Modeling the Austenite Ferrite Transformation by Cellular Automaton

Improving Interface Stability

Delft University of Technology

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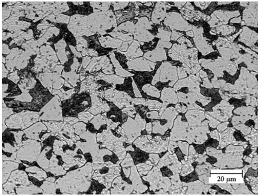
TATA STEEL

Outline

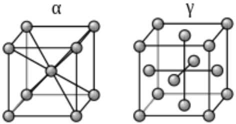
Next Subsection

Steel microstructure

Microstructure determines mechanical properties of steel.



Ferrite/Pearlite microstructure

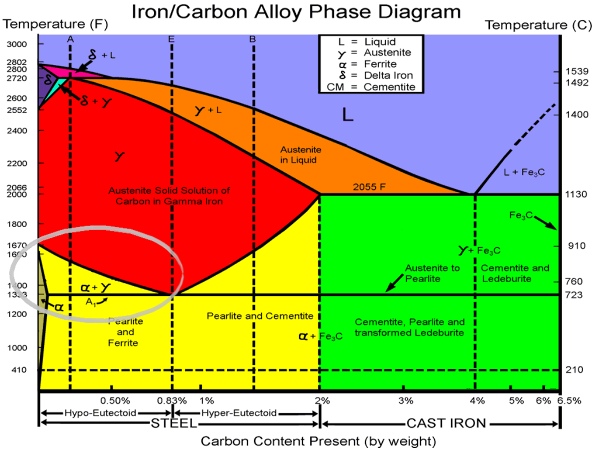


Iron atom lattices

Ferrite nucleation and growth (by Kees Bos, Principal researcher at TATA Steel)

Cooling

High temperature: austenite (γ)
Low temperature: ferrite (α)



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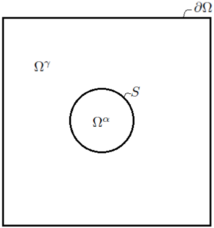
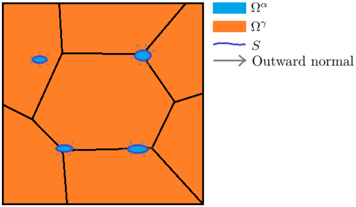
Moving boundary problem

The problem of the moving interface S can be stated as

$$
\begin{cases}
v_n = M\Delta G(X_s^\gamma) & \text{the normal velocity of } S \\
\dfrac{\partial X}{\partial t} = \nabla(D(X,z)\nabla X) & \text{in } \Omega^\gamma, \quad t > 0 \\
\dfrac{\partial X}{\partial n} = 0 & \text{on } \partial\Omega \\
\dfrac{\partial X}{\partial n} = -(X_s^\gamma - X^\alpha)v_n & \text{on } S \\
X(t=0) = X_0 & \text{on } \Omega
\end{cases}
$$





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Cellular Automaton

Model built of cells with properties

- ★ state
- ★ neighbourhood
- ★ transformation rule

example:

Next Subsection

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

Next Subsection

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

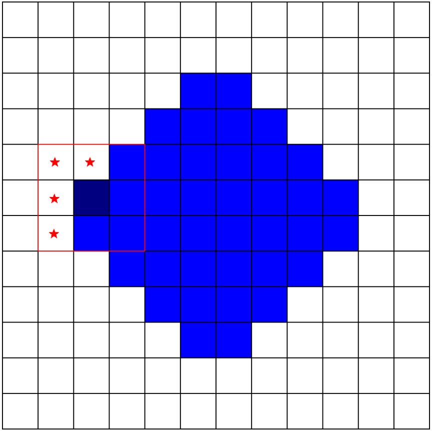
$$v = M \underbrace{\Delta G(X^{\text{interface}}, T)}_{\text{driving force}}, \qquad \text{where} \quad \Delta G : \mathbb{R}^3 \to \mathbb{R},$$

and M the interface mobility.

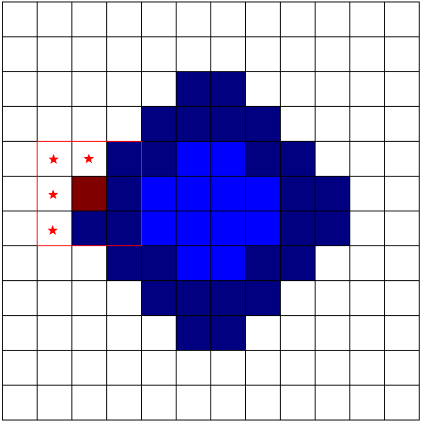
$$\lambda_i = \sum_{j \in \mathcal{M}_i} w_{ji} \ell_j$$

$$w_{ji} = \frac{1}{\sqrt{k}} \qquad \text{where cells } i \text{ and } j \text{ are } k\text{-level neighbours}$$

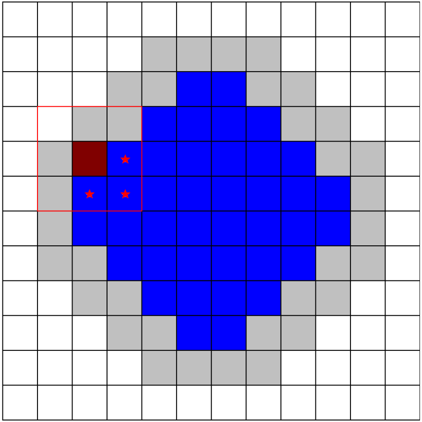
How to determine $X^{\text{interface}}$?



Growth dynamics(2)



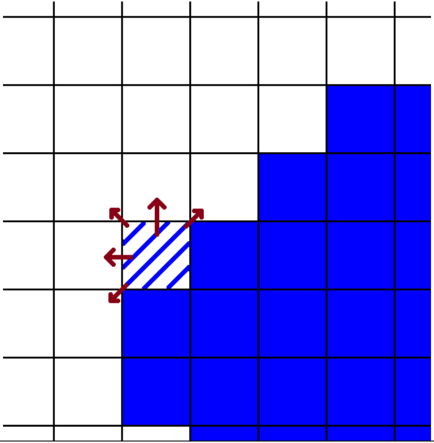
Transformation rule: ℓ



Transformation rule: λ

Carbon Redistribution Mechanics

$$X_j = X_j + \frac{X_i - X^\alpha}{\sum_n w_{ni}} \cdot w_{ji}$$

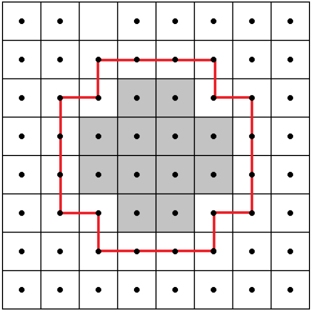


Diffusion Time Step

Find $X(t+\Delta t)$ on $\Omega^\gamma(t)$ such that

$$\begin{cases} \frac{\partial X}{\partial t} = \nabla \cdot (D(z)\nabla X) & \text{in } \Omega^\gamma(t), \qquad t < \tilde{t} \leq t + \Delta t \\ \frac{\partial X}{\partial n} = 0 & \text{on } \partial\Omega^\gamma(t) \end{cases}$$

given $X(t)$ on Ω^γ and $D(z)$ on Ω.



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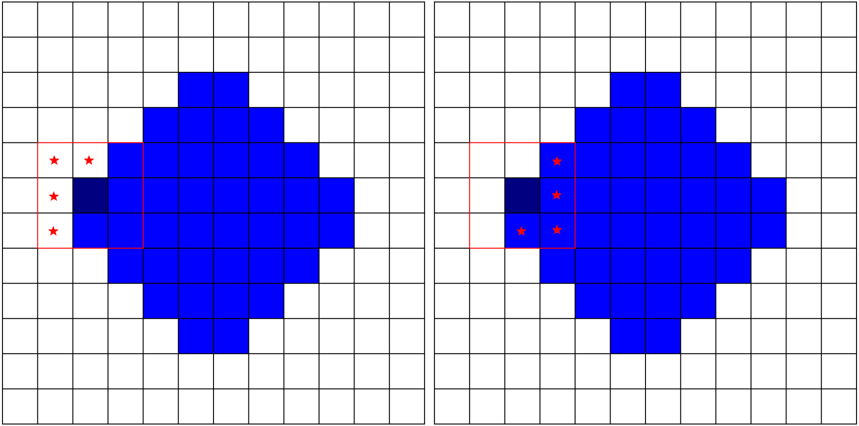
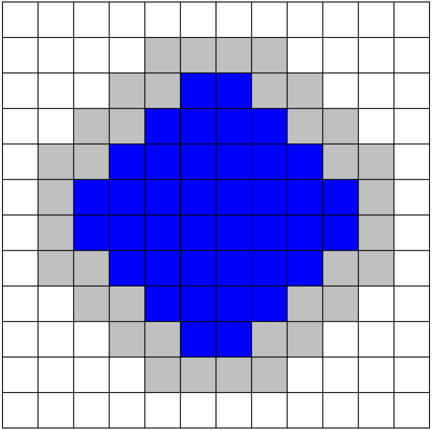
Interface Carbon Smoothing



Increased Diffusion at Interface

$$D = D_0 \cdot e^{-\frac{Q(z)}{RT}}$$



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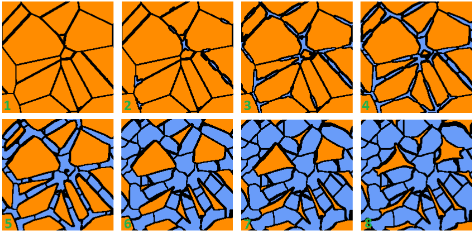
1-dim CA in comparison to Murray-Landis

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

Unstable interfaces → Dendrites

Unknown parameters

- Mobility $M_0 \cdot e^{\frac{-Q^{\alpha,\gamma}}{RT}}$
- Nucleation process
- Increased interface growth at boundaries
- Smoothe range/Increased diffusion factor
- Initial austenitic structure



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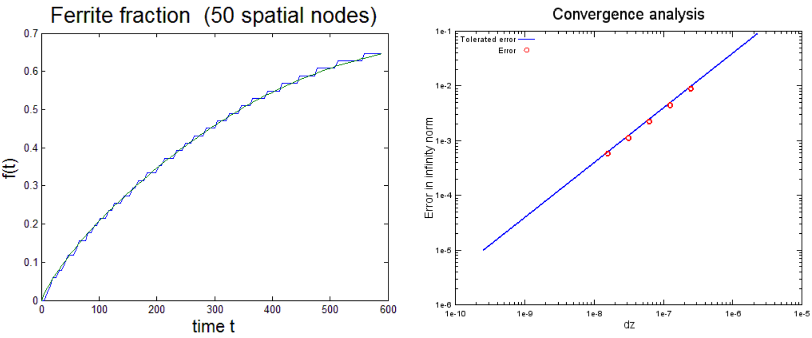
Comparison: CA to Murray-Landis

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



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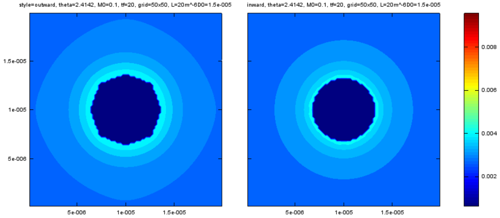
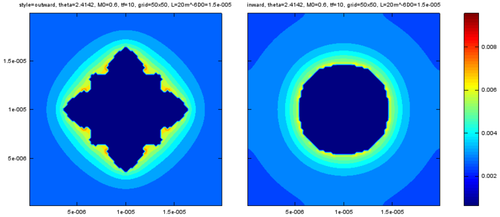
Inward growth results

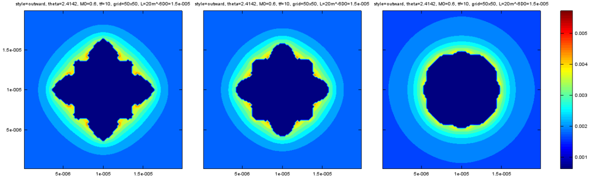


$M_0 = 0.1$

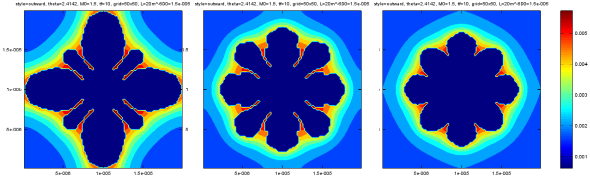


$M_0 = 0.6$

Carbon smoothing results



$M_0 = 0.6$



$M_0 = 1.5$

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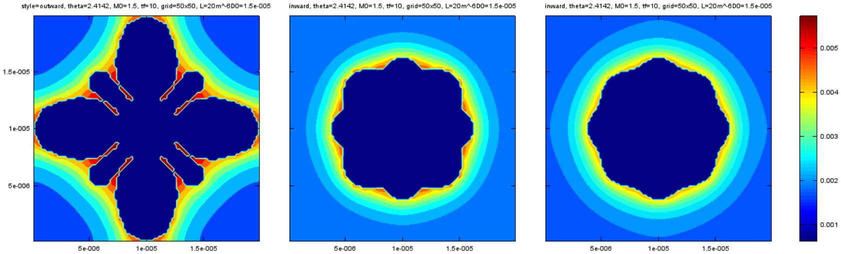
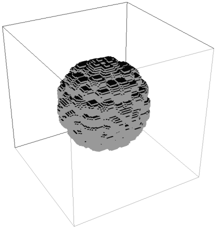
Combined results: Inward growth & Carbon smoothing



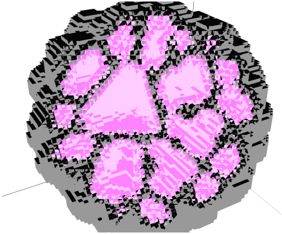
$M_0 = 1.5$

Fast Interface Diffusion

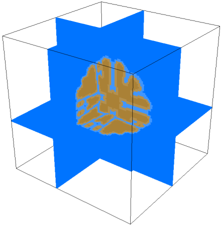
Test Example: Unwanted behaviour for $M_0 = 0.5$



A wobbly shape from the outside.



A look from the inside reveals the dendritic structure.

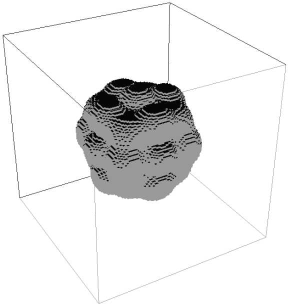


Slices of the grain.

Fast Interface Diffusion

$$D = D_0 \cdot e^{-\frac{\rho Q^{\gamma}}{RT}}$$

5× higher diffusion coefficient



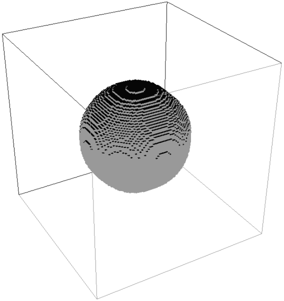
Outer grain view, $\rho = 0.9$.

Inner grain view, $\rho = 0.9$.

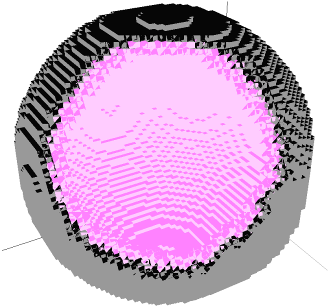
Fast Interface Diffusion

$$D = D_0 \cdot e^{-\frac{\rho Q^{\gamma}}{RT}}$$

30× higher diffusion coefficient



Outer grain view, $\rho = 0.8$.



Inner grain view, $\rho = 0.8$.

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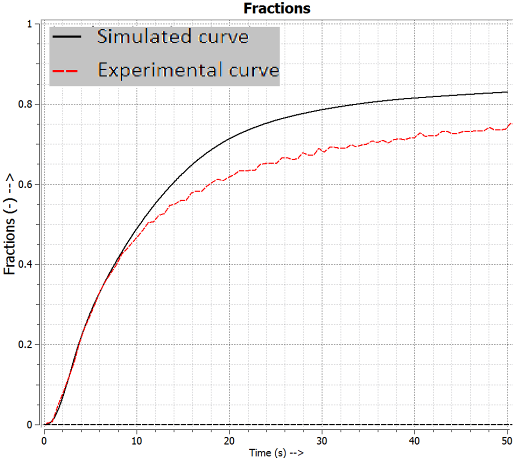
Fraction Curve Fitting



The modeled fraction curve and the experimental fraction curve.

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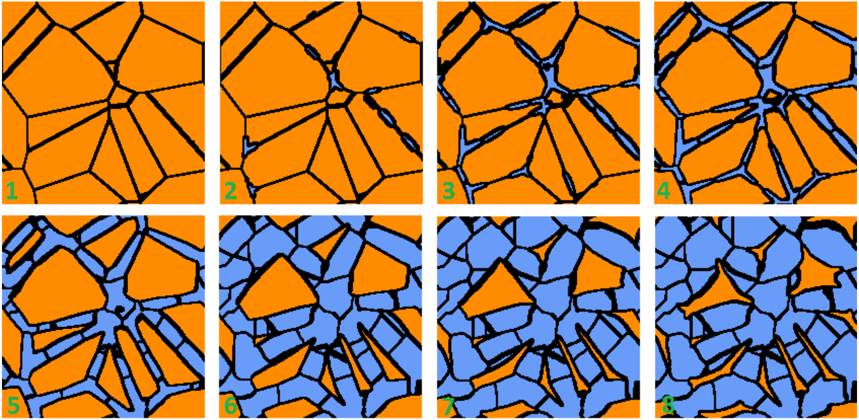
Fraction Curve Fitting



T = 873.15 K
M_0 = 0.05
Fast grain boundary growth factor = 0.85
Fast interface diffusion factor = 0.75

Initial austenite grain density = 5.0e14 m^-3
Number of ferrite nucleations = 2.225e15 m^-3

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Conclusions

- ★ Inward growth seems to reduce dendritic growth and results in less extreme grain shapes
- ★ Carbon smoothing reduces dendritic growth, smoothing area can be scaled up at higher computational costs
- ★ An increased interface diffusion coefficient reduces dendritic growth in an easy-to-implement way, at higher computational costs
- ★ Cellular Automaton is a useful framework for phase transformation models with local concentration differences.

Future Research

- *Experimentally determine parameters for mobility and interface diffusion.*
- *Adaptive grid refinements for a thinner interface*
- *Finite Elements for a better conditioned problem*
- *Parallel implementation for parts of the linear solver*
- *Develop cellular automaton hardware on a chip for fast computation and communication between cells*

Steel structure by *Olafur Eliasson*
Source: www.mymodernmet.com