Modeling the Austenite Ferrite Transformation by Cellular Automaton Improving Interface Stability Delft University of Technology

Mathias Mul September 19, 2014

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Outline

1 Introduction

Microstructure The moving boundary problem

2 Model and Methods

Cellular automaton Model outline Implementation Problems

3 Results

Convergence of CA to Murray-Landis method Improving interface stability Fraction curves

4 Conclusions

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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





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Cellular Automaton

Model built of cells with properties

★ state

- ★ neighbourhood
- ★ transformation rule

example:



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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 $\ell_i \ge 0$ Growth velocity $v_i \ge 0$ Inward growth $\lambda_i \ge 0$

The velocity v is calculated according to the classical equation

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

and M the interface mobility.

$$\lambda_i = \sum_{j \in \mathcal{M}_i} \mathsf{w}_{ji} \ell_j$$

 $w_{ji} = \frac{1}{\sqrt{k}}$

where cells i and j are k-level neighbours

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





Growth dynamics(2)



Transformation rule: ℓ

Transformation rule: λ

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Carbon Redistribution Mechanics



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Diffusion Time Step Find $X(t + \Delta t)$ on $\Omega^{\gamma}(t)$ such that

$$\left\{ egin{array}{rcl} rac{\partial X}{\partial t} &=&
abla \cdot (D(z)
abla X) & ext{in } \Omega^{\gamma}(t), & t < ilde{t} \leq t + \Delta t \ rac{\partial X}{\partial n} &=& 0 & ext{on } \partial \Omega^{\gamma}(t) \end{array}
ight.$$

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



$\mathbf{Unstable\ interfaces} \rightarrow \mathbf{Dendrites}$

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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

$$\Delta z
ightarrow 0, \qquad \Delta t = 0.9 rac{\Delta z}{v_{
m max}}$$



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Inward growth results





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Carbon smoothing results



$$M_0 = 0.6$$

agierocabasel, thetar0.4142, ND=15, th=15, gil=50.650, L=02m/400+1.5+005 agierocabasel, thetar2.4142, M0=1.5, th=16, gil=50.600, L=02m/400+1.5+005 agierocabasel, thetar2.4142, ND=1.5, th=15, gil=50.600, L=02m/400+1.5+005



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Combined results: Inward growth & Carbon smoothing



Indext, Hastr-2 442, M0-16, H-10, guideded, L-20-480-154-005



 $M_0 = 1.5$

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Fast Interface Diffusion

Test Example: Unwanted behaviour for $M_0 = 0.5$



A wobbly shape from A look from the inside Slices of the grain. the outside. reveals the dendritic structure.



Fast Interface Diffusion

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

$5 \times$ higher diffusion coefficient



Outer grain view, ho= 0.9.

Inner grain view, $\rho = 0.9$.

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Fast Interface Diffusion

$$D = D_0 \cdot e^{-rac{
ho Q^{\gamma}}{RT}}$$

$30 \times$ higher diffusion coefficient



Outer grain view, ho = 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



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

