GRAIN SIZE PREDICTION BY USING A MESHLESS ROLLING SIMULATION SYSTEM*

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Abstract
A rolling simulation system has been developed to calculate the macroscopic rate of deformation, stress, strain, and temperature fields by using a novel meshless method. The model is based on two-dimensional traveling slice assumption. The slices are aligned towards the rolling direction. The initial size of the billet, bloom or slab and the geometry of the grooves at each rolling stand, the distances between the rolling stands, and continuous or reverse rolling can be arbitrarily considered. The purpose of this paper is to complement these development by predicting and visualizing also the grain size of steel over the strand cross-section for each position in the rolling mill. The grain size models have been in one-way coupled to the macroscopic calculations. First the critical strain for dynamic recrystallization is being checked. If the calculated strain is higher than that, considering also the time for meta-dynamic recrystallization, dynamic or meta-dynamic grain size calculations are carried out. If the strain is too low then only the static recrystallization is considered together with its required time. Finally, austenite grain size and ferrite grain size are calculated respectively as the steel cools down. The listed physical models are based on collection of empirical relations found in literature. The user of the system is free to choose or create the model he wants with his own parameters. The simulation system has been coded as a user friendly computer application for an industrial use based on C# and .NET framework and runs on regular PCs. The computational time for a rolling simulation is usually less than one hour and can thus be straightforwardly used for optimization of the rolling mill design in a reasonable time.
Keywords: Hot rolling; grain size prediction; meshless methods; radial basis functions.

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1 INTRODUCTION

The rolling simulation is analyzed based on a meshless method [3] where all the unknown fields are interpolated over the collocation nodes distributed over each computational domain and boundary. The solution procedure is 2D where the computational domains are slices aligned towards the rolling direction as shown in Figure 1 below.

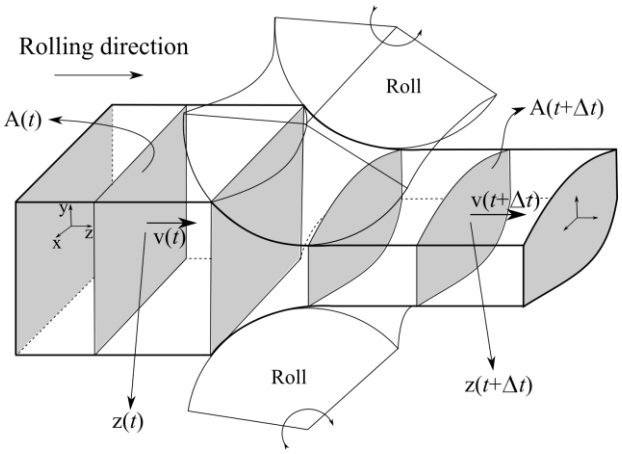


Figure 1. Scheme of the slice model used in the rolling simulations.

During any metal forming process such as the hot rolling, plastic deformation occurs when the stress level exceeds the minimum amount required to move the dislocations. This level is the yield stress and it mostly depends on the current dislocation density. Dislocation density depends on the metal's deformation and temperature history. Exceeding the yield stress, work hardening is observed because of the increased dislocation density. If the strain rate and temperature values are high enough dynamic crystallization occurs. This critical level of deformation is determined by the critical strain. New grain sizes should be calculated at this stage either locally or globally over the computational domain. However, not all the recrystallization takes place immediately after exceeding of the critical strain. After a certain time meta-dynamic crystallization may take place.

When the deformation is very small or there is no deformation at all, with sufficient time at high temperatures, a softening process may take place. A partial or full static recrystallization is followed by grain growth which puts the dislocations into a lower energy configuration.

The grain size prediction models constitute an important aspect of the microstructure studies. Smaller grains may be desired since they lead to higher strength because it is harder for dislocations to pass into another grain. Or the other way around for the ductility. Overall, it is important for steel industry to be able to predict the mechanical properties of their final product and this is only possible together with the microstructure analysis.

In this paper multiple grain size prediction models [1,2] are coupled with the macroscopic rolling simulation system and compared. These models consists of empirical equations to determine the critical strain and grain size after meta-dynamic, dynamic or static recrystallization.

2 SOLUTION PROCEDURE

Sellars [4] pointed out that the experimental tests or industrial trials are not enough to understand the details of hot rolling process. Because it is not possible to monitor or control all the parameters of the sample or billet even in the laboratory conditions. Therefore the best solution he suggested is the combination of the numerical simulation with empirical models based on experiments.

A macro scale numerical simulation of the deformation of steel during hot rolling process has been previously studied [5,6,7] with the present in-house simulation system. Stress-strain and temperature fields over each slice at desired position towards the rolling direction may be obtained. After the verification and

industrial validation of the rolling simulation results, micro structure models are for the first time included in it.
After running a successful simulation of a user defined rolling schedule, a microstructure model is chosen by the user from a database and a one way coupling of the macro-micro model is done in a few seconds of computer power.

2.1 Grain Size Prediction Models

In this work critical strain, time for meta-dynamic recrystallization or static recrystallization and grain sizes after different types of recrystallization are implemented through multiple empirical models. Grain size prediction models are obtained for the austenite phase. Solution steps are adopted from Hodgson and Gibbs [8] as shown in Figure 2.

2.1.2 Critical Strain

The first step is to check if the critical strain (ε_c) over the deformed slice has been reached or not. Exceeding this value will lead to dynamic recrystallization.

$$\varepsilon_c = A\underbrace{\left(\dot{\varepsilon}\exp\frac{Q_d}{RT}\right)^p}_{Z} D^q \quad (1)$$

The central part of this equation (Z) is called Zener-Hollomon parameter (s^{-1}) and will be used multiple times in this paper. $\dot{\varepsilon}$ is strain rate, Q_d is activation energy ($J/mol\ \mathrm{K}$), R is ideal gas constant taken as 8.314, T is temperature in Kelvin and D is the initial austenite grain size. Different coefficients are used in Equation 1 by different authors, the ones that are considered in this paper are listed in Table 1 below.

Table 1. Parameters used in the critical strain definition for carbon-manganese steel in [9,10,12] and low carbon steel in [11].

	[9]	[10]	[11]	[12]
A	$6.82\text{x}10^{-4}$	$4.76\text{x}10^{-4}$	$4.9\text{x}10^{-4}$	$4.9\text{x}10^{-4}$
Q_d	312000	66500	300000	312000
p	0.13	0	0.17	0.15
q	0	0	0.3	1

2.1.3 Meta-Dynamic Recrystallization

Post dynamic recrystallization is usually not considered by most of the researchers which also effects the grain size. There is a time based criteria which includes strain rate. It is defined by Manohar et al [13] as

$$t_{0.9MDRX} = 1.166\varepsilon^{-0.8} \quad (2)$$

If the time during the simulation exceed this value ($t > t_{0.9MDRX}$), it is assumed that meta-dynamic recrystallization (MDRX) occurs. If so, the grain size after the recrystallization is determined from the equation,

$$D_{MDRX} = AZ^r \quad (3)$$

The necessary parameters required in Equation 3 are defined in Table 2 below.

Table 2. Parameters used in the grain size equation for meta-dynamic recrystallization for carbon-manganese steel in [8,12,13] and low carbon steel in [11].

	[8]	[11]	[12]	[13]
A	26000	25000	1600	26000
r	-0.23	-0.23	-0.11	-0.23
Q_d	312000	312000	312000	300000

2.1.4 Dynamic Recrystallization

If the time is not enough for meta-dynamic recrystallization, but the critical strain is still exceeded, then dynamic recrystallization (DRX) occurs. The grain size prediction model is in the flowing form,

$$D_{DRX} = AZ^r \quad (4)$$

The grain size prediction model is just like the meta-dynamic one but with different coefficients as shown in Table 3 below.

Table 3. Parameters used in the grain size equation for dynamic recrystallization for carbon-manganese steel.

	[8]	[10]	[12]	[13]
A	16000	22600	1800	16000
r	-0.23	-0.27	-0.15	-0.23
Q_d	312000	267100	312000	300000

2.1.5 Static Recrystallization

There is a time criteria for static recrystallization (SRX) to occur and in this paper a model defined by Zhang et al. [14] for high carbon steel is used. It has the following form,

$$t_{0.9SRX} = 1.944\times10^{-4}\varepsilon^{-1.0}D_0^{0.6}\left(\frac{3.6}{\dot{\varepsilon}}\right)^{0.28}\exp\left(\frac{6900}{RT}\right) \quad (5)$$

When the time during the simulation is larger than $(t > t_{0.9SRX})$ then a static recrystallization may be expected. The grain size after the recrystallization is obtained from

$$D_{SRX} = A\varepsilon^m D_0^q \quad (6)$$

where $A = 0.5$, $m = -0.67$, and $q = 0.67$ as defined by Zhang et al. [14].

2.1.6 No-Recrystallization Temperature

Dynamic and static recrystallizations depend also on the temperature, however there is a required minimum temperature which determines if it is possible for a material to recrystallize or not. A no-crystallization temperature (T_{nr}) prediction model [15] is used in this paper base on

$$T_{nr} = A\varepsilon^m \dot{\varepsilon}^n t^k \quad (7)$$

where $A = 905$, $m = -0.045$, $n = -0.005$ and $k = -0.024$ for high strength low allow steel and obtained from experiments in [16]. Time is accounted for only during the deformation process.

2.2 Implementation

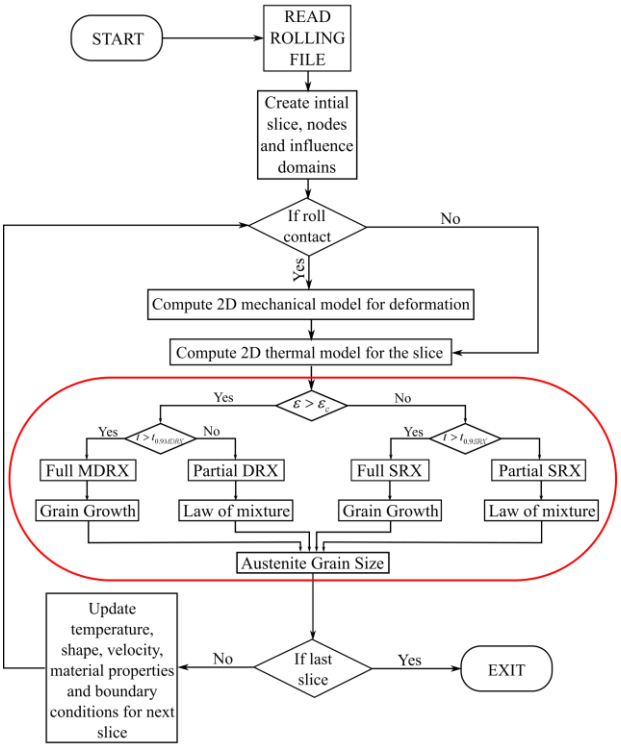


Figure 2. Flowchart of the microstructure implementation (surrounded by red ellipse) to the macroscale rolling simulation system.

A previously developed rolling simulation system based on meshless solution [4,5] is used here to obtain the macro scale deformation results. The solution procedure is based on 2D slices aligned towards the rolling direction. Once the simulation is done, each computational domain is recalculated with the desired microstructure model based on the multiple empirical equation described above. The results are visualized over each slice, in particular at the exit from each rolling stand. Temperature, strain and strain rate fields are the inputs of the micro scale model and obtained from the macro scale

simulation results. This is the solution procedure of a one way coupled system.

All the grain size prediction models are implemented in the simulation system as one of the post process options. A database is created for all the models, together with their coefficients. A user is free to add more of these models into this database with different coefficients without running the simulation over and over again. Once the simulation is run, all the microstructure models are ready to be used and compared. It is very easy to switch in-between the models and the results are updated according to the new model in a few seconds. There are two major outcomes of this microstructure coupling in the simulations. The first outcome is to observe the type of the recrystallization for each slice position such as meta-dynamic, dynamic, and static recrystallizations or no recrystallization at all. The second one is the grain size prediction after recrystallization again for each slice position and scaled from minimum to maximum.

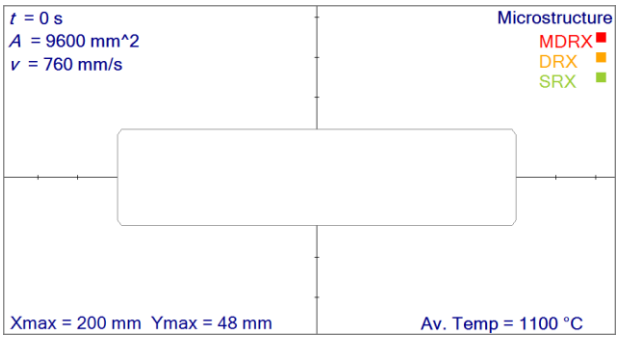
3 RESULTS AND DISCUSSION

A rolling schedule consisting of 8 rolls is chosen here for comparing different microstructure models. Results are demonstrated as slices at the exit of each rolling stand where the deformation is the highest. Two major objectives are analyzed here, first one is to define the type of the recrystallization, if there is any. The second one is the austenite grain size prediction. Three types of recrystallization are shown in different colors over the slices positioned at the exit of each rolling stand.

The process parameters and some of the material properties required for solving the thermo-mechanical rolling process are shown in Table 4 below. The material properties that are not explicitly listed are obtained from JMatPro data base.

Table 4. Parameters used in the rolling simulation.

GENERAL DATA	
Initial size of the slab	200×48 mm
Initial temperature field of the slab	1100 °C
Entry velocity towards the rolling direction	760 mm/s
Coefficient of friction	0.1
MATERIAL MODEL	
$\bar{\sigma}\left(\bar{\varepsilon},\dot{\bar{\varepsilon}},T\right)=589\bar{\varepsilon}^{0.214}\dot{\bar{\varepsilon}}^{0.2}\exp\left(\frac{38000}{RT}\right)$ MPa, for 16MnCr5 alloyed steel	
GROOVE AND ROLL DATA	
Roll radii	230 mm
Roll gaps	34.5 - 26.5 – 118 - 22.5 - 112-20 - 107.4 - 18.2 (mm)
Groove geometries (H-horizontal, V-vertical)	flat (H) – flat (H) - oval box (V) - flat (H)- flat box (V) – flat (H) - flat box (V) – flat (H)
Distance between rolling stands	3 m (for the first five rolling stands), 4.5 m (after the fifth rolling stand).



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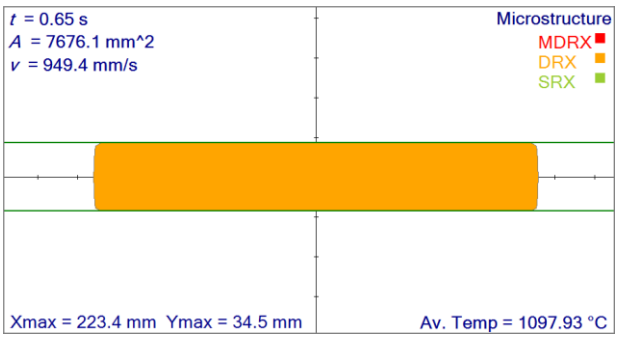

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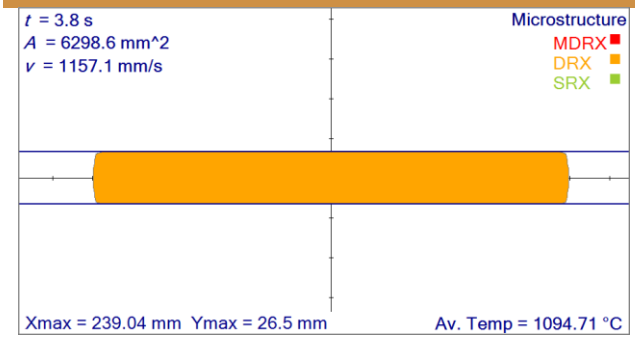

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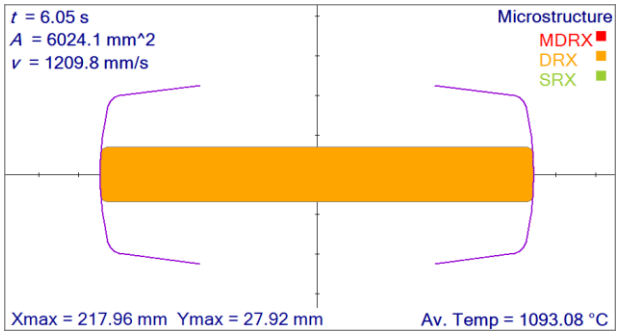

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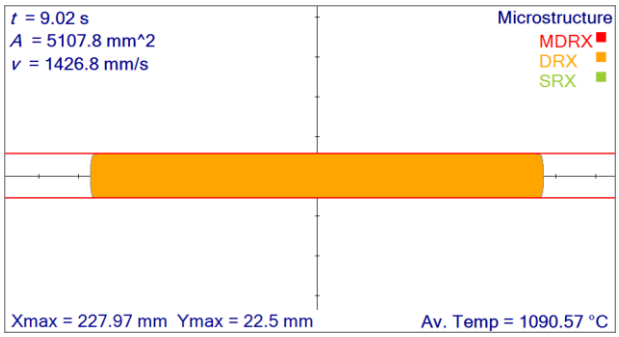

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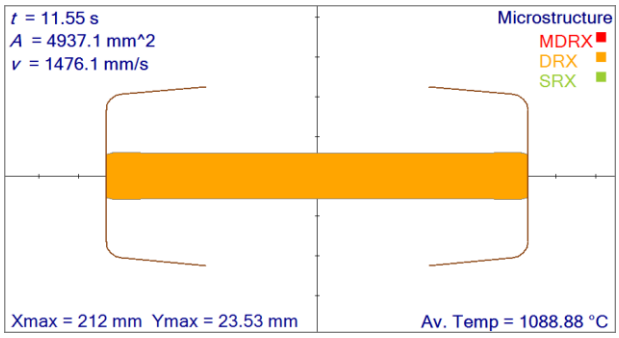

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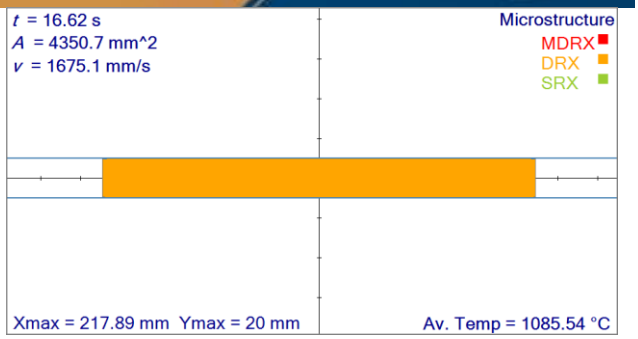

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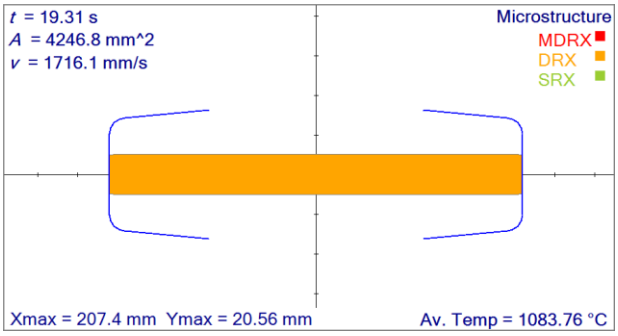

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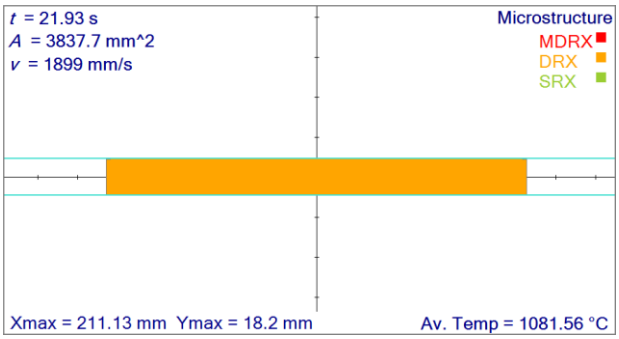


i)

Figure 3. Recrystallization types during finishing rolling of steel. a) initial size b) at the exit of first rolling stand (horizontal), continued by c) second (horizontal), d) third (vertical), e) forth (horizontal), f) fifth (vertical), g) sixth (horizontal), h) seventh (vertical) and i) eighth (horizontal) rolling stands.

The results in Figure 3 show that the critical strain is exceeded in each pass based on Sellars's model [12]. Yada's model [10] predicted similar results except for the forth rolling stand where it predicted very local recrystallization only near the free surface boundaries as shown in Figure 4. Laasraoui and Jonas's model [9] predicted almost no recrystallization at all through all the passes. Kwons's model [11] also predicted dynamic recrystallization at each pass just like in Figure 3.

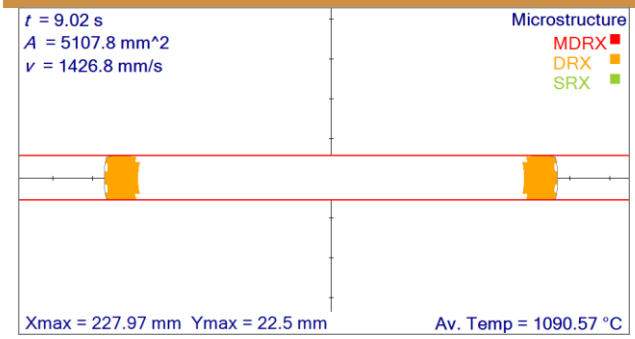
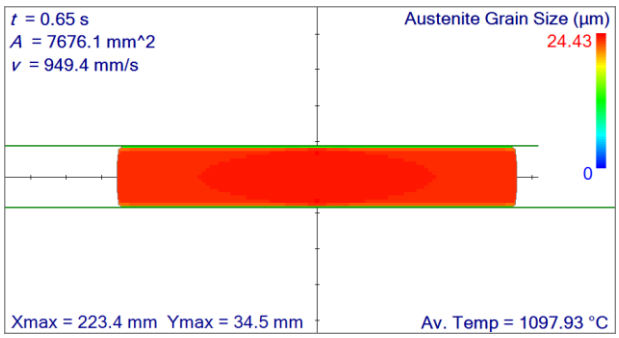


Figure 4. Recrystallization type at the forth rolling stand calculated by Yada's model.

In none of the cases neither meta-dynamic nor static crystallization has been observed. This is due to the specific time requirement of both cases. Even though the reduction are not very large during the finishing rolling, the contact time is very short and it is about 0.05 seconds. The steel moves faster and faster as it deforms and it does not allow material to meta-dynamically or statically recrystallize. On the other hand this short time intervals lead to very high strain rates and this makes it very easy to dynamically recrystallize.

The grain size prediction based on the recrystallization type may also be calculated in a similar way. The grain size model as in Equation 4 and coefficients from Table 3 are implemented and the grain size prediction based on Sellars's [12] model is shown in Figure 5 below. As can be easily noticed, the dynamic recrystallization leads to larger grain sizes, especially towards the center of the material.



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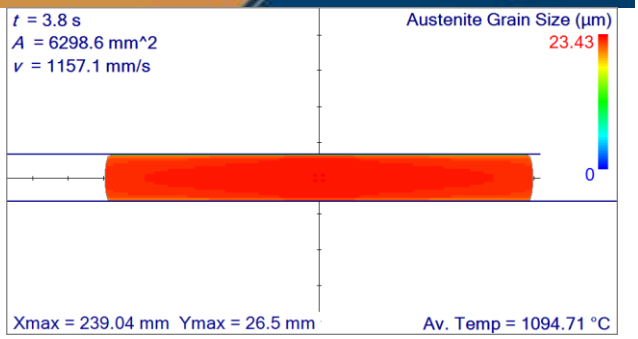

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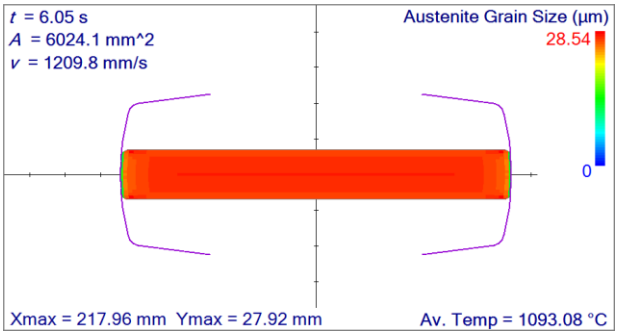

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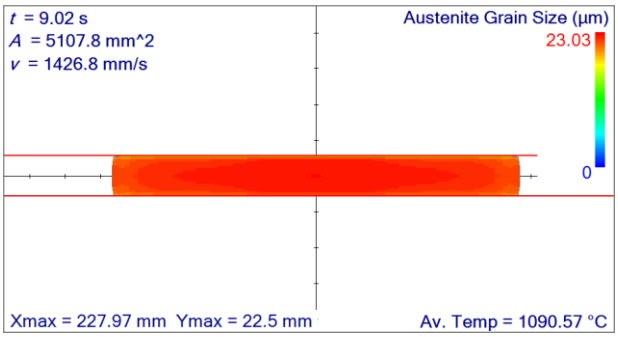

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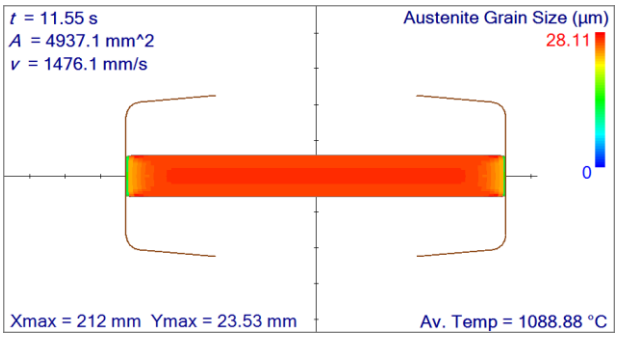

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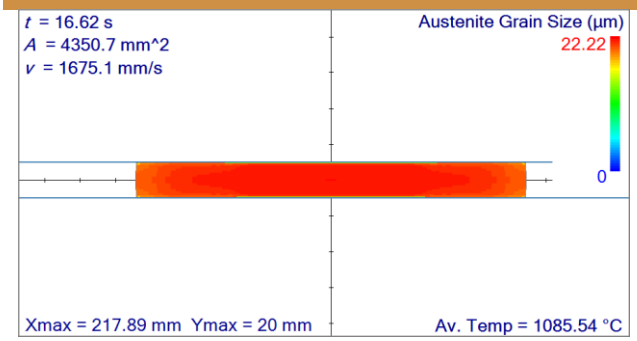

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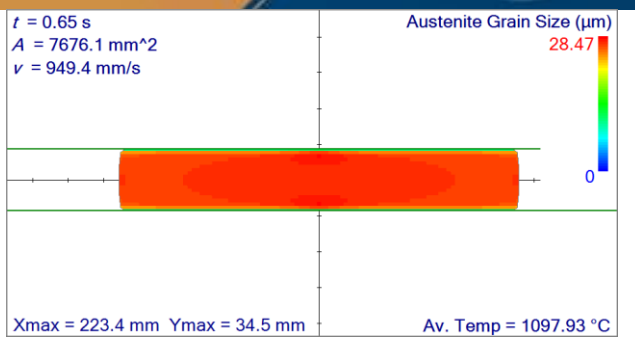

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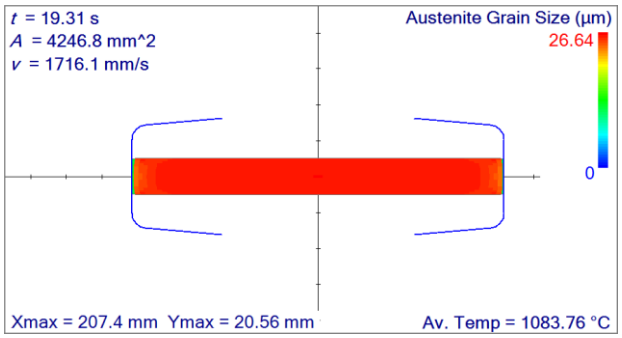

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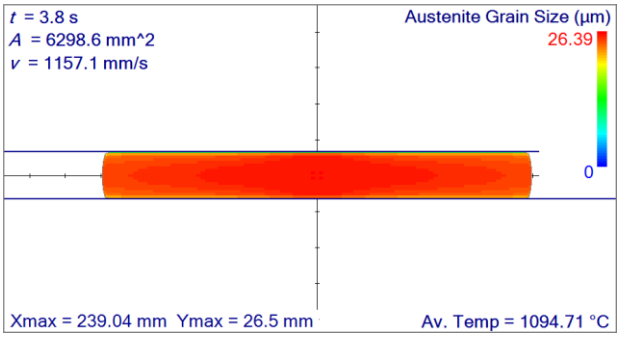

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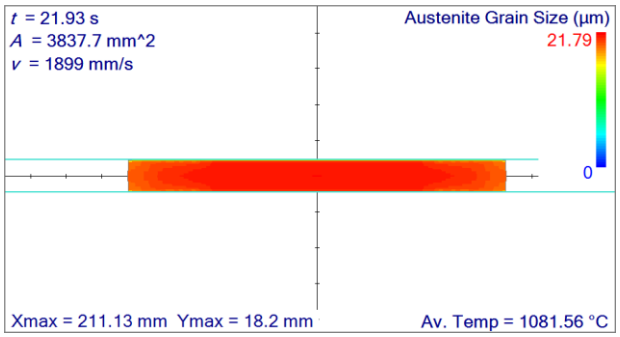

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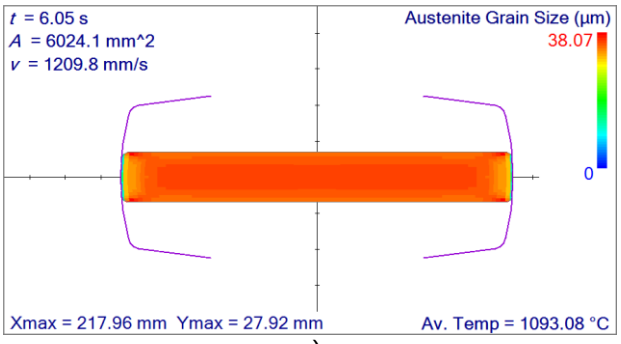

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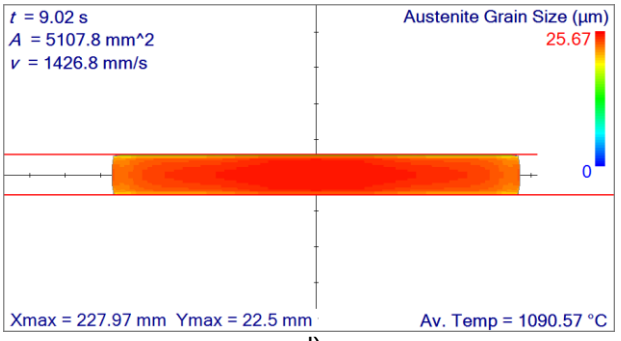

d)

Figure 5. Recrystallized grain sizes based on Sellars's model [12] at the exit of the a) first, b) second, c) third, d) fourth, e) fifth, f) sixth, g) seventh and h) eighth rolling stands.

Another example of the grain size prediction may be obtained by using Yada's [10] model. The results from this model is shown in Figure 6 below and it can be compared with Sellars's model from Figure 5. In both cases the same rolling schedule with same material properties are used.

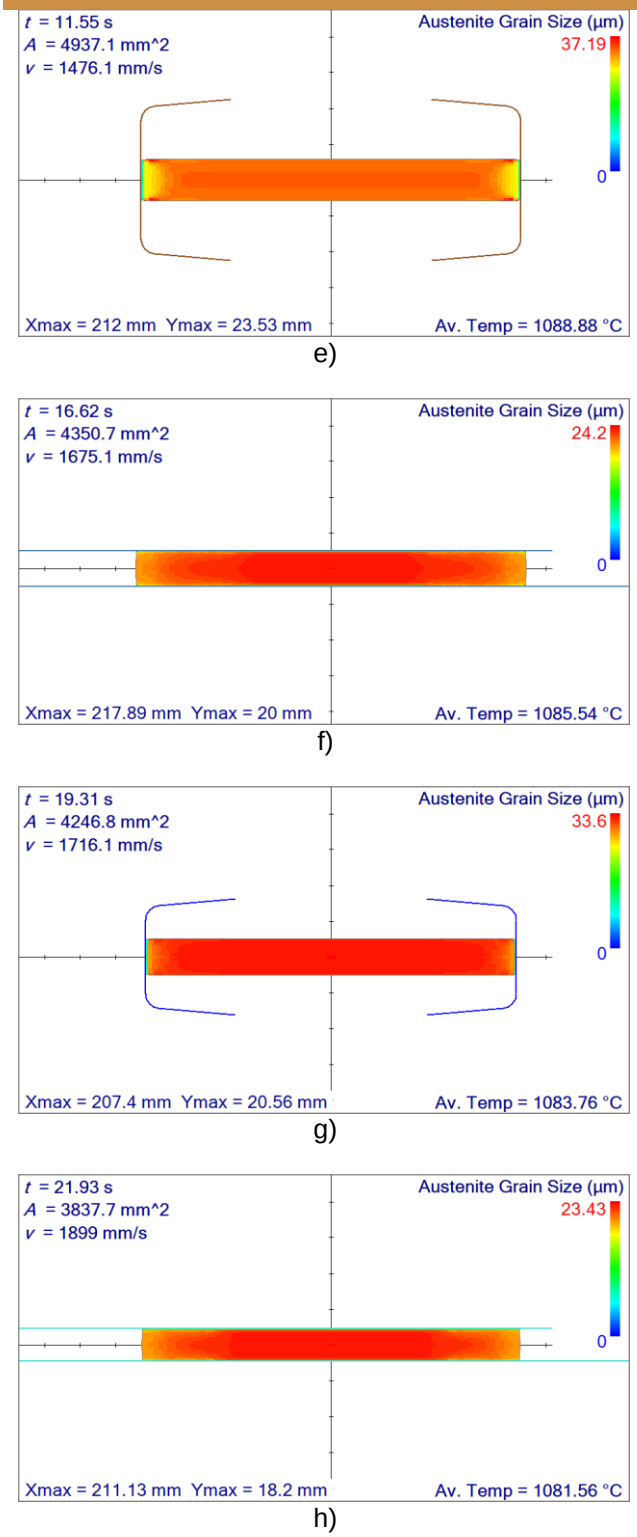

Figure 6. Recrystallized grain sizes based on Yada's model [10] at the exit of the a) first, b) second, c) third, d) fourth, e) fifth, f) sixth, g) seventh and h) eighth rolling stands.

Since the coefficients used in the dynamic crystallization models are so different, the grain size prediction results look similar as expected. Manohar's model [13] predicted relatively smaller grain sizes and Hodgson and Gibbs's [8] model also gave very similar results. Due to limited space it is not possible to show all the results from all the models here.

Another aspect which is calculated in this analysis is the no-recrystallization temperature described in Equation 7. The average values for each slice is obtained and plotted in Figure 7. As the steel first contacts the roll, the calculated no-recrystallization temperature immediately gets a high value and then slowly decreases as the deformation continues. This is repeated 8 times in this figure which is the total number of passes.

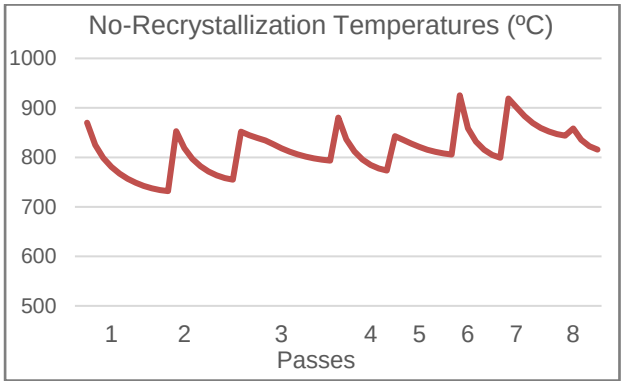

Figure 7. No-Recrystallization temperatures calculated from the simulation results.

There are also many other no-recrystallization temperature models in the literature which depend on the composition of steel. However, a model based on deformation parameters is chosen here for a better coupling of the macro-micro simulation system.

4 CONCLUSION

In this work, various micro structure models are numerically implemented into a macroscopic rolling simulation system from where they obtain all the necessary data in a one-way coupling. They account for the following phenomena: critical strain definition, necessary time for meta-dynamic or static recrystallization and grain size prediction based on recrystallization

types. A continuous finishing rolling schedule (details are given in Table 4) is chosen for feeding the data of the microstructure models. A no-recrystallization temperature model is chosen and used in all microstructure models. The dynamic recrystallization is observed based on models by Yada's [10], Kwons's [11] and Sellars's [12]. A comparison of grain size prediction is done between Yada's and Sellar's models. The austenite grain size will be followed in the future by multiple grain growth models and ferrite grain size predictions. Furthermore, additional calculations that predict yield stress and ultimate tensile strength as a function of the deformation during rolling and chemical composition of steel may be included as well from the obtained results.

Another common and much more detailed approach for analyzing the micro-mechanical behavior is the crystal plasticity [17]. This implementation will be the authors' future target in complementing the described rolling simulation system.

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