Modeling the Austenite to Ferrite Transformation by Cellular Automaton

Improving Interface Stability

Delft University of Technology

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TATA STEEL

Outline

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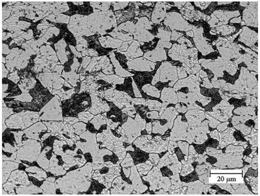
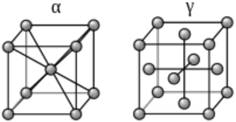
Steel microstructure

Microstructure determines mechanical properties of steel.



Ferrite/Pearlite microstructure

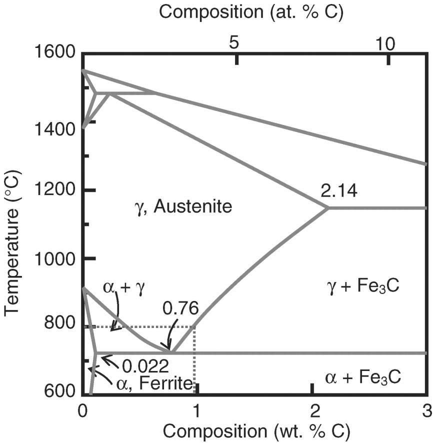


Iron atom lattices

Ferrite nucleation and growth (by Richard Huizenga, TU Delft Materials Science and Engineering)

Cooling down steel

High temperature: austenite
Low temperature: ferrite



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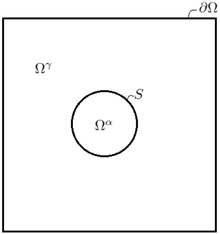
Moving boundary problem

The problem of the moving interface S can be stated as

$$\begin{cases} v_n = M\Delta G(x_s^\gamma) & \text{the normal velocity of } S \\ \frac{\partial x}{\partial t} = \nabla(D(x)\nabla x) & \text{in } \Omega^\gamma, \quad t > 0 \\ \frac{\partial x}{\partial n} = 0 & \text{on } \partial\Omega \\ \frac{\partial x}{\partial n} = -(x_s^\gamma - x^\alpha)v_n & \text{on } S \end{cases}$$



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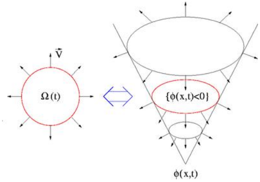
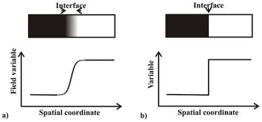
Methods for moving boundaries

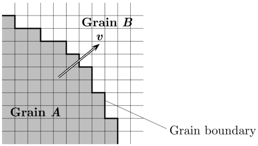
(a) Level Set Method
(b) Phase Field Method
(c) Cellular Automaton



(a)



(b)



(c)

Methods for moving boundaries

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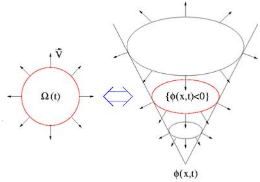
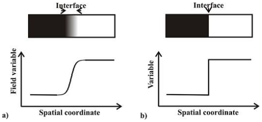
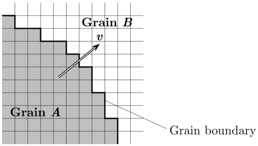


(a)



(b)



(c)

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Cellular Automaton

Model built of cells with properties

- ★ state
- ★ neighbourhood
- ★ transformation rule

example:

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1-dim CA in comparison to Murray-Landis

CA: Interface S always lies on pre-set points
ML: Interface S may freely move

Unstable interfaces

Reasons: Absence of surface tension in model, discretized spatial grid

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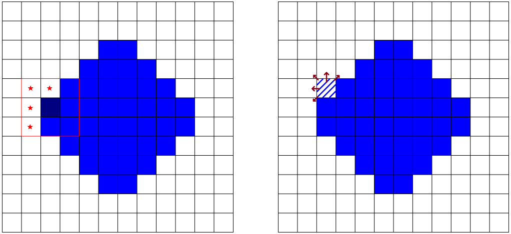
Model outline

1. Compute carbon concentration at interface cells
2. Compute growth velocity of interface cells
3. Compute growth length of interface cells
4. Transform cells according to a transformation rule
5. Redistribute excess carbon from newly transformed cells
6. Solve a time step of carbon diffusion in austenite



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Growth dynamics

For every interface cell i we define:

Growth length $\ell_i \geq 0$

Growth velocity $v_i \geq 0$

Inward growth $\lambda_i \geq 0$

The velocity v is calculated according to the classical equation

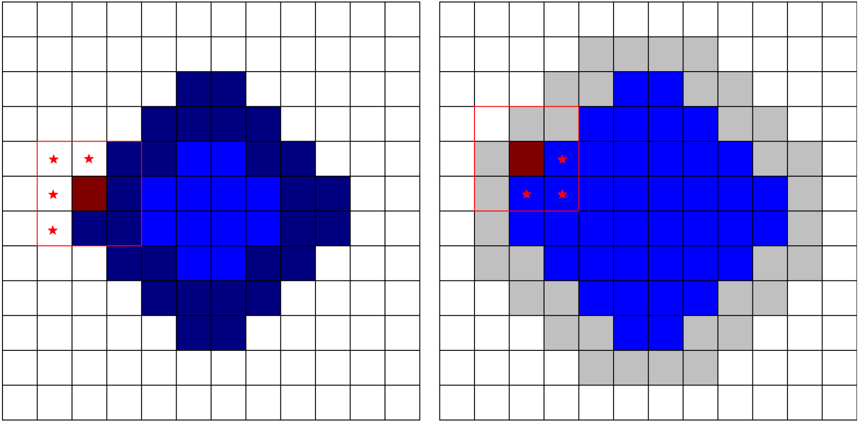
$$v = M \underbrace{\Delta G(x^{\text{interface}}, T)}_{\text{driving force}}, \qquad \text{where} \quad \Delta G : \mathbb{R}^2 \to \mathbb{R},$$

and M the interface mobility.

$$\lambda_i = \sum_{j \in \mathcal{M}_i} w_{ji} \ell_j$$

$$w_{ji} = \begin{cases} 1 & \text{cells } i \text{ and } j \text{ are direct neighbours} \\ \frac{1}{\sqrt{2}} & \text{cells } i \text{ and } j \text{ are diagonal neighbours} \end{cases},$$

Growth dynamics(2)

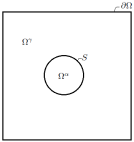


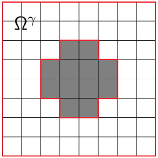
Forward Euler: $\ell_i^{k+1} = \ell_i^k + v_i^k$
Transformation rule: $\ell > \Delta z$
Transformation rule: $\lambda(\ell) > \theta(\Delta z)$

Carbon diffusion

Find $x(t_0 + \Delta t)$ on Ω^γ such that

$$\begin{cases} \frac{\partial x}{\partial t} = \nabla(D(x)\nabla x) & \text{in } \Omega^\gamma, \quad t_0 \leq t \leq t_0 + \Delta t \\ \frac{\partial x}{\partial n} = 0 & \text{on } \partial\Omega^\gamma \\ x(t_0) = x_{t_0} & \text{on } \partial\Omega^\gamma \end{cases}$$





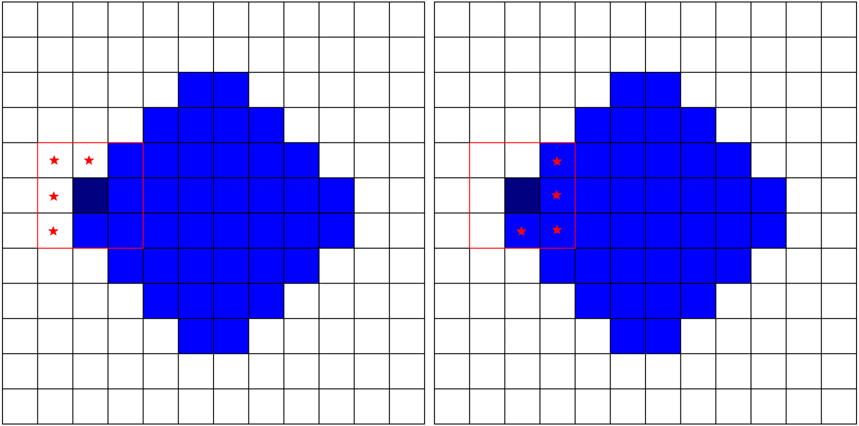
1. Implicit Euler
2. Finite Differences
3. Conjugate Gradient

Interface carbon smoothing

Why? As an attempt to reduce instability.

How? In two steps.

example



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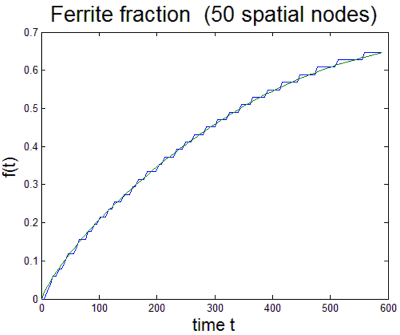
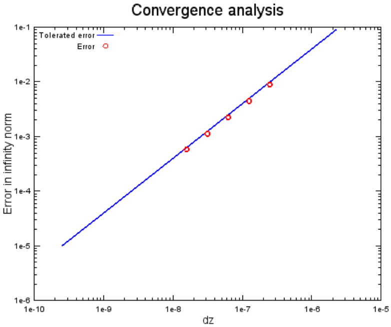
Comparison: CA to Murray-Landis

$$\Delta z \to 0, \qquad \Delta t = 0.9 \frac{\Delta z}{v_{\max}}$$





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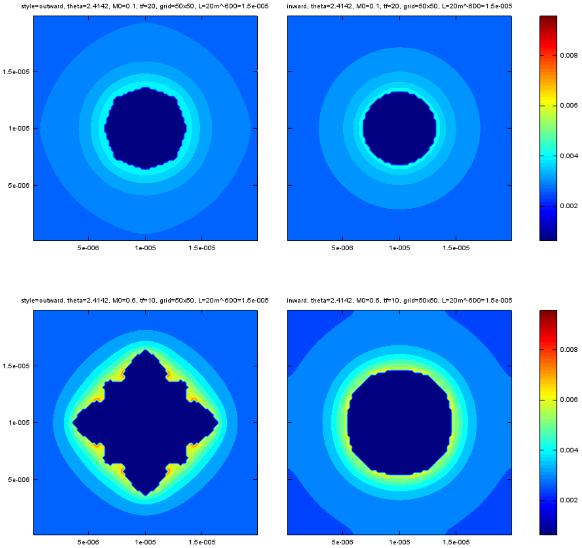
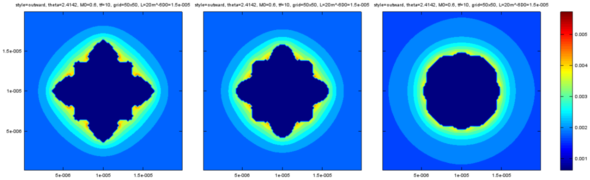
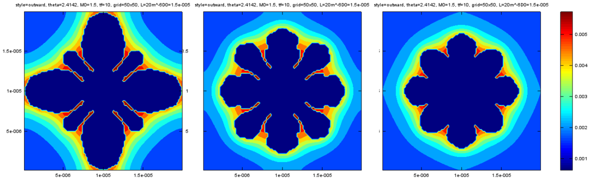
Inward growth results

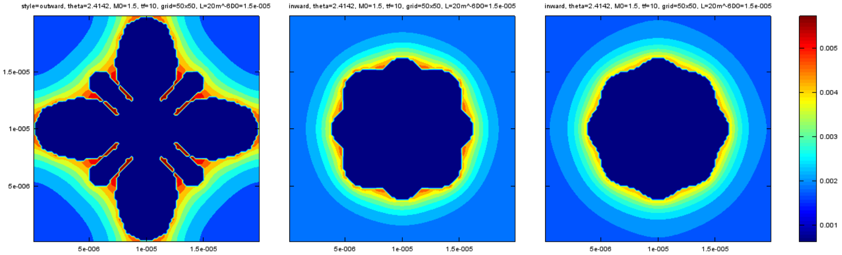


Carbon smoothing results





Combined results:
Inward growth & Carbon smoothing



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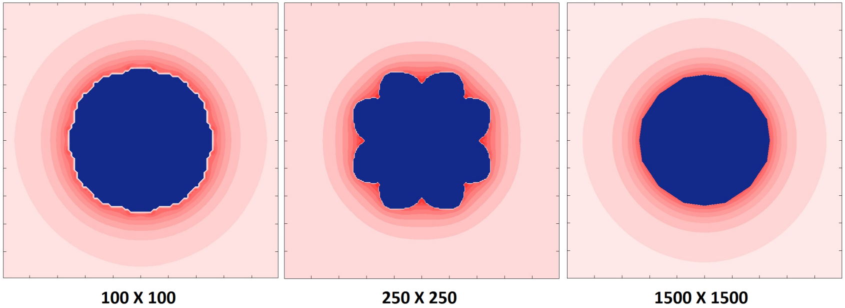
Results on grid analysis



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Conclusions and Research Questions

- ★ Inward growth seems to reduce dendritic growth and results in a circular shape
- ★ Carbon smoothing also reduces dendritic growth, smoothing area can be scaled up

- ? *Is it possible to incorporate surface tension in the model to avoid dendritic grain growth without paying for heavy computational costs?*
- ? *Are the new approaches enough for the current application?*