A new unified approach for modeling hot rolling of steel Part 1: Comparison of models for recrystallization

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Abstract

Models for the microstructure evolution during hot rolling are reviewed. The basic macroscopic phenomena related to recrystallization are summarized. Constitutive models based on semi empirical equations are compared to more sophisticated models based on cellular automata, vertex and Monte-Carlo-Potts methods. The applicability of each kind of model approach for online and offline process control in steel industry is discussed. While constitutive models are still state-of-the-art for online process control, mesoscale models with a spatial representation of the microstructure can provide better predictive capabilities at the cost of long computation times. To fill this gap a new approach based on modeling the interaction of an ensemble of multiple grains is outlined and first simulation results are presented. The proposed approach allows the unified modeling of dynamic, static and metadynamic recrystallization as well as grain growth.

Keywords: Recrystallization, Model, Simulation, Process Control, Grain Growth, Hot Rolling, Microstructure

1. Introduction

The microstructure evolution during hot rolling is of great interest for the industrial production of steel and has therefore been subject of research in the past decades. Recrystallization during and after rolling is one of the mechanisms that can be used for grain refinement \cite{1}. The resulting microstructure after rolling is also important for the following phase transformation during cooling having a significant influence on the mechanical properties of hot rolled products. In consequence, controlling the recrystallization is one opportunity for controlling the mechanical properties and in turn gives room for saving expensive alloying elements. Therefore models with good predictive capabilities are necessary.

Since dynamic recrystallization had been observed by Greenwood and Worner \cite{2}, many theories and models for the description of recrystallization during and after deformation have been developed. These models differ in terms of complexity, characteristic length scale, practical usability and the considered materials. Some of them have been reviewed by Senuma et al. \cite{3}, Militzer \cite{4} and more recently by Hallberg \cite{5} and Xiao et al. \cite{6}.

Additionally the usability of the different model types for technical applications, like process control or numerical simulations of hot forming processes, is discussed. One important aspect is the required experimental effort necessary for determining material parameters. Constitutive models use a large number of empirical parameters whereas models with long computation times are not applicable for inverse analysis methods which are often necessary for parameter identification in an industrial context. Therefore a new approach that combines benefits from constitutive and more sophisticated physical models is proposed.

2. Phenomena related to recrystallization

Several phenomena on macroscopic and microscopic scale can be related to recrystallization. Some of them are summarized below.

- During deformation recrystallization can occur after exceeding a critical strain referred to as dynamic recrystallization (DRX) \cite{7}. In figure 1 flow curves from cylindrical hot compression tests with 42CrMo4 steel are shown. For strains larger than the peak strain a decrease of the flow stress can be observed that is considered to be caused by DRX.

- At high strain rates the flow stress monotonously tends to a lower steady state stress after reaching the peak stress. For lower strain rates a damped oscillation of the flow stress can be observed instead what is referred to as cyclic recrystallization \cite{7}.

- The strain \( \varepsilon_p \) at the peak stress increases with strain rate and decreases with temperature \cite{7}.

- The criteria for the transition from continuous to cyclic recrystallization resulting in grain coarsening depends on the Zener-Holomon-parameter and the initial grain size \cite{8}.
• The grain size during deformation in the steady state regime correlates with the steady state stress as shown by Sakai et al. [11].

• Recrystallization after deformation is called static recrystallization (SRX). If DRX has occurred during deformation the recrystallization kinetics strongly depends on the strain rate of the previous deformation. This case is often referred to as metadynamic recrystallization (MDRX).

• After rapid changes of strain rate or temperature during deformation the flow stress settles on a new steady state value. Before steady state is reached transient oscillations can be observed [11][9][10].

• If DRX is completed, the austenite grain size after deformation depends on temperature. In figure 2 this is shown for two specimens of 42CrMo4 that have been deformed to the logarithmic strain \( \varepsilon \) = 0.8 with a strain rate of 5 s\(^{-1}\) at temperatures of 900 °C and 1000 °C. The specimens have been quenched directly after deformation.

Figure 1: Flow stress curves at different temperatures measured in cylindrical hot compression tests of 42CrMo4 steel samples. After exceeding a specific plastic strain the flow stress decreases due to dynamic recrystallization.

Figure 2: Revealed prior austenite grain boundaries after hot deformation and quenching of 42CrMo4 to \( \varepsilon \) = 0.5 with a strain rate of \( \dot{\varepsilon} \) = 5 s\(^{-1}\).

3. Models for recrystallization

One way to model the microstructure evolution is to model the observed phenomena summarized above with a set of suitable mathematical functions as proposed by Sellars and Whiteman [11]. These functions include several material parameters that are derived from experimental data. Another way is to model the physical mechanism like work hardening, grain boundary movement and nucleation of new grains that lead to the observed phenomena. To do so it is necessary to have some kind of representation of the state of the microstructure. This can be a set of scalar variables, a set of distribution functions or a spatial representation of the microstructure. Such models are described in subsection 3.2 and 3.3. In this paper we focus on model approaches that play a major role in the development of microstructure models for practical applications. Machine learning techniques like artificial neural networks and fuzzy logic can be used for the prediction of the microstructure [12-13]. However, these methodologies provide “Black-Box” models that do not allow for an insight view of the processes and are therefore not discussed in this paper.

In the following major approaches for modeling recrystallization are described. At the end of each section the features and constraints of each model are pointed out.

3.1. Constitutive models

Constitutive models provide a simple way of describing the microstructure evolution mostly by closed form equation, which makes it possible to use them even in simple spread sheet applications.

3.1.1. Classical models for process control applications

Sellars and Whiteman [11] proposed a constitutive model designed for the application of the simulation of the microstructure evolution during hot rolling that built the starting point for many other models developed by several groups [15][20][3][21]. In this paper we only want to give a brief outline of the basic concept behind this type of model. It has to be noted that a multitude of modified or extended versions of the empirical submodels below exist in literature. As input parameter these models use temperature \( T \), strain \( \varepsilon \) and strain rate \( \dot{\varepsilon} \) of each deformation step, the initial average grain size \( d_0 \) and the time \( t \) after the prior deformation. The output parameters are the recrystallized volume fraction \( X \) and the average grain size \( d \). Constitutive microstructure evolution models distinguish between different recrystallization phenomena (DRX, MDRX, SRX and grain growth) that are modeled separately. Each model contains material parameters to be derived from experiments. The recrystallized volume fraction and the prior austenite grain size have to be determined after thermomechanical treatments under various processing conditions, to allow for the determination of material parameters by inverse analysis methods. Many models use the parameter

\[
Z = \dot{\varepsilon} \exp \left( \frac{Q_{\text{def}}}{RT} \right)
\]

introduced by Zener and Hollomon [22] with \( Q_{\text{def}} \) as an activation energy and \( R = 8.314 \frac{J}{\text{mol} \cdot \text{K}} \) as the universal gas constant.
to combine the dependency of strain rate \( \dot{\varepsilon} \) and temperature \( T \) into one parameter. The activation energy can be determined with the method proposed by \([23]\). The recrystallized volume fraction is often described by a modified version of the Johnson-Mehl-Avrami-Kolmogorov equation \([24]\). For SRX it can be written as

\[
X = 1 - \exp \left( -0.693 \left( \frac{t}{t_{0.5}} \right)^{n} \right) \tag{2}
\]

with \( t_{0.5} \) being the time elapsed until the volume has recrystallized. The time \( t_{0.5} \) is calculated with an empirical equation of the common form

\[
t_{0.5} = A_{SRX} \rho_{SRX} d_{0}^{q} Z_{SRX} \exp \left( \frac{Q_{SRX}}{RT} \right) \tag{3}
\]

with \( n, A_{SRX}, \rho_{SRX}, q, r_{SRX} \) and \( Q_{SRX} \) as material parameters and \( d_{0} \) as the average grain size prior to the previous deformation. The equation can also be extended to take the effect of niobium into account as proposed by Hodgson and Gibbs \([25]\). The average diameter of the recrystallized grains is then calculated with

\[
d_{SRX} = \varepsilon^{p_{d}} d_{0}^{n_{d}} \exp \left( \frac{Q_{d}}{RT} \right) \tag{4}
\]

where \( p_{d}, q_{d} \) and \( Q_{d} \) are material parameters.

The onset of DRX during deformation is described by a critical strain

\[
\varepsilon_{c} = A_{c} d_{0}^{m_{c}} Z^{m_{c}} \tag{5}
\]

that has to be exceeded with \( A_{c}, p_{c}, r_{c} \) as material parameter. For the volume fraction recrystallized by DRX the time is replaced by strain resulting in

\[
X_{DRX} = 1 - \exp \left[ B \left( \frac{\varepsilon - \varepsilon_{c}}{\varepsilon_{X}} \right)^{k} \right] \tag{6}
\]

with \( \varepsilon_{X} \) being the strain at which the volume fraction \( X \) has been recrystallized. The strain \( \varepsilon_{X} \) can be described by an empirical equation of the same form as equation \([5]\). \( B \) and \( k \) are material constants. The grain size of the recrystallized grains can be calculated using

\[
d_{DRX} = CZ' \tag{7}
\]

where \( r \) and \( C \) are material parameters. If DRX has occurred the kinetics of recrystallization after deformation depends on the strain rate, i.e. metadynamic recrystallization. The time \( t_{0.5} \) decreases with increasing strain rate \([25]\). Taking this effect into account Hodgson and Gibbs give \( t_{0.5, MD} \) as

\[
t_{0.5, MD} = k_{MD} Z^{n_{MD}} \exp \left( \frac{Q_{MD}}{RT} \right) \tag{8}
\]

with \( k_{MD}, n_{MD} \) and \( Q_{MD} \) as material parameters \([25]\). The recrystallized grain size by MDRX can be calculated with an equation of the form of equation \([7]\) with an extra set of material parameters for MDRX \( (C_{MDRX}, r_{MDRX}) \). For multistage deformation the effect of work hardening of the previous deformations and of recrystallization on the dislocation density has to be taken into account. To do so the concept of accumulated strain is used by many authors \([15, 18, 25]\). The strain of each pass is accumulated to \( \varepsilon_{ACC} \). This accumulated strain is decreased depending on the recrystallized volume fraction \( X \) resulting in an effective strain \( \varepsilon_{ eff,i } \) that can be used for the calculation of the flow stress. For the calculation of \( \varepsilon_{ eff,i } \) various approaches have been discussed by Hodgson and Gibbs \([25]\). One of them is a linear law of mixtures as

\[
\varepsilon_{ eff,i } = \varepsilon_{i} + \lambda (1 - X) \varepsilon_{i-1} \tag{9}
\]

with \( \lambda = 1 \) for C-Mn steels.

Since only average values are considered it is not possible to track multiple volume fractions that have been recrystallized at different time steps. The large number of material parameters make such models easily adjustable to experimental data but also makes them demanding on the scope of the experiments. Although such models cannot describe the influence of the previous processing path due to the lack of inner state variables, they show good agreement with experimental results at steady state conditions, whereas cyclic recrystallization and transient oscillations cannot be described.

### 3.2. Inner state variable models

#### 3.2.1. Luton and Sellars model for cyclic recrystallization

While the models above aim for practical applications the following model was a starting point for later models considering cyclic recrystallization. Observing DRX during hot torsion tests with nickel and nickel-iron alloys Luton and Sellars \([7]\) propose a model that describes the transition from cyclic to steady state behavior. They assumed that DRX is initiated after exceeding a critical strain \( \varepsilon_{c} \) and introduced a strain \( \varepsilon_{c} \) to characterize the strain related to the time \( t_{k} \) needed for a large fraction \( X \) to recrystallize under constant strain rate conditions. If \( \varepsilon_{X} < \varepsilon_{c} \) they suppose cyclic recrystallization and otherwise continuous recrystallization behavior.

They calculate the recrystallized volume fraction \( X \) with

\[
X = 1 - \exp \left( -k \rho^{e} \right) \tag{10}
\]

where \( t \) is the time after initiation of DRX and \( k \) and \( n \) are constants.

The flow stress is calculated as superposition of the flow stress \( \sigma_{r}(\varepsilon) \) and \( \sigma_{f}(\varepsilon) \) for each time increment \( i \). The function \( \sigma_{r}(\varepsilon) \) describes the flow stress without recrystallization at the considered constant temperature and strain rate. For each time increment \( i \) a new function \( \sigma_{i}(\varepsilon) = \sigma_{e}(\varepsilon - \varepsilon_{i}) \) is introduced. The flow stress is then given as a superposition by

\[
\sigma = \sum_{0}^{j} X_{i} \sigma_{i} + \left( 1 - \sum_{0}^{j} X_{i} \right) \sigma_{e} \tag{11}
\]

where \( X_{i} \) is the volume fraction that has been recrystallized in the increment \( i \).

This model is able to describe the transition from periodic to continuous recrystallization. However, it does not describe the damping of the oscillation for cyclic recrystallization.

#### 3.2.2. Inner state variable models

Since microstructure evolution depends on the current microstructure, models using inner state variables have been in-
3.2 Inner state variable models

3.2.1 Stüwe and Ortner

Stüwe and Ortner [26] suggest a model for DRX that describes the recrystallized volume fraction and the resulting flow stress during deformation depending on strain rate and temperature based on the evolution of the dislocation density. In this model the average dislocation density can be seen as an inner state variable. They calculate the flow stress $\sigma$ with

$$\sigma = AGb \sqrt{\rho}$$

(12)

with $b$ as the length of the burgers vector, $G$ as shear modulus, $\rho$ as average dislocation density and $A$ as a material parameter.

The increase of the dislocation density during deformation due to work hardening is

$$\frac{d\rho}{d\epsilon} = \frac{2(l + c)}{lcb}$$

(13)

where $l$ and $c$ are the dimensions of the area swept by one dislocation loop of the burgers vector $b$. In contrast to Luton and Sellars [7] Stüwe and Ortner [26] assume that DRX starts after the time

$$t = t_0 = \frac{\rho_n}{\hat{\rho}}$$

(14)

for a constant $\rho$ after a critical dislocation density $\rho_n$ has been exceeded instead of using a critical strain criterion. For spherical growth with a constant grain boundary velocity $v_0$ the recrystallized volume fraction $X$ after the time $t_0$ is given by

$$X = \left(\frac{v_0(t_0 - t_0)}{R}\right)^3$$

(15)

where $R$ is the traveling distance and for the given assumptions the radius of the recrystallized grains. It has to be noted that $v_0$ depends on the grain boundary mobility that is a function of the temperature. The average dislocation density $\overline{\rho}$ needed for the calculation of the flow stress by equation (12) is determined by integrating over the radius of the grains with

$$\overline{\rho} = \frac{3}{4\pi R^3} \int_0^R \rho(r) 4\pi r^2 dr$$

(16)

to take into account that the volume behind a moving boundary has a very low dislocation density producing a gradient of $\rho$ from the inner to the outer region of the grain.

While the model can describe a transition from single peak to multiple peak behavior for the combination of low strain rates and high temperatures, the theoretical stress strain curves published by [Stüwe and Ortner] show a saw like shape that has not been observed in experiments. In contrast to the constitutive models described above recrystallization and the calculation of flow stress are combined into one model. The model also relies on the assumption of constant strain rate and temperature. Hence the model does not include the evolution of the grain size, its effect on nucleation rate and grain boundary movement are not considered. This issue has been addressed with the model developed by [Sandström and Lagneborg] described below.

3.2.2 Sandström and Lagneborg

In response to the models by [Luton and Sellars] and [Stüwe and Ortner] Sandström and Lagneborg [27] point out, that the current grain size should also be taken into account. They proposed a new model that describes the evolution of the dislocation density distribution. They distinguish between the dislocation density in the subgrain walls $\rho_d$ and the homogeneous dislocation density between the subgrain walls $\rho$. The volume distribution of both kinds of dislocations are described by the functions $g(\rho, t)$ and $G(\rho_d, t)$.

$$\int g(\rho, t) d\rho = 1$$

(17)

$$\int G(\rho_d, t) d\rho_d = 1.$$  

(18)

The time derivative of $\rho$ is given by

$$\frac{d\rho}{dt} = \frac{\dot{\epsilon}}{bl} - 2M\tau\rho^2$$

(19)

considering work hardening and recovery. Here $l$ is the mean free path of the dislocation and $M$ the mobility. Recovery for the dislocations in the subgrain walls is neglected so that their evolution is given by

$$\frac{d\rho_d}{dt} = \frac{\dot{\epsilon}}{bl_d}$$

(20)

where the mean free path $l_d$ is directly related to the subgrain size. They conclude, that $l$ has to be much larger than $l_d$ if the main part of the dislocations are accumulated in the subgrain walls which is reported by Stüwe and Ortner [26] to be also necessary for the calculation of realistic values of the flow stress. According to equation (20) the relation between the critical strain $\varepsilon_{cr}$ and the critical dislocation density $\rho_{cr}$ for the onset of recrystallization is given as

$$\varepsilon_{cr} = bl_d\rho_{cr}.$$  

(21)

The time derivative of the recrystallized volume fraction is given by

$$\frac{dX}{dt} = \int_{\rho_{cr}}^{\infty} \frac{\dot{\varepsilon}\gamma_0}{D} v(\rho_d) G(\rho_d, t) d\rho_d$$

(22)

where $D$ is the grain diameter and $\xi$ a constant given as $\xi = 3$. The velocity of the grain boundary $v(\rho)$ is given by

$$v(\rho) = m\tau\rho$$

(23)

with the grain boundary mobility $m$ and $\tau$ as dislocation line energy. The parameter $\gamma_0$ is called mobile fraction and describes the effect that some of the grain boundaries do not move. In the model of [Sandström and Lagneborg] $\gamma_0$ is assumed to be constant.

The average stress is assumed to depend on the dislocation density in the subgrains and is also calculated using equation (12) but with the average dislocation density being

$$\overline{\rho} = \int_{\rho_{cr}}^{\infty} \rho g(\rho, t) d\rho.$$  

(24)
3.3 Models with spatial representation

where

\[ \rho_s = \sqrt{\frac{\dot{\varepsilon}}{2bm\gamma T}} \]  

is the dislocation density when work hardening and recovery are in balance. While the dislocation density is described by distribution functions the grain size is only represented by an average grain diameter \( D \). The evolution of \( D \) is described as

\[ \frac{dD}{dt} = m \gamma - D \frac{dX}{dt} \ln N(D) \]

with the grain boundary mobility \( m \), the grain boundary energy \( \gamma \) and the amount of grains \( N \) nucleated per parent grain after one recrystallization cycle.

Like the model by Stöwe and Ortner the model proposed by Sandström and Lagneborg [28] describes the recrystallization combined with the evolution of the dislocation density. Additionally it also considers the evolution of the average grain size. It is able to describe the damped oscillations in flow curves at low strain rates. In comparison with data from experiments with nickel the calculated peak strain at high strain rates is too low. This is explained by not taking into account the strain rate dependency of the mean free path \( l \) and the dislocation mobility \( m \).

3.3 Models with spatial representation

Instead of describing the microstructure only with average values some more sophisticated models use a 2D or 3D spatial representation of the microstructure. This representation then evolves according to a set of certain rules that represent the physical mechanisms. The common principle here is the minimization of the free energy. For this there are various methodologies that are not only used for modeling recrystallization but for a broad range of applications. As for the models above temperature and strain rate are the input parameters but here both parameters can exceed a certain transition strain during the first deformation stage. They also performed numerical experiments with two deformation stages for the analysis of the simulated post deformation recrystallization. They found that exceeding a certain transition strain during the first deformation results in a transition from weak to strong strain rate dependency of the recrystallization kinetics. It can be concluded that a model of this kind can describe the transition from SRX to MDRX without introducing submodels or special case handling for each recrystallization process as it is necessary for the constitutive models described earlier.

3.3.1 Cellular Automata

The Cellular Automata (CA) method is based on the work of Ulam [29] and Von Neumann [30]. A CA consists of a set of cells that are commonly ordered in a lattice. Each cell has a state described by a set of variables and is related to a defined set of cells that are called neighborhood. The transition of one state to another is defined by a set of rules that is applied at each evolution step. These rules can only rely on the state of one cell and its neighborhood at the previous evolution step. Starting with Hesselbarth and Göbel [41] many groups have developed models for recrystallization utilizing the CA method [32–40].

In particular Kugler and Turk [41] used a two-dimensional CA with a rectangular grid for the simulation of multistage deformations. To use the CA to describe a virtual microstructure the state of one cell consists of four variables including one variable for the dislocation density \( \rho_s \) and the crystal orientation. The evolution of the dislocation density is calculated by integration of

\[ \frac{\partial \rho_s}{\partial \gamma} = k_1 \sqrt{\rho_s} - k_2 \rho_s \]

for each cell where \( \gamma \) is the shear strain, \( k_1 \) a hardening coefficient and \( k_2 \) a strain rate and temperature dependent parameter describing recovery. The flow stress is calculated with equation [12] using

\[ \dot{\rho} = \frac{1}{n} \sum_{i=1}^{n} \rho_i \]

where \( n \) is the number of cells. Adjacent cells with the same orientation belong to the same grain. At the grain boundary the transition from one orientation to another occurs depending on the grain boundary velocity calculated by

\[ v = m \Delta f \]

with \( \Delta f \) as the driving force per unit area that is a function of the difference of the dislocation densities and the grain boundary energy. The grain boundary mobility \( m \) is given by

\[ m = \frac{b_0 D}{k_B T} \exp\left( \frac{Q_b}{RT} \right) \]

taking the characteristic grain boundary thickness \( \delta \) and the boundary self-diffusion coefficient \( D \) into account. \( R \) is the universal gas constant, \( k_B \) the Boltzmann constant and \( Q_b \) is an activation energy. New grains are created at the grain boundary if a critical dislocation density \( \rho_c \) is exceeded with a probability

\[ P = k_2 \exp \left( -\frac{\omega}{T} \right) \Delta t \]

where \( k \) and \( \omega \) are material parameters and \( \Delta t \) the time increment of one simulation step.

Kugler and Turk show that their model is able to describe the transition from continuous to cyclic softening at a constant temperature with decreasing strain rate and for constant strain rate with increasing temperature. They also performed numerical experiments with two deformation stages for the analysis of the simulated post deformation recrystallization. They found that exceeding a certain transition strain during the first deformation rate resulting in a transition from weak to strong strain rate dependency of the recrystallization kinetics. It can be concluded that a model of this kind can describe the transition from SRX to MDRX without introducing submodels or special case handling for each recrystallization process as it is necessary for the constitutive models described earlier.

3.3.2 Monte Carlo Potts method

The application of the Monte Carlo Potts algorithm for modeling grain growth and recrystallization started with the work of Sahni et al. [42]. Similar to CA models a lattice is used as representation of the microstructure. Each of the cells, also called Monte Carlo Units (MCU), has a state \( Q \) that indicates the misorientation and the affiliation of the cell to one specific grain. Neighboring cells with different values of \( Q \) define a
grain boundary. A basic algorithm for the simulation of grain growth has been described by Zöllner and Streitenberger [43]. A random MCU with the current state \( Q_i \) is temporarily set to a state \( Q_j \), with \( Q_j \neq Q_i \). The difference of the energy \( \Delta E \) between the states \( Q_i \) and \( Q_j \) is then calculated by a Hamiltonian \( H \) that depends on the possible misorientation between the cell and its neighbor cells. The resulting energy difference \( \Delta E \) is used to calculate a probability

\[
p = \begin{cases} m, & \Delta E \leq 0 \\
m \exp\left(\frac{-\Delta E}{k_B T}\right), & \Delta E > 0 \
\end{cases}
\]

with \( k_B \) as Boltzmann constant and \( m \) as grain boundary mobility for the transition from the state \( Q_i \) to \( Q_j \). During one Monte Carlo step one of these reorientation attempts is performed for each cell.

Hence this approach mimics the principle of least actions it can be used to model the grain boundary movement without the definition of specific evaluation rules, but to the cost of additional computation time compared to CA models.

3.3.3. Vertex models

Vertex models also use a spatial description of the microstructure. In contrast to CA models these models do not use a lattice. Instead, the shape of the grains is only described by a set of geometrical features like the vertices illustrated in figure 3. This reduces the needed amount of memory and allows the simulation of larger grain ensembles compared to the CA method. The initialization is often done by a Voronoi tesselation, sometimes followed by a simulated annealing [44, 45], that can be performed with the Lloyd-algorithm [46].

Nagai et al. [47] use a mesh with vertices at the triple points of the grain boundaries in the 2D case. The grain boundaries were modeled by straight lines connecting the vertices. They introduced a force attached to the triple points resulting from the energy minimization by optimizing the angles between the grain boundaries. This model has been extended by several authors to allow curved boundaries. Weygand et al. [45] insert additional vertices that divide the lines or planes representing the grain boundary into multiple segments. Cocks and Gill [44, 48] use cubic splines for modeling curved boundaries in the two dimensional case. They also show that the variational principle can be applied to derive equations for the velocity of the vertices to model curvature-driven grain growth. Telley et al. [49] and Schüle [50] utilize the Laguerre tesselation, a Voronoi tessellation with radial weighting, for the simulation of grain growth so only the coordinates of the center and the weighting are needed to describe one grain.

While the utilization of the vertex approach for the simulation of grain growth is common, models are very rare that also consider nucleation. Hence only the geometry of the grain boundaries is described this approach does not provide a spatial dislocation density in the interior of the grains like models based on the CA approach or the Monte Carlo Potts method. For modeling nucleation the dislocation density has to be stored in an additional data structure.

4. Ensemble model

In the following the new model is outlined combining features of more physical based approaches like CA models mentioned above with short computation times needed for process control applications. A more detailed description of this model will follow in the second part of this publication.

4.1. Outline of a new approach

The processes involved in recrystallization are time dependent and influence each other as outlined in figure 4. In the model strain rate \( \dot{\varepsilon} \) and temperature \( T \) are the input parameters. Instead of using a spatial representation of the microstructure or

![Figure 3: Illustration of two grains in a simple 2D vertex model. Additionally to the vertices (filled) at the triple points each grain boundary line is divided into segments by virtual vertices.](image)

![Figure 4: Graph of the processes considered for the new model to be involved in DRX and their dependencies. The arrows indicate the direction of an influence. Arrows labeled with (-) indicate a decrease of the influenced quantity. Strain rate \( \dot{\varepsilon} \) and temperature \( T \) are the input parameters. The state is defined by a generalized variable \( r_i \) describing the size and the dislocation density \( \rho_i \) of each grain. The state is changed by the processes of work hardening (WH), dynamic recovery (DR) and static Recovery (SR) effecting the time derivative of the dislocation density \( \dot{\rho}_i \) by nucleation of new grains (\( N \)) and grain growth (\( \dot{r}_i \)).](image)
grains. Similar to a cell in a CA model each grain $i$ has state variables like the average dislocation density $ρ_i$ and a generalized variable $r_i$ describing the grain size. These can be evolved by the processes of nucleation of new grains ($N$ in figure 4), grain growth ($r_i$), dynamic recovery (DR), static recovery (SR) and work hardening (WH). WH and SR are considered by the use of equation [27] for the time derivative of the dislocation density $ρ_i$. Each grain has its own constant shape represented by a ratio $V(r_i)/S(r_i)$ between grain volume $V(r_i)$ and surface $S(r_i)$ with $κ_i$ as a geometric constant that has to be set at the initialization of the simulation. The ensemble consists of grains in a specified volume that has to be kept constant. During the simulation the size $r_i$ of each grain is adjusted by the integration of $r_i$ to reduce the free energy of the system in terms of grain boundary energy and energy stored by dislocations in the volume of the grain. During the grain boundary movement the power

$$W_{Diss} = \frac{1}{2m} r_i^2 S(r_i)$$

is dissipated with $m$ as grain boundary mobility. The time derivative of $r_i$ is given by

$$\dot{r}_i = m \left( -3κ_i (τρ_i + λ) - \frac{2}{r_i^2} ρ_i γ \right)$$

where $τ$ is the dislocation line energy, $γ$ the grain boundary energy per unit area and $λ$ a Lagrange multiplier. Similar to the approach chosen by Kugler and Turk [41] new grains are generated with a temperature dependent probability if a critical dislocation density $ρ_{crit}$ is exceeded. Preliminary simulation results of this model are discussed below.

4.2. Simulation results

In order to investigate the dynamic behavior of the model simulations under transient conditions were carried out. In figure 5 the results from a simulated deformation at a temperature of 1000 °C with a rapid change of the strain rate form 5 s$^{-1}$ to 1 s$^{-1}$ are shown. The flow stress first increases until the available time is high enough to induce a high nucleation rate by a high work hardening rate.

Recrystallization is faster there is still grain refinement. The minimum of the grain size is at the lowest temperature in a strain rate regime where DRX is completed and the strain rate is high enough to induce a high nucleation rate by a high work hardening rate.

Figure 5: Results from simulated deformation under transient conditions. The calculated flow stress at a temperature $T = 1000°C$ for an initial average grain diameter $d_0 = 70 μm$ is shown. At the strain $ε = 0.5$ the strain rate is changed from 5 s$^{-1}$ to 1 s$^{-1}$. Following transient oscillation average grain size and flow stress settle on new steady state values.

To illustrate the dependency on strain rate and temperature the average grain size after a deformation step is shown in figure 6. For the combination of low strain rate and high temperature the model predicts grain coarsening. In this case the nucleation rate is relatively low in relation to the growth rate of the grains. At high strain rates $ε > 20 s^{-1}$ the available time for recrystallization decreases, so at low temperatures the grain size remains at the initial state. At higher temperatures where

$\dot{ε}$ [s$^{-1}$]
constraints are summarized in figure 7. For the use of microstructure evolution models in technical applications, like forming simulations or process control, a minimum of computational effort is preferred. Constitutive models for the recrystallization during hot deformation as described in subsection 6.4.3 support fast calculations of average values describing the microstructure like grain diameter or recrystallized volume fraction. Due to their simplicity and low computation times these kinds of models are popular for process control applications. However, there are some drawbacks for the practical application that give motivation for the development of models that include more knowledge about the physical processes.

Constitutive models describe the microstructure evolution in a phenomenological way, so each phenomenon like flow stress, DRX, SRX, MDRX and grain growth are described individually by empirical submodels with their own sets of material parameters. To determine these parameters for one steel grade each phenomenon has to be investigated experimentally under a wide range of process conditions. However, steel companies for example produce a wide range of different steel grades, so there is a great interest in reducing the required experimental work. In particular the determination of the grain size is difficult since the prior austenite grain boundaries cannot easily be revealed with metallographic techniques for a lot of modern low carbon steels.

Another motivation for the use of less phenomenological but more physical based models is to increase the predictive capabilities. Numerical simulation of an industrial hot rolling process using models developed on the basis of laboratory tests are in most cases extrapolations of the underlying experimental data. In a typical hot rolling process strain rates up to $150 \frac{1}{\text{s}}$ and overall strains up to $\varepsilon = 5$ are possible. These conditions are difficult to simulate experimentally on a laboratory scale. During multistage deformation recrystallization may not always be completed. The microstructure can consist of multiple generations of grains that have been recrystallized at different points of time. This can not be modeled adequately when only considering average values of the grain size and the recrystallized volume fraction.

Mesoscale models that use a spatial representation of the microstructure give an opportunity to simulate the physical processes involved in recrystallization during hot rolling. In particular models based on the Cellular Automata method show promising results like the simulation of DRX under transient conditions by Kroc et al. [33] that show similar patterns as the experimental results from Frommert [9] and Sakai et al. [1]. The simulation results of post-deformation recrystallization by Kugler and Turk [41] show that MDRX and SRX can be described with one unified model. This can be explained by the influence of the current grain size on the recrystallization kinetics. The size of the grains recrystallized by DRX depends on strain rate and temperature. Hence the kinetics of MDRX also depends on strain rate and temperature of the previous deformation. However the initial grain size for SRX does not change due to the deformation condition because in this case no DRX is involved. So SRX depends more on temperature and the grain size prior to deformation than on strain rate. Other benefits of such models are, that the virtual microstructure can easily be compared with a real microstructure. It is also possible to track multiple generation of recrystallized grains. However, the CA method is very computationally and memory intensive, especially if a three-dimensional lattice is used. It is therefore not suited yet for a direct usage in forming simulations or process control applications.

The proposed ensemble model describes each grain with a set of scalar variables. Compared to CA models this reduces the required amount of memory and computation cycles proportional to the number of cells needed to describe one grain in a CA lattice. A spherical grain with a grain diameter of $20 \mu m$ fills approximately 4200 cells in a three-dimensional lattice with an edge length of $2 \mu m$ of each cell. The trade off is that the model only provides the distribution of the grain size rather than a spatial representation of the microstructure. The model holds no information about the relationship between the grains. It is not possible to take into account the difference of the misorientation between the grains for the calculations of the grain boundary energy, so an average value is used. But like in vertex models the grains are not discretized so stress boundary movement can be described continuously. Similar to CA models the ensemble model can describe the transient oscillation that can be observed at transient conditions during deformation. The system does not change its state instantly to the configuration with the lowest free energy. Instead, work has to be performed to move the grain boundaries. This is a time dependent and dissipative process that follows the principle of least actions. The path with the lowest energy dissipation is in some cases an oscillation of the average grain size and the flow stress.

6. Conclusion

Mesoscale models allow the modeling of the microstructure evolution during and after hot deformation by describing the underlying physical processes. Phenomena modeled separately by constitutive models like DRX, SRX, MDRX and grain growth can be described in a unified manner. The outlined ensemble model makes some approaches known from mesoscale models practically usable for through process modeling and process control application by a massive reduction of the required computational effort.

All models rely on proper material parameters. Future work should therefore focus on methods for the determination of model parameters, especially for the models based on physical approaches. One way to determine the parameters from experimental data is the use of the inverse analysis method. This implies the execution of many simulation cycles that are time consuming for complex models. The usage of the ensemble model can be a solution to make such analysis feasible.
### Models for Recrystallization

| Stateless | Stateful |
|-----------|----------|
| + Direct computation possible | + Precondition for considering variable temperature, strain rate and grain size |
| + Short computation times | - Numerical integration necessary |
| - Only for constant conditions (T, \(\dot{\varepsilon}\)) | |
| - Microstructure described by average values | |

#### Constitute Models for Process Control [3, 15-21, 25]

| + Models for a wide range of materials | + Multiple grain populations |
| Separate modeling of DRX, SRX, MDRX and grain growth | + Path dependent evolution |
| Model parameter for each phenomenon necessary | + Short computation times |

#### Scalar Values

| + Short computation times | + Multiple grain populations |
| - Multiple grain populations cannot be handled | + Path dependent evolution |

#### Distribution Functions

| + Short computation times | + Shape of distribution predefined |
| - Shape of distribution predefined | + Visual comparison of the morphology |
| - Only average values for grain size | - Long computation times |

#### Luton and Sellars [7]

| + Cyclic DRX | + Simple data input and output |
| - No influence of grain size changes during deformation on RX | + Inhomogeneous interior of the grains possible |
| - No damping during cyclic DRX | + Provides grain size distribution |
| | - Memory consumption limits number of grains in simulation domain |
| | - Lattice spacing has to be finer than the smallest particle |

#### Sandström and Lagneborg [27]

| + Takes current grain size into account | + Less memory consumption and computation time compared to CA |
| + Distribution of dislocation density | + Large differences in length scales possible |
| - Only average values for grain size | - Complex description in 3D |
| - Grain size evolution not considered | - No grain interior |

#### Cellular Automata [31-40]

| + Describes transient behaviour | + Continuous description of the grain boundaries |
| + Unified modeling of DRX, MDRX and SRX | - Complex evolution rules in 3D |
| - Physical parameters on microscopic scale necessary | - Difficult to include local representation of the dislocation density |
| - Long computation time, but parallelizable | |

#### Monte Carlo Potts [42, 43]

| + Unified modeling of DRX, MDRX and SRX | |
| - Longer computation time than CA | |
| - Physical parameter on microscopic scale necessary | |

#### Ensemble Model

| + Multiple grain populations | |
| + Path dependent evolution | |
| + Short computation times | |

#### Geometrical Description

| + Simple data input and output | |
| + Inhomogeneous interior of the grains possible | |
| + Provides grain size distribution | |
| - Memory consumption limits number of grains in simulation domain | |
| - Lattice spacing has to be finer than the smallest particle | |

#### Vertex Approach [44-50]

| + Continuous description of the grain boundaries | |
| - Complex evolution rules in 3D | |
| - Difficult to include local representation of the dislocation density | |

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Figure 7: Hierarchical overview of the features and constraints of different model approaches for recrystallization. The models (highlighted with a thick border) are divided in several branches based on the underlying modeling techniques.
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