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№ 13755

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Aarne Pohjonen, Oskari Seppälä, Olli Väinölä and Jari Larkiola

July 2, 2024

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Aarne Pohjonen * **Oskari Seppälä** ** **Olli Väinölä** *** **Jari Larkiola** ****

* *University of Oulu, Pentti Kaiteran Katu 1, Materials and mechanical engineering department (e-mail: Aarne.Pohjonen@Oulu.fi).*
** *University of Oulu, Materials and mechanical engineering department (e-mail: Oskari.Seppala@Oulu.fi).*
*** *University of Oulu, Materials and mechanical engineering department (e-mail: Olli.Vainola@Ouraring.com).)*
**** *University of Oulu, Materials and mechanical engineering department (e-mail: Jari.Larkiola@Oulu.fi).*

Abstract: Understanding the steel microstructure formation during thermal treatments is crucial for controlling the mechanical properties of a steel product. One of the important factors affecting the subsequent microstructure development is the austenite grain size. To gain understanding of the effect of temperature dependent nucleation and growth rates, as well as providing the tools for quantitatively control the austenite grain size distribution, we have implemented a cellular automata (CA) model for describing austenite nucleation and growth during heating, as well as austenite grain growth during holding in temperatures above the austenitization temperature. The model implementation is based on previous study of Sieradzki and Madej for grain growth during recrystallization now augmetned with the relevant equations for describing the austenite nucleation and growth. The model parameters and their effect on austenite grain size distributions are tested with numerical experiments. The developed computational tool will serve as a basis that can be parameterized with experimental data in the future, which will then enable quantitative predictions for austenite phase transformation and grain size development.

Keywords: cellular automata, austenization, numerical modeling, steel, grain size

1. INTRODUCTION

The mechanical properties of metals and alloys depend on their chemical composition and microstructures. During processing, various mechanisms drive microstructural changes, including recovery, recrystallization, and grain growth. Accurately predicting and controlling these evolutions is vital for achieving desired mechanical properties.

By using models, engineers and designers can optimize processing parameters (e.g., temperature, deformation, strain rate) to achieve desired microstructures. This optimization leads to improved mechanical properties, such as strength, ductility, and toughness.

Different types of models can be used for simulating microstructure evolution. For example mean field models Pohjonen et al. (2018); Seppälä et al. (2023) provide rapid calculation method which can be coupled with macroscopic heat conduction calculations Pohjonen et al. (2021). Full field models, such as phase field Loginova (2003); Pohjonen (2023), level-set Hallberg (2011) and cellular automata Sieradzki and Madej (2013) allow for simulating the actual microstructure topology evolution.

Cellular Automata (CA) is a method which can be used to simulate microstructure evolution during recrystallization. CA is capable of representing topological features and realistically reflecting grain boundary migration. It allows for accurate predictions of grain size distribution and texture evolution. Zhu et al. (2020)

In previous studies by authors, CA has been used to simulate phase transformation from austenite to bainite and martensite. The base model for phase transformations has been described in Seppälä et al. (2018), martensite growth has been studied in more detail in Kaijalainen et al. (2019), bainite growth has been studied in more detail in Seppälä et al. (2021) and the bainite growth model has been utilized in Seppälä et al. (2023), where in-situ SEM experiments were conducted to study the growth of bainite during cooling.

In the current study, phase transformation from ferrite to austenite during heating will be simulated with another

⋆ This research has received funding from the European Commission under the European Union's Horizon Research and Innovation programme (Grant Agreement No. 101091912)

CA model. It is based on Sieradzki and Madej (2013), where static recrystallization and grain growth are simulated. The equiaxial grain growth and grain boundary development algorithms are utilized. The equations for nucleus formation and driving force for growth are modified to suit phase transformation instead of recrystallization.

2. THEORY

In this section we describe the theory and approximations of the models for austenite nucleation from initial ferrite during heating, the growth of the austenitic regions to the surrounding ferrite and the evolution of the austenitic grain structure due to interaction of the neighbouring distinct austenitic grains. The nucleation model is based on the classical nucleation theory Porter and Easterling (2022) with using simplifications that allow the model to be used with only few fitting parameters Kirkaldy (1983); Luukkonen et al. (2023). The austenite growth is described as a thermally activated process. In the current study the diffusion effects are not explicitly included in the model, but both the nucleation and growth rate are limited by the equilibrium constraints, which dictate the temperature where austenite can form and the maximum austenite fraction.

2.1 Austenite nucleation and growth in ferrite

During heating, austenite regions nucleate in the initial ferritic phase. Since it is energetically favourable for austenite to nucleate at certain sites, such as defects, ferrite interfaces, high-carbon regions, etc., the nucleation during heating is heterogeneous. The heterogeneous nucleation rate N_{het} can be described by Eq. (1)

$$N_{\text{het}} = \omega C \exp\left(-\frac{\Delta G^*}{RT}\right) \exp\left(-\frac{\Delta G_m}{RT}\right) \tag{1}$$

where C is the concentration of nucleation sites, ω is the attempt frequency for the nucleation, ΔG_m is the activation energy per atom for atomic migration between the austenitic and ferritic regions and ΔG^* is the energy barrier for nucleation of austenite from ferrite, which is strongly dependent on the temperature relative to the austenite ferrite equilibrium temperature T_{eq}. Theoretically, the energy barrier ΔG^* can be obtained by calculating the total Gibbs energy change as a function of nucleating austenite region size Porter and Easterling (2022). Such a detailed approach could be viable, if the energy values associated with the nucleus volume and surface, as well as possible misfit strain energies and the effect of local chemical inhomogeneities could be quantitatively estimated. However, as it is difficult to estimate all the effects, we take in the current study the widely used pragmatic approach and replace $\omega C \exp\left(-\frac{\Delta G^*}{RT}\right)$ in Eq. (1) with the expression $A(T - T_{\text{eq}})^a \left(1 - \frac{\chi}{\chi_{\max}(T)}\right)^b$, where χ is the transformed austenite fraction, $\chi_{\max}(T)$ is the temperature dependent maximum austenite fraction, which can be obtained from thermodynamic databases. The factor $\left(1 - \frac{\chi}{\chi_{\max}(T)}\right)^b$ was added to limit the austenite transformation to the maximum fraction that can be transformed in temperature T. The parameters A, a and b are kinetic fitting parameters that can be obtained by fitting the model to experimental data. This expression yields Eq. (2), which we have implemented in the CA model.

$$N_{\text{het}} = A(T - T_{\text{eq}})^a \left(1 - \frac{\chi}{\chi_{\max}(T)}\right)^b \exp\left(-\frac{\Delta G_m}{RT}\right) \tag{2}$$

Austenite growth to the surrounding ferrite matrix is simulated as thermally activated process using the Arrhenius type Eq. (3).

$$v = F \left(1 - \frac{\chi}{\chi_{\max}(T)}\right)^c \exp\left(-\frac{Q_G}{RT}\right) \tag{3}$$

where F is a constant prefactor containing the attempt frequency and average atomic sites per unit length as well as the length of austenite interface progression due to one transformation event, and Q_G is the activation energy for growth.

2.2 Austenite-austenite grain interface evolution

The evolution of austenite-austenite interfaces, i.e. the grain growth stage, is calculated based on the reference Sieradzki and Madej (2013). When austenite grains have impinged to each other, grain growth occurs to minimize the surface energy. The effect of crystal orientations is neglected in the current model, and in this case, the surface energy minimization becomes dependent only on the surface curvature κ. The speed of the interface between the two austenite grains v is described by Eq. (4)

$$v = \frac{H}{kT} \exp\left(-\frac{Q_b}{RT}\right) \kappa \tag{4}$$

where H and Q_b are parameters for fitting the thermally activated, curvature dependent interface mobility.

2.3 Cellular automata method

In Cellular Automata (CA), a simulation area is divided into equal-sized, square-shaped cells. Each cell has an individual value, which is manipulated using neighborhood rules, which change the cell value based on user-defined conditions. In this study, CA is used to simulate microstructural evolution of solid state steel, so the cell value describes its phase instance. The CA model essentially reshapes a graphical two-dimensional representation of the steel microstructure.

The user-defined neighborhood rules are the main way to customize the general CA solver. The neighborhood rules, found in Sieradzki and Madej (2013), are applied for ferrite-to-austenite phase transformation and austenite grain growth. Phase transformation starts at nucleation, which can occur anywhere on the simulation area, but grain boundaries and similar high-energy areas have a higher nucleation chance. From the point-of-view of the CA algorithm, nucleation simply means that a single cell of the simulation area is set to an austenitic phase instance. A pseudo-hexagonal rule is used for equiaxial grain growth. The rule works so that every cell checks its neighboring cells for each time step, using the pseudo-hexagonal pattern. Each neighboring cell that belongs to an austenitic phase instance cumulatively increases the total phase transformation pressure of the checked cell, and

after the total transformation pressure increases higher than a set level, the cell transforms to the neighboring phase instance.

With this growth algorithm, the new austenitic grains gradually grow freely into the old ferritic microstructure, until the grains collide with each other. At this point, the second neighborhood rule, which controls austenite grain growth, activates. The basic principle for the rule is that boundaries of two grains strive to be straight. For each cell near a grain boundary, the amount of grain cells are calculated in a long Moore (5x5 cells) neighborhood. In a 2D case, this means that there are a total 25 cells in the neighborhood. If more than 15 of those cells belong to the same grain as the checked cell, nothing happens. Otherwise, the total pressure to change into the neighboring grains cumulatively grows, which increases according to the number of neighboring grain cells, and after the total change pressure reaches a set level, the cell transforms to the neighboring grain. when calculated for all cells, this algorithm causes austenite grain boundaries to gradually become more straight and some grains grow at the expense of other, smaller grains, which gradually disappear.

3. NUMERICAL EXAMPLES

To test the operation of the mathematical model, we picked some parameter values in the order of magnitude range, that could be expected in realistic cases. In the current study, the parameter values are not fitted to experimental data, but the aim is to demonstrate the operation of the model and the relative effect of nucleation and growth rates on the simulation outcome. We do not consider specific steel in the current study, and the thermodynamic equilibrium temperatures were chosen based on a textbook example Callister and Rethwisch (2000), p. 381. In that example, the equilibirium austenite formation temperature is 727 °C, and the temperature dependent maximum austenite fraction $\chi_{\max}$ was calculated using the usual lever rule construction Callister and Rethwisch (2000).

Four simulation test cases were performed, where the effect of changing nucleation and growth rates was examined. In all of the simulation cases, the heating rate was defined as 10 °C/s and initial temperature of the simulation was set to 700 °C, which is well below assumed austenitization temperature of 727 °C. Heating was continued for 25 seconds, until the maximum temperature of 950 °C was reached. During the simulation, all the relevant mechanisms operated, nucleation and growth primarily affected the results until the austenite regions became more impinged, and after this the grain growth phenomena had more influence, and it became the dominating effect in the later stages of the simulation.

To demonstrate the operation of the model, the following parameters were used in the simulations: $\Delta G_m = 170$ kJ/mol, $Q_G = 140$ kJ/mol, $F = 25 \times 10^{-5}$, $a = 1$, $b = 1$, $c = 1$. Parameter A is dependent on the local probability of nucleation in the initial ferritic microstructure, and it was set to obtain reasonable effect within simulated times. This approach is capable of taking in to account the fact that the nucleation is heterogeneous, i.e. there usually are

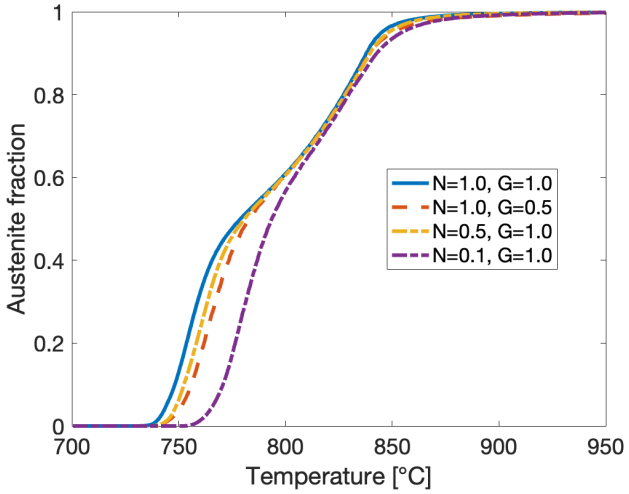

Fig. 1. Overall transformed austenite fraction as function of temperature during heating for the four examined cases where the nucleation and growth rate were scaled with parameters N and G respectively.

sites that are more probable for nucleation, as well as including the randomness to the simulation. In simulating more realistic cases, the parameter values will be fitted to data that can be obtained for example from simplified laboratory experiments.

The model was tested for four different cases, scaling the nucleation rate with factor of N and growth rate with factor of G. This shows what kind of effect the relative change in nucleation and growth rates have in the formation of the microstructure.

Figure 1 shows overall transformed austenite fraction as function of temperature during heating for the four examined cases. The deflection of the curve at a range of 50-70 % is mainly due to the temperature dependent maximum austenite fraction $\chi_{\max}$, which is a realistic effect similar to that shown in Savran et al. (2010).

Figure 2 shows the development of austenite grain structure during heating for the case 1 (N=1, G=1). This case serves as the baseline where the other simulation cases can be compared.

Figure 3 shows the development of austenite grain structure during heating for the case 2 (N=1, G=0.5). This case shows that when the growth rate is halved, there is much more available nucleation sites at higher temperature, and the resulting austenite structure becomes more refined.

Figure 4 shows the development of austenite grain structure during heating for the case 3 (N=0.5, G=1). This case shows not much difference to the baseline case (case 1). The reason appears to be that the growth rate has more effect to the nucleation by removal of the available nucleation sites than actually halving the nucleation rate.

Figure 5 shows the development of austenite grain structure during heating for the case 4 (N=0.1, G=1). This case shows that when the nucleation rate is more drastically diminished, it has significant effect to the resulting austenite structure, as less austenite grains are formed and they grow bigger.

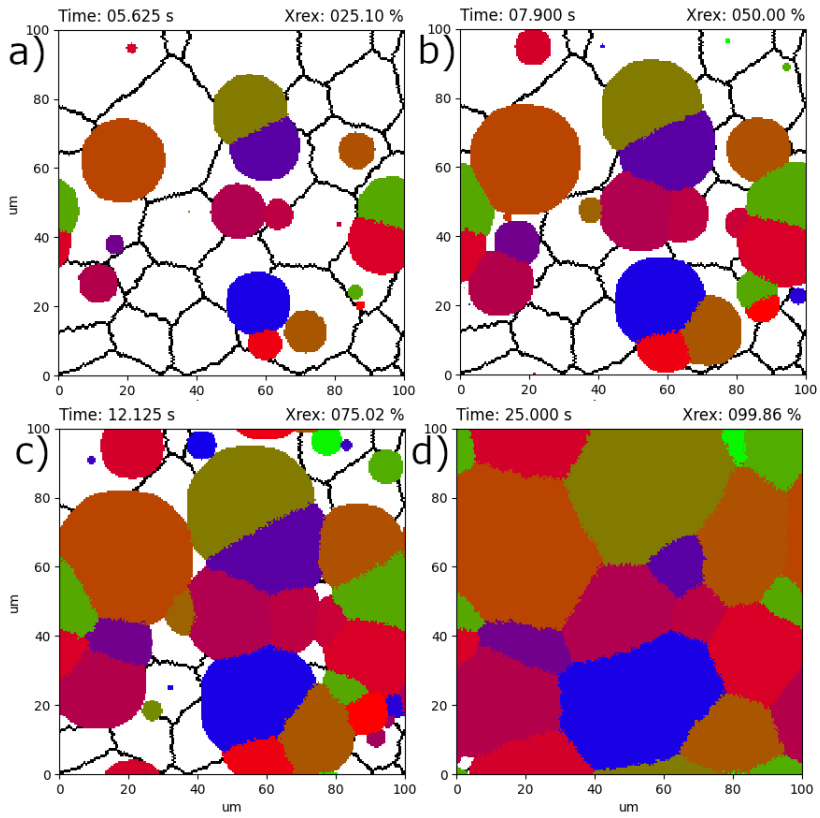

Fig. 2. The baseline simulation with scaling parameters $N = 1$ and $G = 1$, where the other simulation cases can be compared. Simulation snapshots where a) 25 %, b) 50 % and c) 75 % austenite has formed and d) at the end of the heating stage 950 °

4. CONCLUSIONS AND OUTLOOK

The austenite nucleation, growth, impingement and grain growth phenomena was implemented as cellular automata model. The model operation was demonstrated with four examples by altering the nucleation and growth rate. In future, the model will be parameterized using experimental data.

ACKNOWLEDGEMENTS

Partial funding from AID4GREENEST project is gratefully acknowledged: This research has received funding from the European Commission under the European Union's Horizon Research and Innovation programme (Grant Agreement No. 101091912). Views and opinions expressed are, however, those of the authors only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

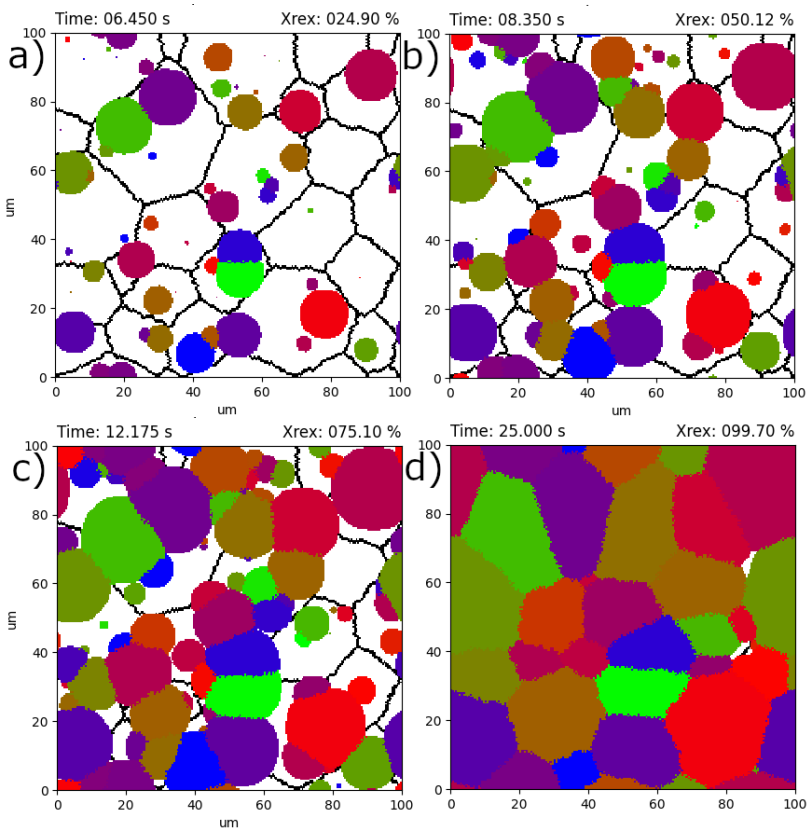

Fig. 3. The development of austenite grain structure during heating for the case 2 (N=1, G=0.5). a), b), c), d) same fractions as in Fig. 2

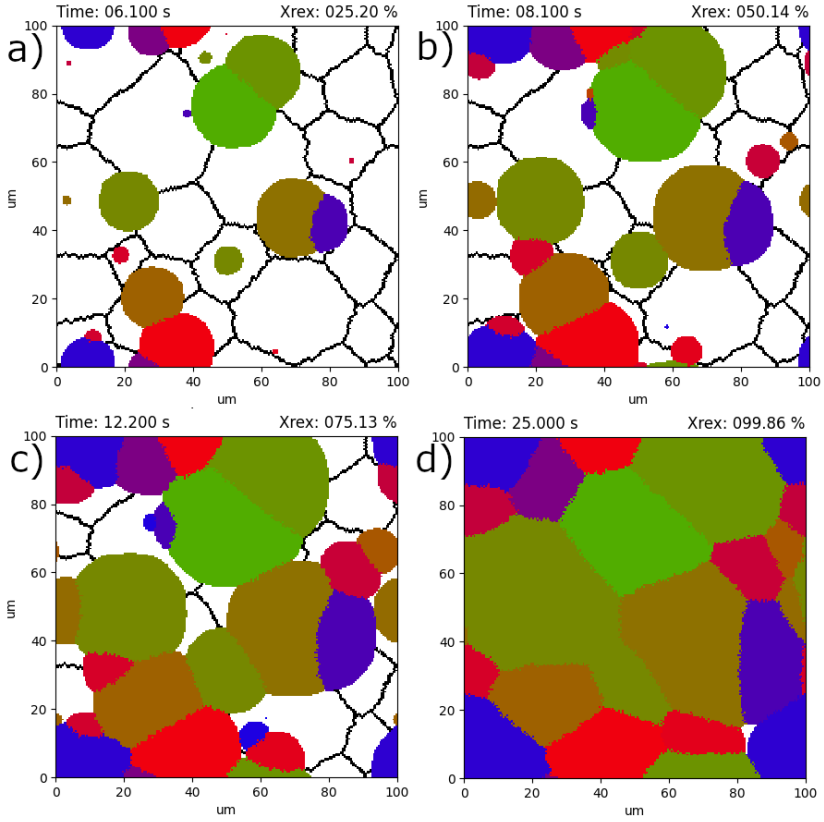

Fig. 4. The development of austenite grain structure during heating for the case 3 (N=0.5, G=1). a), b), c), d) same fractions as in Fig. 2

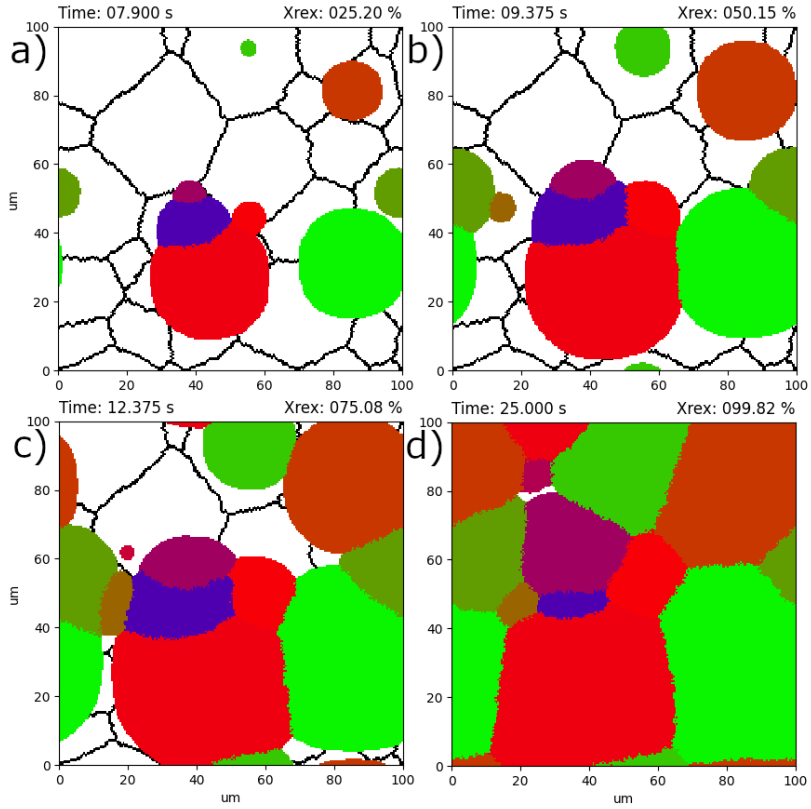

Fig. 5. The development of austenite grain structure during heating for the case 4 (N=0.1, G=1). a), b), c), d) same fractions as in Fig. 2

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