

LITERATURE REPORT

part of the MSc project

Modeling Austenite Ferrite Transformation by Cellular Automaton: Improving Interface Stability

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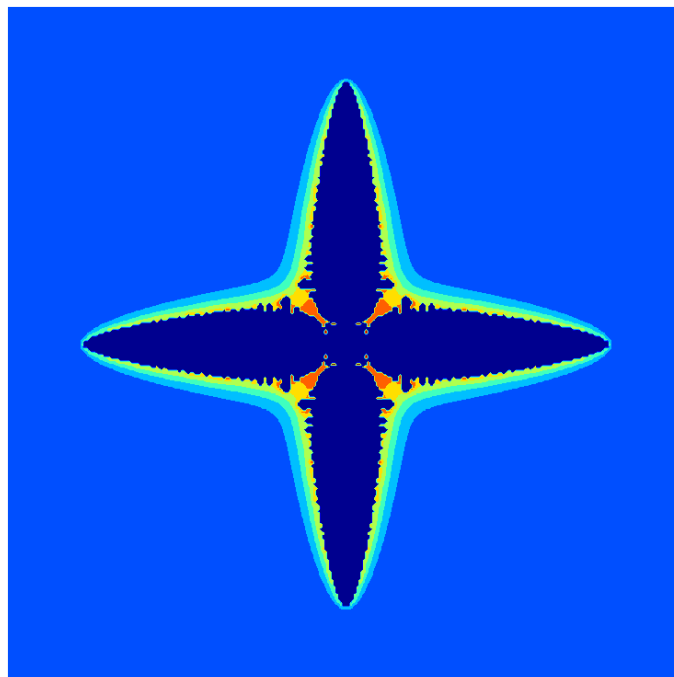
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1 Introduction

The steel industry is large in size and essential to our ever-developing society. Construction, transport and packaging are three examples of sectors that are highly dependent on steel production. Sometimes high quality steel is required as in the automotive industry, sometimes high quantities are required when constructing railways. This confirms the importance of developing steel production processes and the impact when improvements can be made. Typically, steel is made by melting iron ore with cokes, resulting in a liquid carbon-rich steel. Then, oxygen is used to reduce the carbon amount. Since this process is exotherm, scrap metal is added to control the temperature. This is the point where other elements can be added to change final steel properties. After this liquid phase, the metal is cast into solid blocks. The steel blocks will be hot or cold rolled into metal sheets, which is the end product of the steel producer. During the process of making steel, the austenite ferrite transformation often plays an important role determining the final mechanical properties of the steel. The final microstructure depends on the whole process of steel making, starting from the resources iron ore and coal. The prediction of the final microstructure given a certain treatment is desired, because mechanical properties of steel are correlated to its microstructure. For the prediction of final microstructure, phase transformation models as described in this literature study are used. Often, deformation and heat treatments are used in the production process. During heat treatment, specially in the region between 1000 K and 1185 K for regular steels, phase transformation between ferrite and austenite occur. This is the result of iron atoms preferring a different iron lattice at different temperatures. For higher temperatures, iron atoms prefer a face centered cubic lattice while for lower temperatures they prefer a body centered cubic lattice. The interface between these types of iron atom lattices depends partly on the local carbon concentration. Sometimes, numerical errors in carbon concentration result in amplified interface solution errors. Since this report only covers the austenite to ferrite transformation, only the case of cooling down steel is considered. This process is typically important for the roll out table of the hot strip mill and for the cooling section of a continuous annealing line.



Figure 1: The end product of a steel manufacturer.

2 Literature

When slowly cooling down steel around 1000K its micro structure will change. Ferrite grains are nucleating and growing inside austenite during this process. As stated in the introduction, this process is typically important for the roll out table of the hot strip mill and for the cooling section of a continuous annealing line.

2.1 Austenite to Ferrite Transformation

Part of the models for the hot strill mill and annealing line are the dynamics of ferrite growth inside austenite. The main point of interest in this model is to simulate the interface movement during austenite ferrite transformation. The velocity of the interface depends heavily on the carbon concentration at the interface^[8]. Since carbon diffusivity in ferrite is large in comparison to austenite, in existing models it is assumed that the carbon concentration in ferrite instantaneously attains its equilibrium value^[9]. There are several ways to find carbon concentration values at the interface. Some make use of an exponential model assumption for the carbon profile^[9], while others determine the carbon concentration in the whole austenite domain by solving the diffusion equation^[11].

2.1.1 Test Problem

The fundamental test problem that will be investigated is the austenite to ferrite phase transformation. This is a concentration-based moving boundary problem. The interface S between the ferrite domain Ω^α and the austenite domain Ω^γ is the main interest. For the whole domain $\Omega = \Omega^\alpha \cup \Omega^\gamma$ the n -dimensional cube with edges of length L is used. Consider the one and two-dimensional case, that is, for one dimension $\Omega = [0, L]$ and for two dimensions $\Omega = [0, L] \times [0, L]$. The magnitude of L is of the order 10^{-6} m. The test problem will be further specified by initial conditions and boundary conditions.

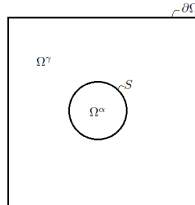


Figure 2: Domain of the moving boundary problem: $\Omega = \Omega^\alpha \cup \Omega^\gamma \cup (\bar{\Omega}^\alpha \cup \bar{\Omega}^\gamma)$

Initial conditions: The initial state is a domain consisting of austenite with a small grain of ferrite situated within the austenite.

Boundary conditions: The diffusion of carbon in austenite requires boundary conditions. The boundary of Ω^γ is $\partial\Omega^\gamma = \partial\Omega \cup S$. The size of the domain for simulating microstructural changes in steel is restricted due to computation times. Since only a small part of the steel is simulated, boundary conditions with symmetric behaviour are chosen. Using Neumann boundary conditions on all sides of the domain, implicitly it is assumed that the microstructural development in time is mirrored on all sides outside the domain. The assumption of constant concentration of carbon in ferrite results in a flux of carbon into the austenite domain, depending on the velocity of the interface v_n . This gives us our boundary condition on S .

The moving boundary problem can be stated as the following system.

$$\begin{cases} v_n & = M\Delta G(x_s^\gamma) & \text{the normal velocity of } S, \\ \frac{\partial x}{\partial t} & = \nabla(D(x)\nabla x) & \text{in } \Omega^\gamma, \quad t > 0, \\ \frac{\partial x}{\partial n} & = 0 & \text{on } \partial\Omega, \quad \forall t, \\ \frac{\partial x}{\partial n} & = -(x_s^\gamma - x^\alpha)v_n & \text{on } S, \quad \forall t, \\ x(t=0) & = x_0. \end{cases} \quad (1)$$

In this system, x is the carbon concentration, M the interface mobility, ΔG the driving force, $D(x)$ the diffusion coefficient, x_s^γ the carbon concentration at the interface S , x^α the equilibrium carbon concentration in ferrite and finally x_0 the initial carbon distribution. Remark that the diffusion coefficient $D(x)$ may depend on the carbon concentration x . Some models assume otherwise to simplify the problem, but experiments show that D really is carbon dependent, see Ågren^[21].

2.2 Cellular Automaton

A popular approach for modeling this transformation is Cellular Automaton(CA), which appears in many articles^[1;3;4;5;6;7;22]. An introductory review of using CA for this type of problem can be found in a paper written by K.G.F. Janssens^[1]. A Cellular Automaton is a discrete model with a regular grid of cells. Each cell has a set of properties, most importantly its state, neighbourhood, and transformation rule. The state represents to which type of grain the cells belong. Given an initial state, each time step the state of a cell is updated by a rule that is a mathematical function of the states of its neighbours.

Grids Any regular grid is allowed in CA models. The most common regular grid is built from squares. But also other grids are used, see figure 3. Hexagonal grids are sometimes used to reduce grid anisotropies^[11;16].

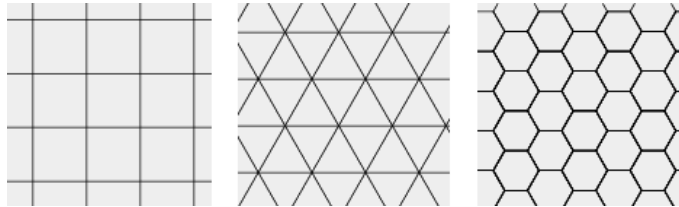


Figure 3: Square grid(l), triangular grid(m), and hexagonal grid(r)

Neighborhoods Two types of neighborhoods will be defined, the Von Neumann neighborhood and the Moore neighborhood. The neighborhood of a cell is usually defined as a set of cells around it, including itself. Using lexicographic numbering on a square $n \times n$ grid, the Von Neumann neighborhood of cell i is defined as the collection of cells

$$\mathcal{N}_i = \{\text{Cells } j : j \in \{i-1, i, i+1, i-n, i+n\}\}. \quad (2)$$

The 3×3 Moore neighborhood of cell i is defined as the collection of cells

$$\mathcal{M}_i = \{\text{Cells } j : j \in \{i+n-1, i+n, i+n+1, i-1, i, i+1, i-n-1, i-n, i-n+1\}\}. \quad (3)$$

Figure 4 illustrates these two definitions.

In general, the $m \times m$ Moore neighbourhood of a cell i consists of all cells within an $m \times m$ square of cells around i .

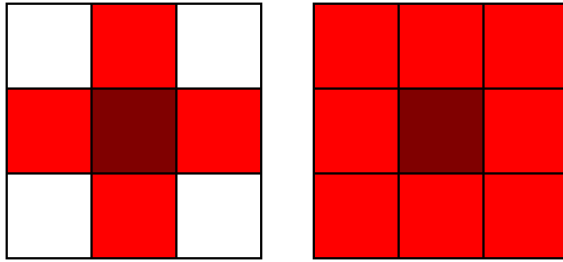


Figure 4: Von Neumann neighborhood(l) and 3×3 Moore neighborhood(r)

Model description A 2-dimensional CA approach from C. Bos et al.^[9] will be described. First, the space domain is discretized into squares of dimension Δz . Ignoring boundary cells, a cell has four *direct neighbours* at distance Δz and four *diagonal neighbours* at distance $\sqrt{2}\Delta z$. Each cell has three properties.

1. The grain to which the cell belongs, austenite or ferrite.
2. The growth length ℓ from the cell centre, updated every time step by Euler time integration using the grain interface velocity v , i.e.

$$\ell(t + \Delta t) = \ell(t) + v\Delta t.$$

3. The grain interface velocity v , which is used to compute the growth length ℓ . Velocity v is computed according to the classical equation $v = M\Delta G$, where the driving force $\Delta G = \Delta G(T, x)$ is a function of temperature T and the interface carbon concentration. The interface carbon concentration is computed by assuming an exponential profile for the carbon distribution in austenite. Knowing the average amount of carbon in an austenite grain, the interface carbon concentration can be computed. This approach for the interface velocity is called a mixed-mode model^[8]. Using this model, the fact that diffusion of carbon in austenite plays a role is acknowledged, but the diffusion equation is not actually solved. The function $\Delta G(T, x)$ can be extracted from the software Thermo-calc[®]. Based on an average carbon concentration and material composition this software produces a table for a range of temperatures and carbon concentrations.

Note that the last two properties are only relevant for the ferrite interface cells. When the growth length of cell i has reached the grid spacing Δz , the direct neighbours of cell i will transform from austenite into ferrite. When ℓ_i has reached the diagonal grid spacing $\sqrt{2}\Delta z$, also the diagonal neighbours of cell i will transform. For the sake of reliability of the model, one should use the excess length $\ell_i - \Delta z$ as initial growth length for the newly transformed cell. The time step Δt will be chosen in such a way that the event of diagonal and direct neighbours simultaneously transforming can not happen. Therefore, Δt is restricted by the criterion:

$$\Delta t < (\sqrt{2} - 1) \frac{\Delta z}{v_{\max}},$$

where v_{\max} is the maximum grain interface velocity of all cells.

2.3 Problem Section

The phase transformation from austenite to ferrite will be modeled using cellular automaton, because CA is advantageous in its simplicity versus phase field^[20] or level set methods^[24]. The CA model framework from Bos et al.^[9] is available and could be improved at some points. Thus, also from a pragmatic point of view it is wise to continue with this type of model. Also, other transformations, recrystallization and nucleation processes are present in this model. The submodel for determining the carbon interface concentration based on an assumed exponential profile will be replaced by solving the carbon concentration using a finite difference grid on the austenite domain, because it is suspected that the exponential carbon profile model is not always accurate enough in the multi-grain model. Another problem lies in the assumption that the interface is restricted to a discrete set of points. Additionally, there are some issues with the interface stability due to the discretized grid.

2.3.1 Jumping interface

The movement of the interface between austenite and ferrite depends partly on the carbon concentration at the interface. Since the carbon diffusivity in ferrite is large in comparison to austenite, it is assumed that the carbon concentration in ferrite instantaneously attains its equilibrium value. The carbon concentration in austenite is determined by solving the diffusion equation on the austenite part of the domain. Using a CA model, the austenite domain does not change continuously, but with jumps every time a cell is transformed. Consider a cell that transforms during time step iteration k , i.e. at time step k it belongs to austenite and at time step $k + 1$ it belongs to ferrite. The excess carbon $x_k - x^\alpha$ then flows instantaneously towards its neighbouring cells. After this redistribution of carbon, a time step for the diffusion equation is applied on the austenite domain. Using this approach, it is possible to exceed the equilibrium concentration of carbon in austenite. This is physically impossible. Therefore, it is necessary to investigate if the CA approach where the interface is restricted to fixed cells can be justified. It would be desirable to observe that the fixed grid method behaves similarly to an adaptive grid method such as the Murray-Landis method^[12].

2.3.2 Unstable interface growth

As found in other literature^[11], the interface between ferrite and austenite is not always stable. According to observable physics, dendritic growth does not happen when ferrite grows in austenite. For the interface mobility large in comparison with the diffusion coefficient, i.e. $M \gg D$, it seems that interface instabilities are unavoidable. Due to discretization into square cells in combination with a freedom restriction on the interface position, a perturbation error is easily introduced. A small perturbation error of carbon concentration will cause perfect spherical growth to evolve into dendritic growth. If an erroneous carbon accumulation area is formed, the interface shape will not recover from the error. When observing the steel microstructure after real experiments, dendritic growth does not seem realistic. The main causes for dendritic growth behaviour are assumed to be the discretized square grid and the absence of surface tension in the model. However, incorporating surface tension in a growth model would complexify the model and drastically increase computation times. Also, the influence of surface tension on the growth kinetics is small. Is it the right way to go to add physical phenomena to reduce numerical error issues? Using curvature in a CA model has been done by Janssens^[1], which he summarized by his conclusion: *as grains get large relative to the cell size, the grain boundary curvature decreases relative to the cell size, and consequently the cellular automaton underestimates the driving pressure.* Another model with curvature incorporated can be found in Raghavan^[3]. In a paper of Lan^[11] a different grid is used in order to reduce instabilities. Using a hexagonal grid reduces instabilities, but it did not eliminate the grid anisotropy. The main point of interest lies in the relationship between surface tension, interface mobility and diffusion. These three parameters determine whether or not dendrites will be formed. It can be stated that there is no golden rule yet to fully avoid unstable interface growth. Dendritic grain growth behaviour will be replicated and analyzed in order to avoid or reduce interface instabilities in a physical realistic way.

3 The Model

The model is constructed based on the moving boundary problem (1), but simplified such that D does not depend on x .

$$\begin{cases} v_n & = M\Delta G(x_s^\gamma) & \text{the normal velocity of } S, \\ \frac{\partial x}{\partial t} & = D\nabla^2 x & \text{in } \Omega^\gamma, \quad t > 0, \\ \frac{\partial x}{\partial n} & = 0 & \text{on } \partial\Omega, \quad \forall t, \\ \frac{\partial x}{\partial n} & = -(x_s^\gamma - x^\alpha)v_n & \text{on } S, \quad \forall t \\ x(t=0) & = x_0. \end{cases} \quad (4)$$

For each cell i its binary state is defined as $\zeta_i \in \{0, 1\}$. The ferrite and austenite domains in problem (4) are defined as collections of cells,

$$\begin{aligned} \Omega^\alpha &= \{\text{Cells } i : \zeta_i = 1\}, \\ \Omega^\gamma &= \{\text{Cells } i : \zeta_i = 0\}. \end{aligned} \quad (5)$$

3.1 CA Framework

To model ferrite grain growth and investigate behaviour, a 2-dimensional Cellular Automaton model with carbon diffusion is constructed. This model is based on existing models from literature, e.g. in Bos et al.^[9]. Consider a square domain Ω with n square row and column cells of dimension Δz . Ignoring boundary cells, a cell has four *direct neighbours* at distance Δz and four *diagonal neighbours* at distance $\sqrt{2}\Delta z$. Initially, a small ferrite grain is nucleated and environmental conditions are imposed such that the ferrite will grow. The ferrite and austenite cells can be subdivided into interface and internal cells.

| Description | Symbol | Defined for |
|---|--------|-------------------------|
| Average carbon concentration at the interface | x_s | Ferrite interface cells |
| Growth velocity | v | Ferrite interface cells |
| Outward growth length | ℓ | Ferrite interface cells |
| Carbon concentration | x | All cells |

Table 1: Cell properties

3.2 Interface Growth Dynamics

For each ferrite interface cell, the growth length $\ell(t)$ is defined as

$$\ell(t) = \int_{t_0}^t v_n(\tau) d\tau, \quad (6)$$

where $v_n(t)$ is the outward normal growth velocity of the interface S and $t_0 = \inf\{t : v_n(t) > 0\}$. This growth length can be interpreted as the radius of a growing ball with radius ℓ centered in the cell. This omnidirectional growth model is a simplification making the consideration for different growth velocities for every direction obsolete. The growth velocity v_n is computed by a model for the interface velocity in the outward normal direction, which can be formulated as

$$v_n = M_0 \cdot e^{-\frac{Q^{\alpha,\gamma}}{RT}} \Delta G(T, x_s), \quad (7)$$

where M_0 and $Q^{\alpha,\gamma}$ are respectively the pre-exponential factor and the activation energy for the interface mobility. Additionally, R is the gas constant and T the temperature. The driving force ΔG is assumed to be a function of the temperature T and the carbon interface concentration x_s . Using the software Thermo-Calc[®] this function can be extracted for the desired steel alloy. Using a transformation method based on the growth length ℓ , cells are transformed from austenite to ferrite.

3.3 Carbon Dynamics

First, the use of atomic fraction as a concentration in the diffusion equation is justified. Let

$$f_C = \frac{a_C}{a_C + a_{Fe}} \quad (8)$$

be the fraction of carbon atoms of a cell with volume $V = (\Delta z)^2$, where a_C and a_{Fe} are respectively the number of carbon and iron atoms inside the cell. Since low-carbon steel is considered, it is assumed that the number of carbon atoms is much smaller than the number of iron atoms, i.e. $a_C \ll a_{Fe}$. Furthermore, it is assumed that a_{Fe} per cell is constant, i.e. density variations of iron atoms are neglected. In reality, these variations are small^[2]. Inserting these two assumptions, the following relationship is obtained

$$\frac{f_C}{V} \approx \frac{a_C}{a_{Fe}V} \propto \frac{a_C}{V} \quad (9)$$

which is a quantity per unit volume and thus the atomic fraction can be used in the diffusion equation.

For an accurate value of the interface carbon concentration, carbon diffusion on the austenite domain has to be implemented. The boundaries of this domain are the interface with ferrite S and the boundary of the whole domain $\partial\Omega$. The diffusion coefficient is computed by

$$D = D_0 \cdot e^{-\frac{Q^\gamma}{RT}}, \quad (10)$$

where D_0 and Q^γ respectively are the pre-exponential constant and the activation energy for carbon diffusion. As stated, remind that D does not depend on the carbon concentration x .

Recall the two boundary conditions on $\partial\Omega^\gamma$, as shown below.

$$\begin{cases} \frac{\partial x}{\partial n} = 0 & \text{on } \partial\Omega \\ \frac{\partial x}{\partial n} = -(x_s^\gamma - x^\alpha)v_n & \text{on } S \end{cases} \quad (11)$$

The non-zero Neumann boundary condition is important when cells transform. Whenever this happens, the excess carbon x^e of a newly transformed cell that corresponds with the term $(x_s^\gamma - x^\alpha)$ is instantaneously distributed over neighbouring austenite cells by the procedure outlined in Section 4.1. Furthermore, assume that no cells transform between t_0 and $t_0 + \Delta t$, i.e Ω^γ is constant and on $[t_0, t_0 + \Delta t]$. Using this approach, the boundary conditions for the diffusion equation reduce to zero-Neumann conditions on the whole boundary $\partial\Omega^\gamma$ and the diffusion problem can be stated as:

Find x on $\Omega^\gamma(t)$ such that

$$\begin{cases} \frac{\partial x}{\partial t} = D\nabla^2 x & \text{in } \Omega^\gamma(t), \\ \frac{\partial x}{\partial n} = 0 & \text{on } \partial\Omega^\gamma(t) \end{cases}, \quad t_0 < t \leq t_0 + \Delta t \quad (12)$$

given $x(t_0)$ on Ω^γ .

4 Methods and Implementation

4.1 Smoothed Carbon Interface Concentration

To compute the growth velocity v_n for a ferrite interface cell, a value for the carbon interface concentration at this cell x_s is required. This interface concentration is determined in two steps. For all neighbouring austenite interface cells a non-trivial value for the carbon concentration is defined. The carbon interface concentration x_s^i of ferrite interface cell i is computed as

$$x_s^i = \frac{\sum_{j \in \mathcal{M}_i} w_{ji} x_j}{\sum_{j \in \mathcal{M}_i} w_{ji}}, \quad (13)$$

where the weights w_j are defined as

$$w_{ji} = \begin{cases} 0 & \text{cell } j \text{ is ferrite} \\ 1 & \text{cells } i \text{ and } j \text{ are direct neighbours and cell } j \text{ is austenite} \\ \frac{1}{\sqrt{2}} & \text{cells } i \text{ and } j \text{ are diagonal neighbours and cell } j \text{ is austenite} \end{cases}. \quad (14)$$

The Moore neighborhood \mathcal{M}_i of cell i , *direct* and *diagonal* neighbours are defined in the literature section(CA).

An attempt is made to reduce the interface instabilities due to numerically introduced errors by smoothing the interface concentrations. Based on the level s of smoothing, the interface carbon concentration is averaged over the $(2s+1) \times (2s+1)$ cells around the reference cell. The smoothed carbon interface concentration of level $s = 1$ \tilde{x}_s^i at reference cell i is computed as

$$\tilde{x}_s^i = \frac{\sum_{j \in \mathcal{M}_i} w_{ji} x_s^i}{\sum_{j \in \mathcal{M}_i} w_{ji}}, \quad (15)$$

where the weights w_j are defined as

$$w_{ji} = \begin{cases} 1 & \text{cell } j \text{ is ferrite interface} \\ 0 & \text{else} \end{cases}. \quad (16)$$

In general, the level s smoothed carbon interface concentration \tilde{x}_s^i at reference cell i is defined as

$$\tilde{x}_s^i = \frac{\sum_{j \in \mathcal{S}} x_s^i \mathbf{1}\{j \text{ is ferrite interface}\}}{\sum_{j \in \mathcal{S}} \mathbf{1}\{j \text{ is ferrite interface}\}}, \quad (17)$$

where \mathcal{S} are the indices of the $(n_s \times n_s)$ Moore neighbourhood of cell i and $\mathbf{1}\{\text{statement}\}$ is the indicator function defined as

$$\mathbf{1}\{\text{statement}\} = \begin{cases} 1 & \text{statement is true} \\ 0 & \text{statement is false} \end{cases}. \quad (18)$$

Remark that for $\Delta z \rightarrow 0$ this method reduces to smoothing over a point, thus using the value of carbon concentration in that point. This is desirable behaviour in the sense that the solution of the discretized problem converges to the exact problem.

Inspiration This method of carbon smoothing at the interface is based on an idea from van Leeuwen^[19]. To guarantee interface stability, the idea was to use an infinite carbon diffusion coefficient at the interface. This results in a constant value for the interface concentration, i.e. a constant interface velocity across the whole interface.

4.2 Adaptive time steps

The concept of adaptive time stepping is based on the combination of accuracy and efficiency. Large changes result in small time steps and small changes allow larger time steps. The time step Δt will be chosen in such a way that the event of diagonal and direct neighbours simultaneously transforming due to one growing ferrite interface cell can not happen. Therefore, the time step is restricted such that the growth length of a cell does not change more than the difference in distance between a direct and a diagonal neighbor. The following time step criterion is the result,

$$\Delta t < (\sqrt{2} - 1) \cdot \frac{\Delta z}{v_{\max}}, \quad (19)$$

where v_{\max} is the maximum grain interface velocity.

4.3 Interface Growth Methods

A transformation method utilizing the growth length ℓ is formulated in Bos et al.^[9], see section 2. This approach can be interpreted from the perspective of growing cells, based on the question whether the ferrite boundary cell expands. Using the Euler forward time integration method, the growth length ℓ after a time step of Δt is computed as

$$\ell(t + \Delta t) = \ell(t) + v\Delta t, \quad (20)$$

where the growth velocity is computed using the classical equation $v = M\Delta G$, as found in Bos et al.^[9].

A different approach is to change the perspective and consider growth based on the question whether an austenite boundary cell will transform. This results in a more sophisticated strategy that also takes the amount of growing neighbouring ferrite cells into account. As an intuitive support for this approach, it does make sense that a cell will transform earlier if there is interface growth coming from multiple directions instead of only one. The latter approach assigns a percentage of transformation to the austenite interface cells.

The inward growth length λ , defined for all austenite interface cells, is introduced here and defined as

$$\lambda_i = \sum_{j \in \mathcal{M}_i} w_{ji} \ell_j \quad (21)$$

$$w_{ji} = \begin{cases} 1 & \text{cells } i \text{ and } j \text{ are direct neighbours} \\ \frac{1}{\sqrt{2}} & \text{cells } i \text{ and } j \text{ are diagonal neighbours} \end{cases}, \quad (22)$$

where w_{ji} are weights and ℓ_j is the growth length. The Moore neighborhood \mathcal{M}_i of cell i , *direct* and *diagonal* neighbours are defined Section 2.2. Austenite interface cell i transforms if $\lambda_i > \theta\Delta z$, where Δz is the grid spacing. Theta can be computed using the fact that a straight interface with a constant velocity v_c should move accordingly. Consider a straight vertical interface as in Figure 5 with velocity $v_c > 0$. Let $\ell_1 = \ell_2 = \ell_3 = \ell$. Then

$$\begin{aligned} \lambda_i &= \frac{1}{\sqrt{2}}\ell_1 + \ell_2 + \frac{1}{\sqrt{2}}\ell_3 \\ &= \frac{2}{\sqrt{2}}\ell + \ell \\ &= (1 + \sqrt{2})\ell. \end{aligned}$$

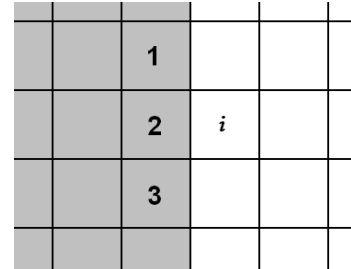


Figure 5: Finding θ .

The transformation happens when $\ell > \Delta z$. It follows that $\frac{\lambda_i}{1+\sqrt{2}} > \Delta z \Leftrightarrow \lambda_i > (1 + \sqrt{2})\Delta z$. Hence, $\theta = 1 + \sqrt{2}$.

4.4 Carbon diffusion

Due to model assumptions discussed in Section 3.3, the boundary conditions reduce to zero-flux conditions. The reduced carbon diffusion problem is stated in Equation (12) as: Find x on $\Omega^\gamma(t)$ such that

$$\begin{cases} \frac{\partial x}{\partial t} = D\nabla^2 x & \text{in } \Omega^\gamma(t), & t_0 < t \leq t_0 + \Delta t, \\ \frac{\partial x}{\partial n} = 0 & \text{on } \partial\Omega^\gamma(t), \end{cases}$$

where x is the carbon concentration, D is the carbon diffusion coefficient and $\partial\Omega^\gamma(t) = \partial\Omega \cup S$ is the complete boundary of the austenite domain. To solve this time step for the diffusion equation, use implicit Euler time integration in combination with finite differences. For every cell the carbon concentration is approximated by x_i . The main reason to apply an implicit method is its property of unconditional stability which allows larger time steps^[13]. Implementing this method yields

$$\frac{x_i^{k+1} - x_i^k}{\Delta t} = \frac{D}{(\Delta z)^2} (x_{i-1}^{k+1} + x_{i+1}^{k+1} + x_{i-n}^{k+1} + x_{i+n}^{k+1} - 4x_i^{k+1}). \quad (23)$$

This expression is rewritten as the matrix equation

$$Ax^{k+1} = x^k, \quad (24)$$

where $A = I - T$ is a sparse symmetric positive definite matrix. Using the Kronecker product \otimes , the matrix T is constructed in three steps. Boundary conditions are treated in step 2 and 3.

1. Compute

$$T = \frac{D\Delta t}{(\Delta z)^2} (S \otimes I + I \otimes S), \quad (25)$$

where I is the identity matrix of dimension $n_z \times n_z$ and S has the structure

$$S = \begin{bmatrix} -1 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -1 \end{bmatrix}. \quad (26)$$

2. Set all rows and columns corresponding to ferrite cells to zero. (The carbon concentration does not change in ferrite, thus all ferrite rows are set to zero. Also, due to zero-flux boundary conditions the ferrite columns are set to zero.)
3. Set the diagonal entries equal to minus the row sum that excludes the diagonal value, due to zero-flux boundary condition between austenite-ferrite, i.e.

$$T_{ii} = - \sum_{j \neq i} T_{ij}. \quad (27)$$

CG method The implicit Euler time integration method includes solving a linear system. In our case, from numerical analysis it is known that by applying finite differences on the diffusion equation with zero-flux boundary conditions, the resulting matrix $A = I - T$ is a sparse symmetric positive definite matrix. An effective way to solve this type of linear system is to apply the a pre-conditioned Conjugate Gradient (CG) method. The CG method is an iterative method for solving large sparse linear systems, first published in 1952 by Hestenes and Stiefel^[23]. A simple-to-implement pre-conditioner like the Jacobi pre-conditioner may be used to speed up convergence results.

4.5 The algorithm

For each iteration in time, the algorithm consists of the following steps.

1. Compute the interface carbon concentration for the ferrite interface cells. It is necessary to compute the interface velocity during the next time step. It takes two steps to compute x_s . For ferrite interface cell i , compute x_s by the weighted average (direct neighbours weight 1, diagonal neighbours weight $\frac{1}{\sqrt{2}}$) of carbon concentration of its austenite neighbours. Then, smooth x_s by taking the average x_s inside the $n_s \times n_s$ cell square around cell i , see the carbon interface smoothing section.
2. Compute v for all relevant cells, using the classical equation $v = M\Delta G$. The driving force ΔG is assumed to be a function of the temperature T and the carbon interface concentration x_s . Using the software Thermo-Calc[®] this function can be extracted for the desired steel alloy.
3. Compute ℓ for all relevant cells, using Euler forward time integration: $\ell(t + \Delta t) = \ell(t) + v\Delta t$.
4. Compute λ for all relevant cells, by taking the weighted sum over its direct and diagonal neighbours. The direct neighbours have weight 1 and the diagonal neighbours have weight $\frac{1}{\sqrt{2}}$.
5. Transform all cells according to outward growth length or inward growth. The outward growth method can be found in the literature^[9], the inward growth method is based on an implementation on a hexagonal grid^[11].
 - **Outward growth method:** Consider the ferrite interface cells. If the growth length of cell i exceeds the direct or diagonal grid spacing, its neighbouring austenite cells will transform into ferrite, respectively. In other words, if $\ell^i > \Delta z$ then its direct neighbours transform, whereas if $\ell^i > \sqrt{2}\Delta z$ then its diagonal neighbours transform. The time stepping will be chosen in such a way that it is not possible that direct and diagonal neighbours of a ferrite interface cell will transform simultaneously, see the time step section.
 - **Inward growth method:** Consider the austenite interface cells. If the inward growth of cell i exceeds $(1 + \sqrt{2})\Delta z$, then cell i transforms into ferrite.
6. Redistribute the excess carbon from newly transformed cells. If cell i transforms, the carbon amount will be set at x^α . The remaining carbon will be distributed to its austenite neighbours, using a weight 1 for direct neighbours and a weight $\frac{1}{\sqrt{2}}$ for diagonal neighbours.
7. Solve the diffusion equation for the carbon concentration on the austenite part of the domain, using Neumann boundary conditions on the interface between austenite and ferrite and on the boundary of our square domain Ω .

5 Results

Even though this is a literature report, some preliminary results will be given.

5.1 Comparison: CA to Murray-Landis

The main point of interest in the transformation model is the interface $s(t)$, which is equivalent to the fraction ferrite $f_\alpha(t)$ for a 1-dimensional model. It is desired to show that the two methods are consistent for $\Delta z \rightarrow 0$. For both methods the time step Δt is coupled to the space increment Δz for stability, $\Delta t = 0.9 \cdot \frac{\Delta z}{v_{\max}}$, where v_{\max} is determined from a previous simulation using the same parameters. Let us denote the fraction of ferrite according to the CA method and the Murray-Landis method as f_1 and f_2 respectively. Then, the error is defined as $e = \|f_1 - f_2\|_\infty$, using the maximum norm of the difference between the two methods. Hence, the task is to show that $e \rightarrow 0$ as $\Delta z \rightarrow 0$.

For a decreasing sequence of space increments Δz and according sequence of time increments Δt , the error $e = \|f_1 - f_2\|_\infty$ was computed. Using a fixed grid, the interface $s(t)$ is restricted to values on the grid. Therefore, an error due to grid spacing is tolerated and expected to occur. Figure 4 shows the results of this sequence of simulations, using logarithmic scaling on both axes.

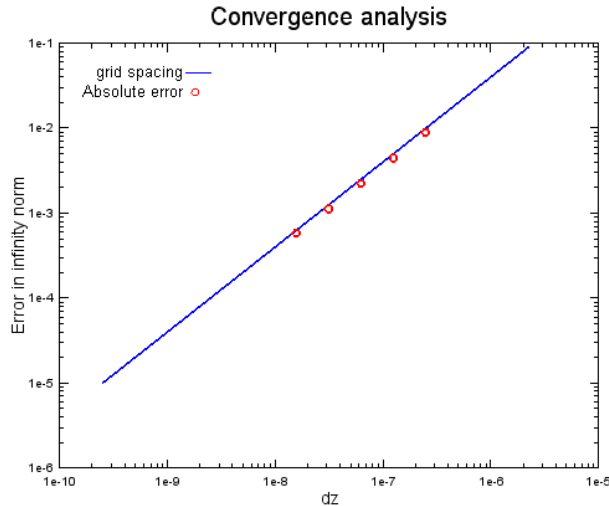


Figure 6: Experimental convergence of the absolute error e .

Analyzing the slope of the errors, an experimental order of convergence of 1 is obtained. The conclusion that the fixed grid method converges linearly to the adaptive grid method can be drawn from this. Furthermore, observe that the error is smaller than the tolerated error due to grid spacing for any Δz tested. In conclusion, it can be stated that the fixed grid method is accurate up to an error induced by the grid spacing.

The convergence analysis has been performed using the parameters in Table 2. Also, the excess length $\ell_i - \Delta z$ should be set as the initial length of a newly transformed cell.

| Description | Variable | Value | Unit |
|---|--------------------|-----------|-------------------------------------|
| Length of interval | L | 25e-6 | m |
| Simulation time | t_f | 600 | s |
| Temperature | T | 1000 | K |
| Gas constant | R | 8.314462 | J K ⁻¹ mol ⁻¹ |
| Pre-exponential diffusion factor | D_0 | 0.15e-4 | m ² s ⁻¹ |
| Pre-exponential mobility factor | M_0 | 0.035 | m J ⁻¹ s ⁻¹ |
| Activation energy for carbon diffusion | Q_D^γ | 142e3 | J mol ⁻¹ |
| Activation energy for ferrite recrystallization | $Q^{\alpha\gamma}$ | 140e3 | J mol ⁻¹ |
| Average carbon concentration | x_0 | 4.1580e-3 | atomic fraction |

Table 2: Parameter Values: Convergence Analysis

5.2 Inward Growth Method

For increasing values of interface mobility M_0 , the transformation rules of outward and inward growth are compared using identical input parameters.

Stable Case First, the two methods using a low value for the interface mobility are compared. The outward growth method does not show any dendritic growth. However, the grain shape did not grow into a circle, but a polygon. This behaviour is analyzed in a paper written by Marek^[16] and is acceptable as an approximation of a circle. When analyzing the output of the inward growth method, a circular shape is observed. The growth behaviour is symmetric on the square grid in this case and thus more realistic.

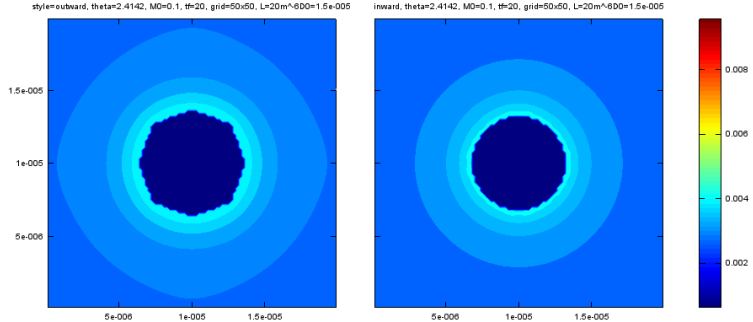


Figure 7: *Outward growth (l) and inward growth (r): $M_0 = 0.1$, $t_f = 20$*

Unstable Case Let us now consider a higher interface mobility which causes interface instability. The outward growth method shows clear accumulation areas of carbon, resulting in dendritic *fingers* that grow faster in the direction of the least carbon concentration. When examining the results of the same test using the inward growth method, significant decrease of dendritic growth is seen. In fact, the grain shape has a realistic circle shape.

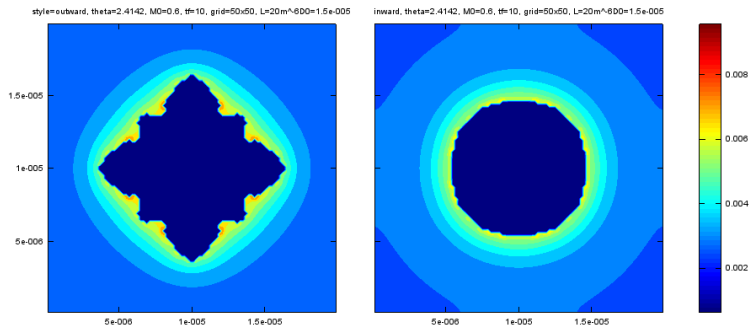


Figure 8: *Outward growth (l) and inward growth (r): $M_0 = 0.6$, $t_f = 10$*

Very Unstable Case The limits of the inward growth method are investigated. When increasing the interface mobility even further, the point is reached where also the behaviour of this method is unsatisfactory. Although one could argue that the grain shape from the inward growth method is 'better', it is not the desired circular shape. Thus, also this method has its limits.

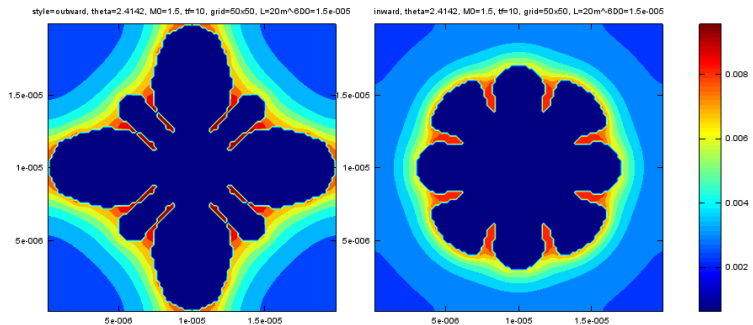


Figure 9: *Outward growth (l) and inward growth (r): $M_0 = 1.5$, $t_f = 10$*

5.3 Carbon Interface Smoothing

For increasing values of the interface mobility M_0 , the effectiveness of carbon interface smoothing is tested using the outward growth model.

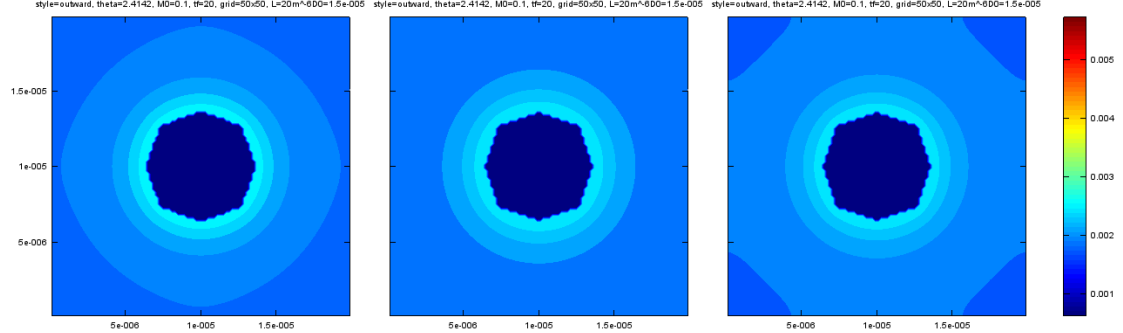


Figure 10: *No smoothing*(l), 3×3 -*smoothing*(m) and 5×5 -*smoothing*(r): $M_0 = 0.1$, $t_f = 20$

Stable Case: Figure 10 For a low interface mobility there is not much to improve. Minor but no significant differences can be found in the isoconcentration lines, but the grain shape seems identical.

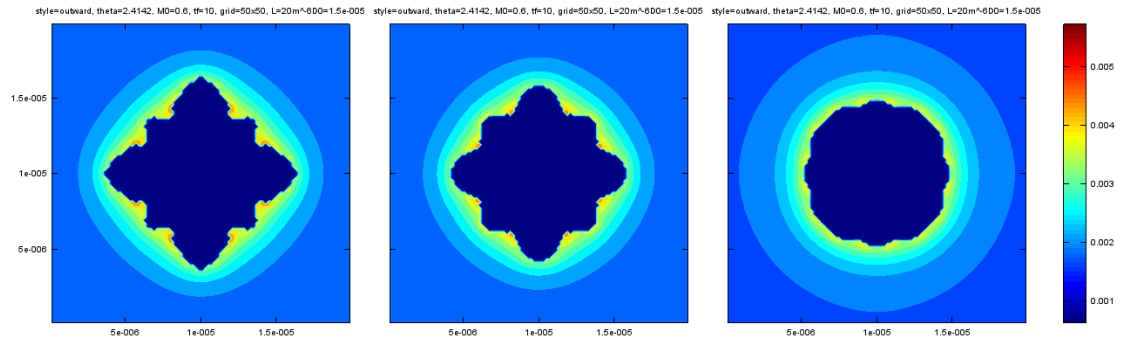


Figure 11: *No smoothing*(l), 3×3 -*smoothing*(m) and 5×5 -*smoothing*(r): $M_0 = 0.6$, $t_f = 10$

Unstable Case: Figure 11 For a higher interface mobility there is more space for improvements. The interface behaves less wildly when the smoothing area is enlarged. The grain shape approximates the circle better when applying the carbon interface smoothing method. It seems that the smoothing has an effect on the interface stability, but is unable to remove the interface instabilities completely.

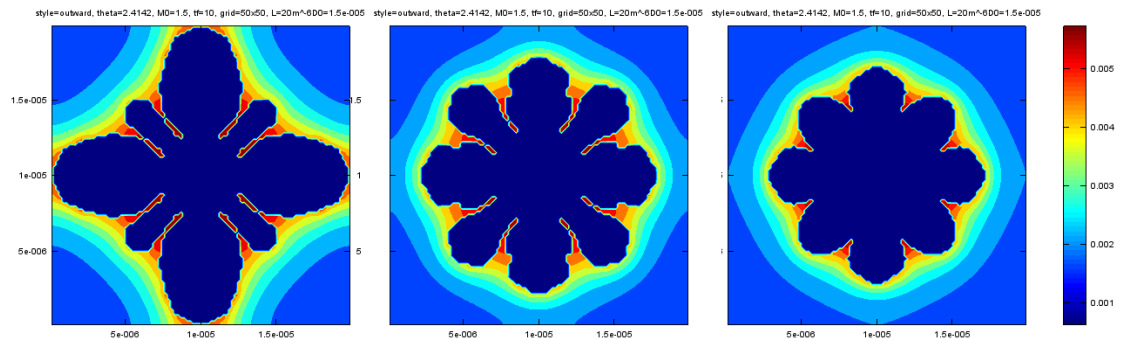


Figure 12: *No smoothing*(l), 3×3 -*smoothing*(m) and 5×5 -*smoothing*(r): $M_0 = 1.5$, $t_f = 10$

Very Unstable Case: Figure 12 When simulating a more extreme case, the same improvements as from less extreme values for interface mobility are observed. The dendritic grain growth is reduced, but the method by itself is unable to avoid dendritic grain growth.

5.4 Stabilizing methods combined

Both improvements on literature models reduce interface instabilities and are unable to eradicate the problem. Therefore, by combining both methods, it is only expected to further reduce dendritic grain growth, not eliminate. A large analysis of different cases can be done, but this is skipped because results seem obvious when starting at the most extreme test case. Combining the inward growth method with the carbon smoothing method of level s , IG&CS(s), the following plots are given as a result.

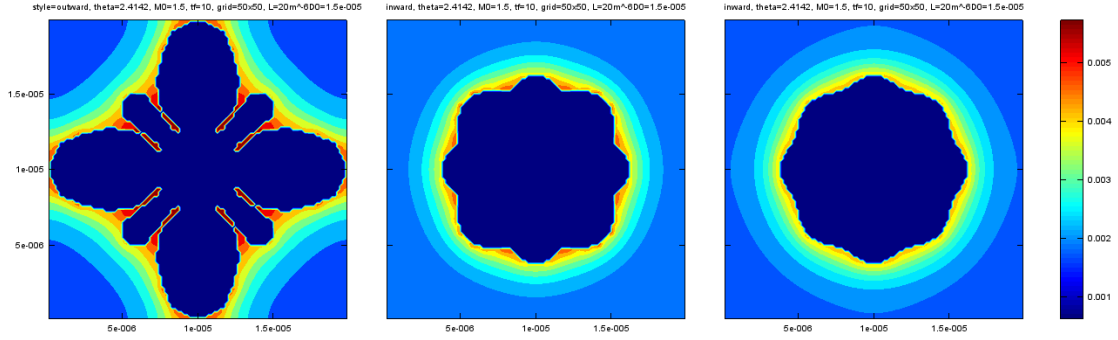


Figure 13: OG&CS(0)(left), IG&CS(1)(middle) and IG&CS(2)(right)

Parameters and Initial State

For all results the parameter values from Table 3 have been used. The initial grain shape used was a small thick cross, depicted in Figure 14. A grid size of 100×100 cells has been used. For low interface mobility values, the simulations have been extended from 10 to 20 seconds. This has been done to increase grain size and therefore visibility of the results.

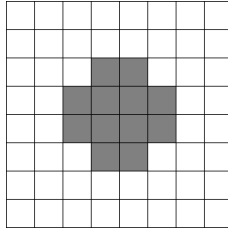


Figure 14: The initial ferrite grain shape

| Description | Variable | Value | Unit |
|---|--------------------|-----------------|-------------------------------------|
| Length of interval | L | 20e-6 | m |
| Simulation time | t_f | 10 or 20 | s |
| Temperature | T | 1000 | K |
| Gas constant | R | 8.314462 | J K ⁻¹ mol ⁻¹ |
| Pre-exponential diffusion factor | D_0 | 0.15e-4 | m ² s ⁻¹ |
| Pre-exponential mobility factor | M_0 | 0.1, 0.6 or 1.5 | m J ⁻¹ s ⁻¹ |
| Activation energy for carbon diffusion | Q_D^γ | 142e3 | J mol ⁻¹ |
| Activation energy for ferrite recrystallization | $Q^{\alpha\gamma}$ | 140e3 | J mol ⁻¹ |
| Average carbon concentration | x_0 | 4.1580e-3 | atomic fraction |

Table 3: Parameter Values: Testing Stability Methods

6 Conclusions

Conclusions A 2-dimensional square grid Cellular Automata model for the austenite ferrite transformation has been reproduced based on literature. The model allows experimenting within the Cellular Automata framework, making it possible to try different approaches for the subproblems. The interface restriction that is a consequence of the Cellular Automata model has been analyzed by comparing the CA model with the Murray-Landis method which allows continuous interface movement. After carefully constructing the model, it has been shown that the 1-dimensional CA model does converge to the Murray-Landis solution as the grid spacing goes to zero. Furthermore, the causes of interface instabilities have been investigated. In the literature, transformation rules found are based on the outward growth(OG). Even in stable cases, the grain shape tends to a octagon when applying the OG method. Changing the perspective to inward growth(IG), a new transformation rule was found. This method works positive in two ways. Firstly, the stable case tends to a circular shape. Secondly, dendritic grain growth is reduced and a higher value for interface mobility is allowed. In order to even further reduce instable interface growth, the carbon concentration at the interface was smoothed. Averaging the concentration over a couple of neighbouring cells, the numerically introduced errors in the concentration are spreaded to reduce impact on interface shape. As a result, this reduces dendritic growth even further.

Summary A CA model for the austenite ferrite transformation has been *reproduced*, the use of CA has been *justified* in some sense and the interface stability has been *improved*. It is recommended to use the inward growth method in combination with carbon smoothing to improve the austenite ferrite interface when using cellular automata.

6.1 Research Questions

The major part of this literature study was about reducing interface instabilities. However, it is known that also surface tension plays a role in grain growth kinetics. Thus, the main question remains: *Is it possible to incorporate surface tension to completely avoid dendritic grain growth without paying for heavy computational costs?* On the other hand, the current increase in stability might be enough for better results in transformation simulations. This thought leads to another question: *Are these new approaches enough for the current application?*

References

- [1] K.G.F. Janssens, *An introductory review of cellular automata modeling of moving grain boundaries in polycrystalline materials*. Mathematics and Computers in Simulation 80.7 (2010): 1361-1381.
- [2] T.A. Kop, *A dilatometric study of the austenite/ferrite interface mobility*. Printed by Print-Partners Ipskamp, Proefschrift, 2000.
- [3] S. Raghavan and Satyam S. Sahay, *Modeling the grain growth kinetics by cellular automaton*. Materials Science and Engineering: A 445 (2007): 203-209.
- [4] S. Raghavan and Satyam S. Sahay, *Modeling the topological features during grain growth by cellular automaton*. Computational Materials Science 46.1 (2009): 92-99
- [5] C. Zheng, D. Raabe, *Interaction between recrystallization and phase transformation during intercritical annealing in a cold-rolled dual-phase steel: A cellular automaton model*. Acta Materialia 61.14 (2013): 5504-5517.
- [6] B.J. Yang, L. Chuzhoy and M.L. Johnson, *Modeling of reaustenitization of hypoeutectoid steels with cellular automaton method*. Computational Materials Science 41.2 (2007): 186-194.
- [7] L. Zhang, Y.M. Wang, C.B. Zhang, S.Q. Wang and H.Q. Ye, *A cellular automaton model of the transformation from austenite to ferrite in low carbon steels*. Institute of Physics Publishing, Modelling and simulation in materials science and engineering, 2003.
- [8] C. Bos and J. Sietsma, *A mixed-mode model for partitioning phase transformations*. Scripta Materialia 57.12 (2007): 1085-1088.
- [9] C. Bos and M.G. Meozzi and J. Sietsma, *A microstructure model for recrystallisation and phase transformation during the dual-phase steel annealing cycle*. Computational Materials Science 48.3 (2010): 692-699.
- [10] Y.J. Lan, D.Z. Li, Y.Y. Li, *A mesoscale cellular automaton model for curvature-driven grain growth*. Metallurgical and materials transactions B, volume 37B, February, 2006.
- [11] Y.J. Lan, D.Z. Li, Y.Y. Li, *Modeling austenite decomposition into ferrite at different cooling rate in low-carbon steel with cellular automaton method*. Acta Materialia 52.6 (2004): 1721-1729.
- [12] W.D. Murray and F. Landis, *Numerical and machine solutions of transient heat-conduction problems involving melting or freezing*. J. Heat Transfer. C, 81, 106-112, 1959.
- [13] J. van Kan, F. Vermolen and A. Segal, *Numerical Methods in Scientific Computing*. Published by VSSD, ISBN 9789065621795, First Edition 2005.
- [14] W.W. Mullins and R.F. Sekerka, *Stability of a Planar Interface During Solidification of a Dilute Binary Alloy*. Journal of applied physics, volume 35, number 2, February, 1964.
- [15] S.M.C. van Bohemen, C. Bos and J. Sietsma *Simulation of Ferrite Formation in Fe-C Alloys Based on a Three-Dimensional Mixed-Mode Transformation Model*. Metallurgical and Materials Transactions A, 42(9), 2609-2618, April 6th, 2010.
- [16] M. Marek, *Grid anisotropy reduction for simulation of growth processes with cellular automaton*. Physica D: Nonlinear Phenomena, Volume 253, p. 73-84, 2013
- [17] H. Pattabhiraman, *MSc thesis: Kinetics of austenite to ferrite transformation and microstructure modelling in steel*. MSc thesis Material Science and Engineering, TU Delft, June, 2013
- [18] D.A. Porter and K.E. Easterling, *Phase Transformations in Metals and Alloys*. Published by Chapman&Hall, First Edition 1981.

- [19] Y. van Leeuwen, *Moving interfaces in low-carbon steel: a phase transformation model*. Published by Ponsen&Looije, ISBN 90-6464-572-8, Proefschrift ter verkrijging van de graad doctor, 2000.
- [20] M.G. Meozzi, *Phase Field Modelling of the Austenite to Ferrite Transformation in Steels*. ISBN-10: 90-77172-26-2, Doctoral thesis, 2006.
- [21] J. Ågren, *A revised expression for the diffusivity of carbon in binary Fe-C austenite*. Scripta Metallurgica, Vol. 20, pp 1507-1510, 1986.
- [22] D. Raabe, *Computational Materials Science: The Simulation of Materials Microstructures and Properties*. Published by Wiley-VCH Verlag GmbH, ISBN: 3-527-29541-0, 1998.
- [23] M.R. Hestenes and E. Stiefel, *Methods of Conjugate Gradients for Solving Linear Systems*. Journal of Research of the National Bureau of Standards, Vol. 49, No. 6, December, 1952.
- [24] E.J. Pérez, *Numerical methods for vector Stefan models of solid-state alloys*. ISBN: 90-8559-240-2, Doctoral thesis, 2006.