^{\gamma\alpha}$,
- ϕ^{θ}.

From $\phi^{\gamma\alpha}, \phi^{\theta}$ we can find the interface points. Adding interface points to T gives enriched mesh T^E. On T^E is defined

- c_γ where $\phi^{\gamma\alpha} \leq 0$ and $\phi^{\theta} \leq 0$,
- c_α where $\phi^{\gamma\alpha} \geq 0$ and $\phi^{\theta} \leq 0$.

Space Discretization

Define fixed background mesh T, on T is defined

- $\phi^{\gamma\alpha}$,
- ϕ^{θ}.

From $\phi^{\gamma\alpha}, \phi^{\theta}$ we can find the interface points. Adding interface points to T gives enriched mesh T^E. On T^E is defined

- c_γ where $\phi^{\gamma\alpha} \leq 0$ and $\phi^{\theta} \leq 0$,
- c_α where $\phi^{\gamma\alpha} \geq 0$ and $\phi^{\theta} \leq 0$.

Discretization: Finding Interface

Level-set function is piece-wise linear on T. Interface point $\boldsymbol{x}^{\boldsymbol{e}}$ can be found over an edge $\boldsymbol{e} = (\boldsymbol{x}_0, \boldsymbol{x}_1)$ by:

$$\begin{aligned} \boldsymbol{x}^{\boldsymbol{e}} &= (1 - \tau^{\boldsymbol{e}})\,\boldsymbol{x}_0 + \tau^{\boldsymbol{e}}\boldsymbol{x}_1, \\ \tau^{\boldsymbol{e}} &= -\frac{\phi(\boldsymbol{x}_0)}{\phi(\boldsymbol{x}_1) - \phi(\boldsymbol{x}_0)}. \end{aligned}$$

Depending on position of $\boldsymbol{x}^{\boldsymbol{e}}$ either shift node from T or add to T^E.

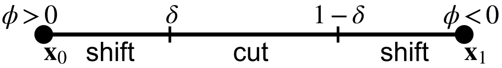
TUDelft

Discretization: Finding Interface

Level-set function is piece-wise linear on T. Interface point $\boldsymbol{x}^{\boldsymbol{e}}$ can be found over an edge $\boldsymbol{e} = (\boldsymbol{x}_0, \boldsymbol{x}_1)$ by:

$$
\begin{aligned}
\boldsymbol{x}^{\boldsymbol{e}} &= (1 - \tau^{\boldsymbol{e}})\, \boldsymbol{x}_0 + \tau^{\boldsymbol{e}} \boldsymbol{x}_1, \\
\tau^{\boldsymbol{e}} &= -\frac{\phi(\boldsymbol{x}_0)}{\phi(\boldsymbol{x}_1) - \phi(\boldsymbol{x}_0)}.
\end{aligned}
$$

Depending on position of $\boldsymbol{x}^{\boldsymbol{e}}$ either shift node from T or add to T^E.



Discretization: Mesh Creation

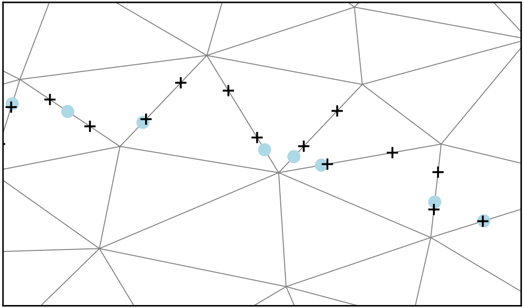


Figure: Position of interface points (light blue) on background mesh T. $+$ show shift/cut regions per edge.

Discretization: Mesh Creation

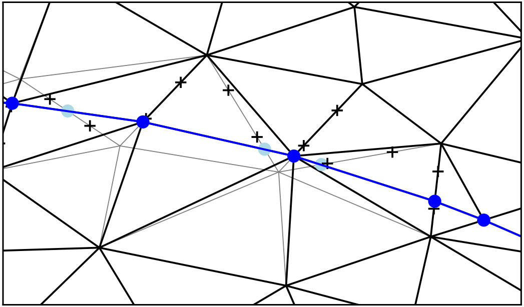
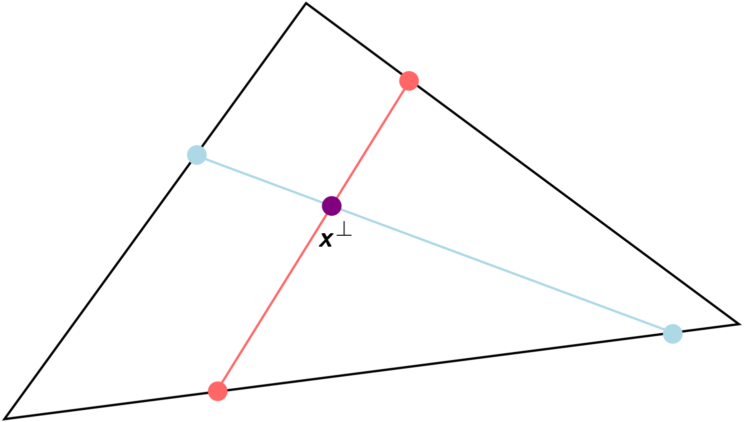


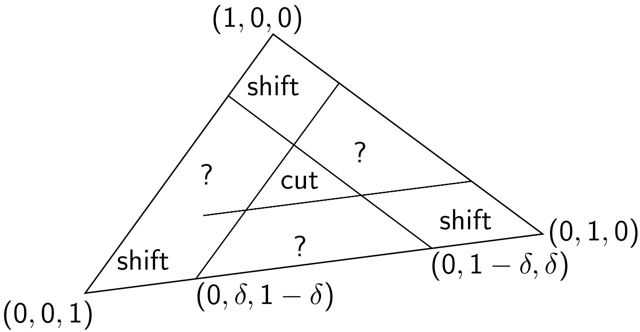
Figure: Enriched mesh T^E with blue interface points.

Discretization: Triple Points $x^{\perp}$



Discretization: Triple Points

Using barycentric coordinates we can find the position of $\boldsymbol{x}^{\perp}$ in the triangle.



Discretization: Shift Triple Point

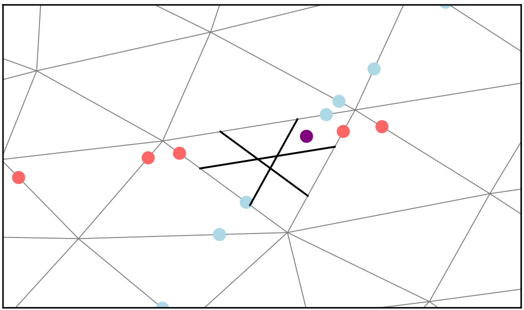


Figure: Triple point in background mesh T with interface points (blue from $\phi^{\gamma\alpha}$ and red from ϕ^{θ}).

Discretization: Shift Triple Point

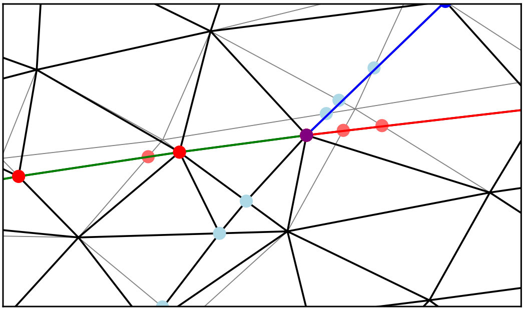


Figure: Shifted to triple point (purple) in enriched mesh T^E with interface points (blue from $\phi^{\gamma\alpha}$ and red from ϕ^{θ}).

Discretization: Bend Triple Point

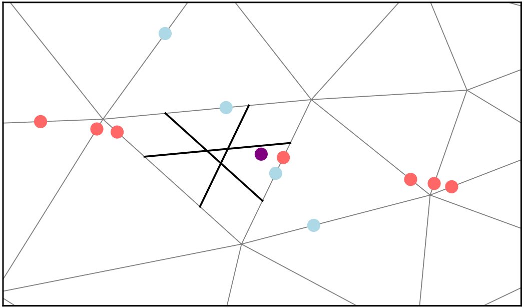


Figure: Triple point in background mesh T with interface points (blue from $\phi^{\gamma\alpha}$ and red from ϕ^{θ}).

Discretization: Bend Triple Point

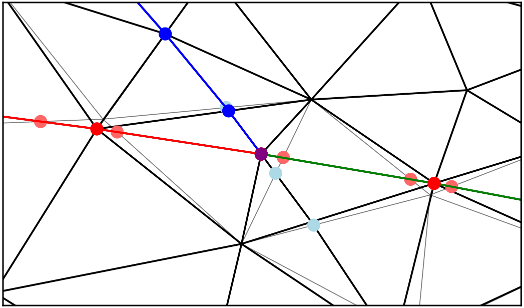


Figure: Bend edge to triple point (purple) in enriched mesh T^E with interface points (blue from $\phi^{\gamma\alpha}$ and red from ϕ^{θ}).

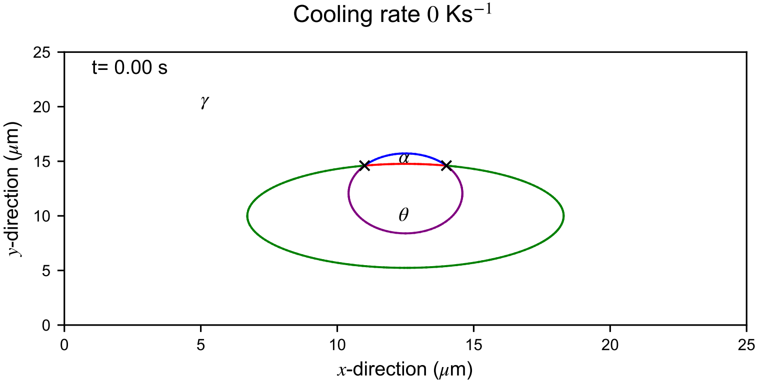
TUDelft

Discretization: Meshing Algorithm

In order:

- Shift triple points;
- Shift vertices to interfaces;
- Shift/cut/bend triple points;
- Cut points;

Back to Results



TU Delft

Triple Point Boundary Condition

$$v_n^{\gamma\theta} = \frac{K^{\gamma\theta}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right), \qquad v_n^{\alpha\theta} = \frac{K^{\alpha\theta}}{c_\theta}\left(c_{\alpha\theta} - c_\alpha\right).$$

In $\boldsymbol{x}^\perp$ these velocities have to be equal and $c_\alpha = c_{\alpha\gamma}$, this gives

$$c_\gamma = c_{\gamma\theta} - \frac{K^{\alpha\theta}}{K^{\gamma\theta}}\left(c_{\alpha\theta} - c_{\alpha\gamma}\right).$$

Only reaction speeds $K^{\gamma\theta}$ and $K^{\alpha\theta}$ have some freedom, as

$$K^{\gamma\theta} = k_{\gamma\theta}\frac{D_\gamma}{a_\gamma}, \qquad K^{\alpha\theta} = k_{\alpha\theta}\frac{D_\alpha}{a_\alpha},$$

$$k^{\alpha\theta} = k_{\gamma\theta}\frac{D_\gamma}{D_\alpha}\frac{a_\alpha}{a_\gamma}.$$

TU Delft

Triple Point Boundary Condition

$$v_n^{\gamma\theta} = \frac{K^{\gamma\theta}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right), \qquad v_n^{\alpha\theta} = \frac{K^{\alpha\theta}}{c_\theta}\left(c_{\alpha\theta} - c_\alpha\right).$$

In $\boldsymbol{x}^\perp$ these velocities have to be equal and $c_\alpha = c_{\alpha\gamma}$, this gives

$$c_\gamma = c_{\gamma\theta} - \frac{K^{\alpha\theta}}{K^{\gamma\theta}}\left(c_{\alpha\theta} - c_{\alpha\gamma}\right).$$

Only reaction speeds $K^{\gamma\theta}$ and $K^{\alpha\theta}$ have some freedom, as

$$K^{\gamma\theta} = k_{\gamma\theta}\frac{D_\gamma}{a_\gamma}, \qquad K^{\alpha\theta} = k_{\alpha\theta}\frac{D_\alpha}{a_\alpha},$$

$$k^{\alpha\theta} = k_{\gamma\theta}\frac{D_\gamma}{D_\alpha}\frac{a_\alpha}{a_\gamma}.$$

TUDelft

Triple Point Boundary Condition

$$v_n^{\gamma\theta} = \frac{K^{\gamma\theta}}{c_\theta}\left(c_{\gamma\theta} - c_\gamma\right), \qquad v_n^{\alpha\theta} = \frac{K^{\alpha\theta}}{c_\theta}\left(c_{\alpha\theta} - c_\alpha\right).$$

In $\boldsymbol{x}^\perp$ these velocities have to be equal and $c_\alpha = c_{\alpha\gamma}$, this gives

$$c_\gamma = c_{\gamma\theta} - \frac{K^{\alpha\theta}}{K^{\gamma\theta}}\left(c_{\alpha\theta} - c_{\alpha\gamma}\right).$$

Only reaction speeds $K^{\gamma\theta}$ and $K^{\alpha\theta}$ have some freedom, as

$$K^{\gamma\theta} = k_{\gamma\theta}\frac{D_\gamma}{a_\gamma}, \qquad K^{\alpha\theta} = k_{\alpha\theta}\frac{D_\alpha}{a_\alpha},$$

$$k^{\alpha\theta} = k_{\gamma\theta}\frac{D_\gamma}{D_\alpha}\frac{a_\alpha}{a_\gamma}.$$

TUDelft

Austenite Carbon Concentration Triple Points

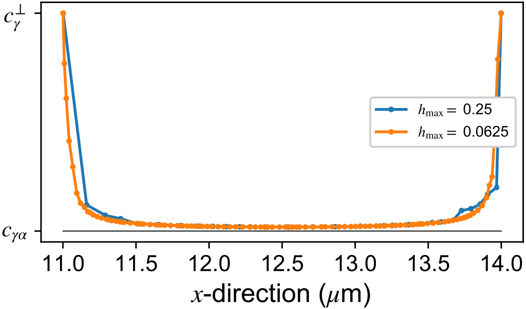


Figure: Austenite carbon concentration over austenite-ferrite interface for two mesh sizes.

Austenite Carbon Concentration Triple Points

Remember that on $\Gamma^{\gamma\alpha}$ in γ:

$$D_\gamma \frac{\partial c_\gamma}{\partial n} = \frac{K^{\gamma\alpha}}{c^{\text{sol}}_{\alpha\gamma}} \left(c^{\text{sol}}_{\gamma\alpha} - c_\gamma\right)\left(c^{\text{sol}}_{\alpha\gamma} - c_\gamma\right) + \frac{D_\alpha}{c^{\text{sol}}_{\alpha\gamma}} \frac{\partial c_\alpha}{\partial n} c_\gamma.$$

The gradient $\frac{\partial c_\alpha}{\partial n}$ has to be recovered over α.

Ferrite Carbon Concentration Gradient

$\frac{\partial c_\alpha}{\partial n}$ is recovered by fitting a second order polynomial $c_\alpha^{h^2}$ to c_α over a patch of mesh points and calculating $\nabla c_\alpha^{h^2} \cdot n$.

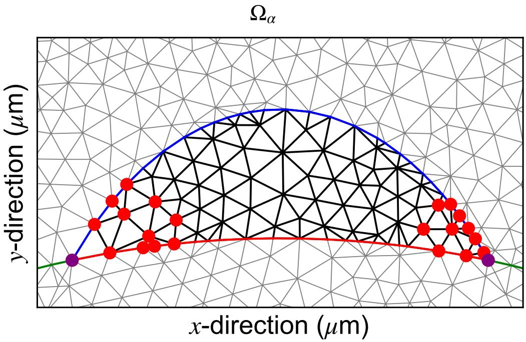


Figure: Patch for left and right triple point.

Ferrite Carbon Concentration Gradient

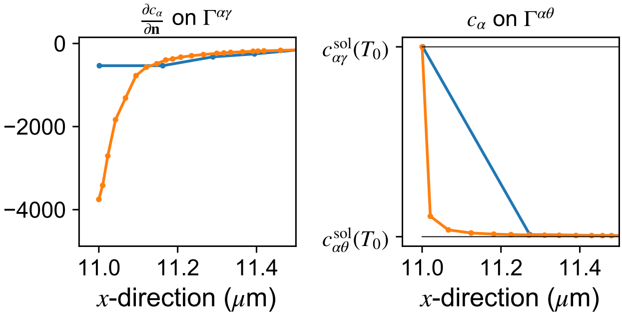


Figure: Ferrite carbon concentration gradient over austenite-ferrite interface (left) and ferrite carbon concentration over the ferrite-cementite interface (right) for two mesh sizes.

TU Delft

$\frac{\partial c_\alpha}{\partial n}$ and $v_n^{\gamma\alpha}$

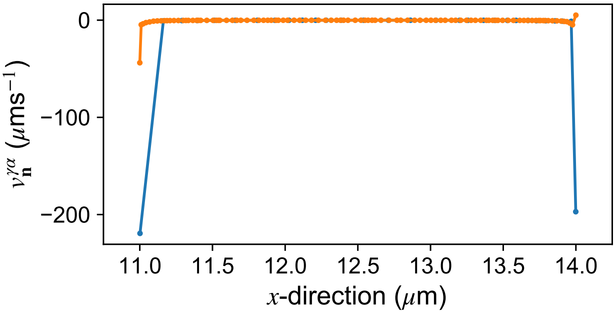


Figure: Austenite-ferrite interface normal velocity for two mesh sizes.

Conclusion Three-Phase Growth

So difference in results of the model and realistic three-phase behavior is due:

- Unknown carbon concentration for austenite in triple points. 'Chosen' concentration value resulted in unrealistic results.
- Resolution issue for the mesh size used. Finer mesh sizes were too computationally heavy.

However the rest of the simulation show results coinciding with the 1D model of the literature study.

Conclusion Three-Phase Growth

So difference in results of the model and realistic three-phase behavior is due:

- Unknown carbon concentration for austenite in triple points. 'Chosen' concentration value resulted in unrealistic results.
- Resolution issue for the mesh size used. Finer mesh sizes were too computationally heavy.

However the rest of the simulation show results coinciding with the 1D model of the literature study.

Conclusion Three-Phase Growth

So difference in results of the model and realistic three-phase behavior is due:

- Unknown carbon concentration for austenite in triple points. 'Chosen' concentration value resulted in unrealistic results.
- Resolution issue for the mesh size used. Finer mesh sizes were too computationally heavy.

However the rest of the simulation show results coinciding with the 1D model of the literature study.

TU Delft

Conclusion Three-Phase Growth

So difference in results of the model and realistic three-phase behavior is due:

- Unknown carbon concentration for austenite in triple points. 'Chosen' concentration value resulted in unrealistic results.
- Resolution issue for the mesh size used. Finer mesh sizes were too computationally heavy.

However the rest of the simulation show results coinciding with the 1D model of the literature study.

Conclusion Three-Phase Growth

So difference in results of the model and realistic three-phase behavior is due:

- Unknown carbon concentration for austenite in triple points. 'Chosen' concentration value resulted in unrealistic results.
- Resolution issue for the mesh size used. Finer mesh sizes were too computationally heavy.

However the rest of the simulation show results coinciding with the 1D model of the literature study.

Thanks for your attention!