UNCERTAINTY OF MICROSTRUCTURE MODELLING DURING HOT ROLLING OF DP STEEL STRIPS

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ABSTRACT: Advanced numerical models, which predict heterogeneity of microstructural features, are essential in designing modern multiphase steels. Models based on stochastic internal variables meet this requirement. Our objective was to account for the random character of the recrystallization and to transfer this randomness into equations describing the evolution of the dislocations and the grain size during the hot deformation of steel. The idea of the internal variable model with the dislocation density and the grain size being stochastic variables is described briefly in the paper. Histograms of the grain size measured in the experimental compression tests were used to identify the coefficients in the model. The model was used to simulations of the industrial process of the hot strip rolling. The same model was used to evaluate the uncertainty of the predictions of phase composition in the final product.

KEYWORDS: Internal variables, stochastic model, microstructure evolution, uncertainty, hot strip rolling

1 INTRODUCTION

Continuous development of the industry is associated with the search for new construction materials that combine high strength with good formability and a high strength-to-density ratio. Steels have met these requirements for many decades. Historically, grain refinement was the main strengthening mechanism for steels investigated during the second half of the 20th century, when High Strength Low Alloyed (HSLA) steels were developed [1]. By controlling the precipitation and its influence on the recrystallization, an improvement of the strength and workability was obtained [2]. Different strengthening mechanism was used in the Advanced High Strength Steels (AHSS), which were developed in the last decades of the 20th century. These steels are composed of soft ferrite with islands of hard constituents of bainite, martensite and retained austenite. The AHSSs benefit from the best features of the phases they are made of [3]. They are locally isotropic but heterogeneous at the macroscopic scale due to spatial variations of phase fractions. Among AHSSs, Dual Phase (DP) and Complex Phase (CP) steels are the two most widely used in car body applications [4]. The correlation between mechanical properties and microstructure has been extensively studied for DP steels [5] composed of the fine ferrite matrix with dispersed hard islands of martensite. The high strength and total elongation of DP steels go side by side with low local formability caused by large gradients of properties at the phase boundaries. CP steels are characterized by the fine microstructure with a heterogeneous mixture of bainite, martensite and ferrite. Compared with DP steel, the volume fraction of hard phases is higher, leading to higher yield and tensile strength. On the other hand, the gradients of properties are smaller than that in DP steels. Thus, CP steels with a more heterogeneous microstructure have better local formability [3]. This feature makes them suitable for stretch-forming processes [6]. It is expected that more balanced properties of multiphase steels can be achieved by tailoring the microstructure gradients [7]. Advanced numerical models are needed to gain knowledge on distributions of microstructural features and to design thermal-mechanical cycles allowing to obtain moderate gradients of properties. These models have to have the capability to predict distributions of various microstructural parameters instead of their average values. Beyond this, since process optimization is the prospective application of these models, they must be characterized by low computing costs.

Numerical tools, which can predict distributions of various parameters in heterogeneous materials, are intensively searched for. Extremely fast progress in this field has been observed during the last decades. Mean-field and full-field material models are distinguished in the literature, see the review in the PhD thesis [8]. In the former, the microstructure is implicitly represented by closed-form equations describing grain size, dislocation density (uniform per grain), the kinetics of phase transformations etc. The latter is based on an explicit microstructure representation using Representative Volume Element (RVE) or Digital Materials Representation (DMR) concept [9]. The predictive capabilities of the full-field models are broader, but they involve much higher computing costs.

Beyond predictions of the microstructure heterogeneity, a problem of the uncertainty of predictions is also essential [10]. Knowledge of the possible spread of the predicted target values, such as microstructural parameters, is needed for a reliable process design. In production, the spread of product properties is due to uncertainties in the processing conditions and the material behaviour.

Thus, the objectives of the work were twofold. The first objective was to apply the fast mean-field stochastic model with extended predictive capabilities. As it was shown in [11], the description of the heterogeneous microstructure of metals and alloys using internal stochastic variables allows for building the mean-field model with the capability to predict gradients of product properties. The internal variables allow accounting for the history of the process. The stochastic character of the variables allows the prediction of distributions of parameters instead of their average values.
The same stochastic model can also be used to evaluate the uncertainty of the predictions of microstructural parameters when the uncertainty of the input parameters (grain size) and boundary conditions (temperatures) is known. This was the second objective of the paper.

2 MODEL

The internal variable stochastic model for hot deformation was proposed in our earlier publication [12]. The model was identified based on the experimental data [11]. In publication [13] the model was applied to simulations of multi-step hot forming processes. The practical application of the model to simulations of the industrial process of the hot rolling of flat rods is described in [14]. The model details are presented in [12] and only the main equations are repeated here for the completeness of the presentation.

2.1 MAIN EQUATIONS

The model origins from the Kocks-Estrin-Mecking (KEM) approach [15,16] with the recrystallization term proposed in [17]. The deterministic model described in [18] was extended in [12], where the critical time for dynamic recrystallization was substituted by a random character of the recrystallization. The evolution of the dislocation density is governed by the equation:

$$\begin{aligned}\rho(t_i) &= \rho(t_0)\left[1-\xi(t_i)\right] \\ &+\left\{\rho(t_{i-1})+\left[A_1\dot{\varepsilon}-A_2\rho(t_{i-1})\dot{\varepsilon}^{1-a_7}\right]\Delta t\right\}\xi(t_i)\end{aligned} \tag{1}$$

where: t - time, $\dot{\varepsilon}$ – strain rate.

Coefficients A_1 and A_2 responsible for hardening and recovery are defined in [12]. The parameter $\xi(t_i)$, accounts for a random character of the recrystallization and its distribution is described by the conditions:

$$\begin{aligned}\mathbf{P}\left[\xi(t_i)=0\right] &= \begin{cases} p(t_i) & \text{if } p(t_i)<1 \\ 1 & \text{otherwise} \end{cases} \\ \mathbf{P}\left[\xi(t_i)=1\right] &= 1-\mathbf{P}\left[\xi(t_i)=0\right]\end{aligned} \tag{2}$$

In equation (3), $p(t_i)$ is a function that bounds together the probability that the material point recrystallizes in a current time step and the present state of the material:

$$p(t_i) = a_4\rho(t_{i-1})^{a_6}\frac{3\gamma(t_i)\tau}{D(t_{i-1})}\exp\left(\frac{-a_5}{RT}\right)\Delta t \tag{3}$$

where: D – grain size in μm, τ – energy per unit dislocation length, a_4, a_5, a_6, a_{17} – coefficients.
In equation (4), coefficient γ represents a mobile fraction of the recrystallized grain boundary and depends on the distribution of $\xi(t_{i-1})$ in the previous step. The model was extended in work [13] by including interpass times and static phenomena in simulations. In consequence, it was possible to reveal numerical distributions of the dislocation density and the grain size. Many trajectories of equation (1) were calculated, each time using randomly generated values of $\rho(t_0)$ and $D(t_0)$. These trajectories were then aggregated into histograms at consecutive time steps t_i. We start with the grain size $D(t_0) \equiv D_0$ which is a random variable described by the Weibull distribution. Based on measured grain size distributions shown in [11] the shape parameter equal to 10 was assumed. The scale parameter $\bar{D}_0$ was established as the average grain size measured after preheating before deformation. The changes in the grain size during deformation and during the interpass times were calculated based on the fundamental works of Sellars [19]. When during the calculation, the random parameter $\xi(t_i) = 0$, the considered point recrystallizes and its new grain size $D(t_i)$ is drawn from the Gauss distribution with the standard deviation being an optimization variable a_{16} in the model. The expected value of the grain size is either dynamically (for $\dot{\varepsilon} > 0$) or statically (for $\dot{\varepsilon} = 0$) recrystallized grain size. The model contains 21 coefficients grouped in the vector **a**. These coefficients were identified based on the experimental data.
Beyond the histograms of the selected parameters, the model calculates the average dislocation density ρ_{av} and further the flow stress σ_p, as follows:

$$\sigma_p = \alpha b G\sqrt{\rho_{av}} \qquad \rho_{av} = \frac{1}{Np}\sum_{i=1}^{Np}\rho_i \tag{4}$$

where: G – shear modulus, b – a module of the Burgers vector, Np – number of points in the Monte Carlo solution, α – coefficient.

2.2 IDENTIFICATION AND VALIDATION

Details of the identification procedure are described in [11,12]. The inverse algorithm developed in [20] was applied. The objective function was extended by including the metric of the distance between measured and calculated histograms of the grain size. The experimental data published in [21] were used. Steel DP600 with the symbol S406 in that publication was considered. The tests composed uniaxial compression of the samples measuring ϕ10×12 mm at various strain rates and temperatures. The total strain was 1 in all the tests and the expected value of the austenite grain size

after preheating was 30 μm. A complete set of experimental data for these tests, including micrographs taken at various stages of the deformation and after the deformation, can be found in the RFCS report [22].
The model with optimal coefficients was validated and selected results are shown in **Figure 1** for the flow stress and in **Figure 2** for the histograms of grain size. The experimental flow stress in **Figure 1** was calculated by the inverse solution following the algorithm described in [20] for the forces measured in the compression tests. Good agreement between measurements and predictions of the model was obtained for all the experiments. The value of the Earth Movers Distance (EMD) metric [23] is given in the bottom left corner of the plots in **Figure 2**. Analysis of all results confirmed the good accuracy of the model. In all the tests the EMD did not exceed 0.5, which is a reasonable limit for the microstructure evolution model.

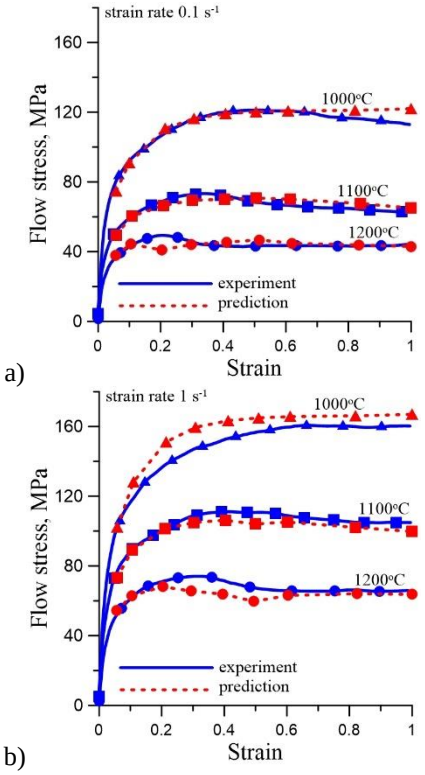

Figure 1: Selected results of a comparison of measured and calculated flow stress in uniaxial compression.

3 RESULTS

3.1 HOT ROLLING

The hot strip mill composed of the reverse roughing mill, 6-stand continuous finishing mill and 2-section laminar cooling was considered. Rolling of the DP600 steel strip measuring 1500×4 mm was simulated. Only the results for the finishing mill and the laminar cooling are presented below. The work roll radius was 450 mm in all stands and the distance between stands was 5.8 m. The rolling schedule is given in **Table 1**, where: h – thickness, r – reduction, v – velocity, t – interpass time.

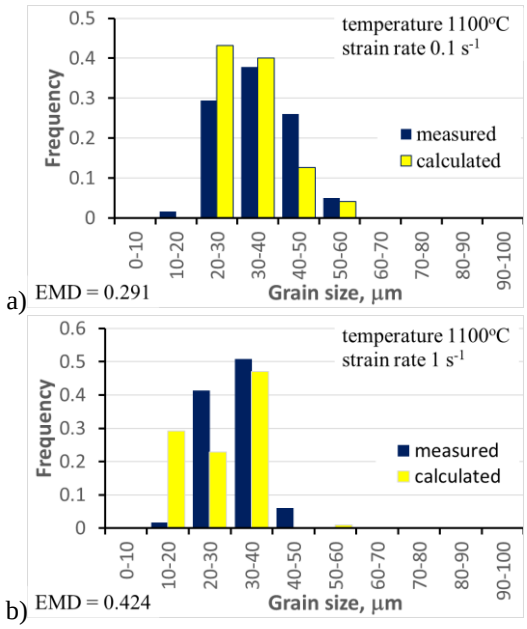

Figure 2: Selected results of a comparison of measured and calculated histograms of the grain size after uniaxial compression at the temperature 1100°C and the strain rate 0.1 s^{-1} (a) and 1 s^{-1} (b).

Table 1: Rolling schedule considered in the paper.

pass	h, mm	r	v, m/s	t, s
0	40	-	0.95	-
1	19.2	0.52	1.98	2.9
2	12.6	0.344	3.02	1.9
3	9.3	0.262	4.09	1.4
4	6.9	0.258	5.51	1.1
5	5.2	0.246	7.31	0.8
6	4	0.231	9.5	0.6

Classical hot strip rolling with the end of the rolling temperature of about 900°C was simulated. After exit from the last stand the strip enters the laminar cooling system. The model predicted full recrystallization after rolling and a model for recrystallized material was applied to simulate phase transformations. Calculated time-temperature profiles during rolling and cooling and load parameters during rolling are shown in **Figure 3**.
Monte Carlo solution with 20000 points was used to calculate distributions of the dislocation density and the austenite grain size during rolling accounting for the random character of the recrystallization, following equations (2) and (3). Calculated histograms (10 bins each) of distributions of the dislocation density and the austenite grain size at various stages of the hot strip rolling are shown in **Figure 4**. It is seen that there is no dynamic recrystallization in any pass, which is due to high strain rates and reasonably low temperature. The static recrystallization is completed during all interpass times, except the interpass between passes 5 and 6, where about 90% of the SRX was predicted. Anyway, as it has been mentioned, the material is recrystallized at the beginning of phase transformations

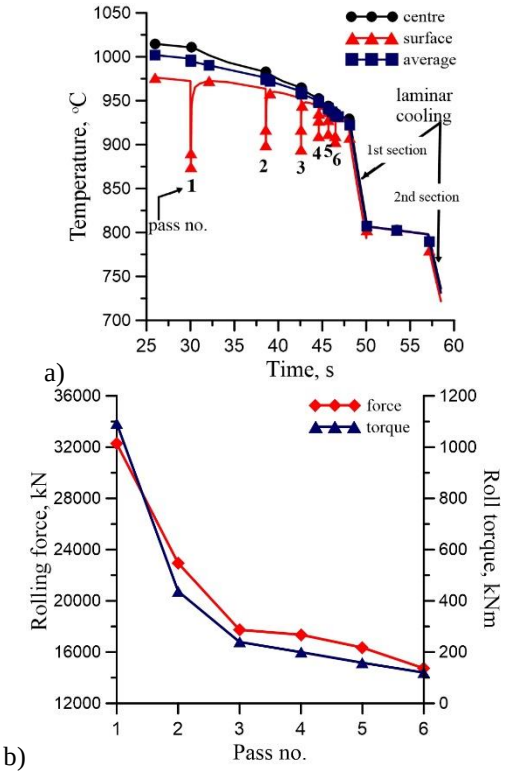

Figure 3: Calculated time-temperature profile (a) and load parameters (b) during hot finishing strip rolling and laminar cooling.

transformations, when the temperature drops to A_{e3}, (for the investigated steel A_{e3} = 842°C).

As far as the austenite grain size is considered, it decreases rapidly in the first two passes and then remains reasonably stable. The histogram of the austenite grain size at the temperature A_{e3} was used as an input for the simulation of phase transformations during laminar colling. Obviously, due to the full recrystallization of the steel, the effect of the dislocation density on the phase transformations was not considered.

3.2 LAMINAR COOLING

The results of calculations of the austenite grain size were used as input data for the simulations of the phase transformations during laminar cooling. At this stage, the deterministic model of phase transformations described in [21] was applied, but the input data, as well as the boundary conditions, were stochastic. The typical laminar cooling system composed of 2 sections with 40 boxes each and described in [24] was considered. This system allows a 3-stage cooling sequence: fast/slow/fast. As a consequence of this sequence, the DP microstructure composed of ferrite and martensite can be obtained. Heat transfer coefficients depending on the water flux and the active number of boxes, which are given in [24], were used in the present work.

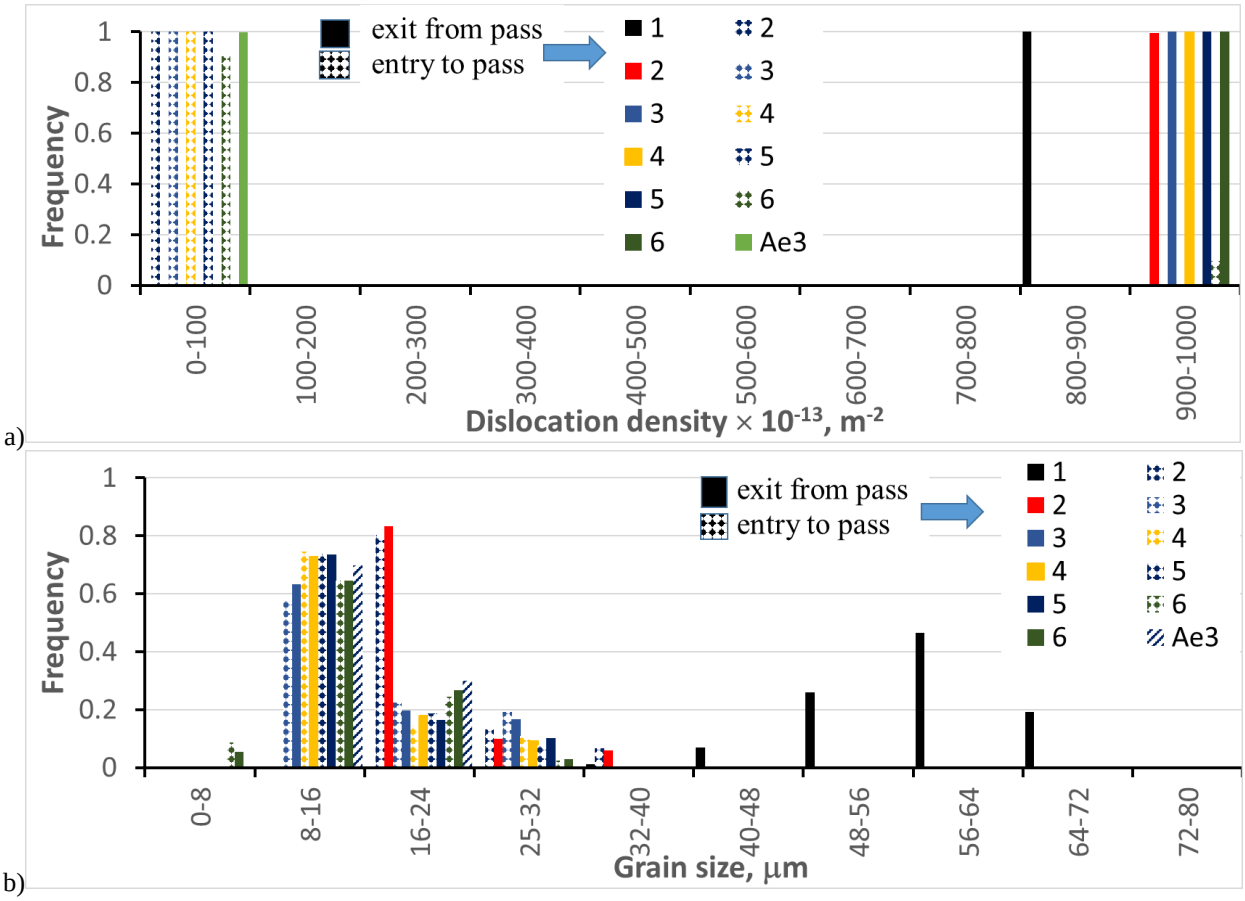

Figure 4: Calculated histograms of the dislocation density (a) and the grain size (b) at various stages of the hot strip rolling.

The kinetics of transformations during laminar cooling calculated by the deterministic model [21] for the average austenite grain size is shown in Figure 5. The microstructure composed of approximately 80% of ferrite and 20% of martensite was obtained.

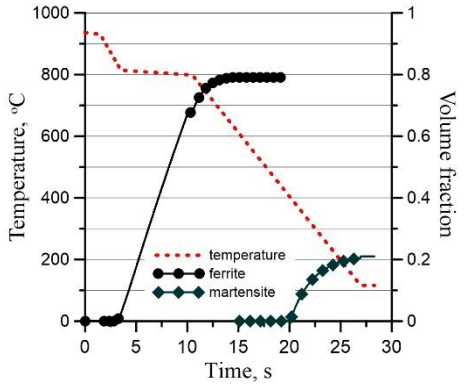

Figure 5: Kinetics of transformations during laminar cooling calculated by the deterministic model**.**

3.3 UNCERTAINTY

Since the input data for the deterministic phase transformation model were stochastic, the calculated phase composition was obtained in the form of histograms. Additionally, the model allows to account for the uncertainty of the boundary conditions. In the first approach, we assumed that the heat transfer coefficient during laminar cooling is given by the Gauss distribution:

$$\mathrm{f}\left(HTC\right)=\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{\left(HTC-\overline{HTC}\right)^2}{2\sigma^2}\right] \qquad (5)$$

$\overline{HTC}$ - the expected value of the heat transfer coefficient calculated following the data in [24], σ - standard deviation, assumed 50 W/m^{2}K.

A histogram of the martensite volume fraction calculated accounting for the random character of the input data and the boundary conditions is shown in **Figure 6**. This histogram represents the uncertainty of the predictions of the phase composition.

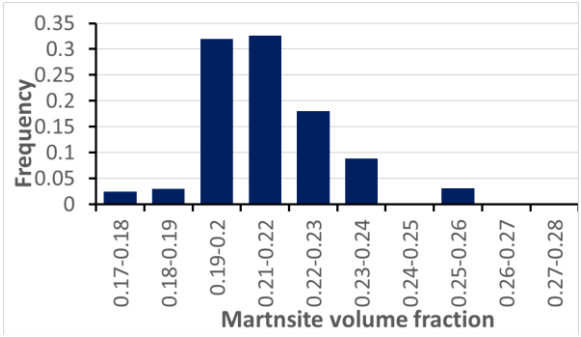

Figure 6: Histogram of the martensite volume fraction calculated accounting for the random character of the input data and the boundary conditions.

4 CONCLUSIONS

The stochastic model describing the evolution of the microstructure during hot strip rolling and laminar cooling is presented in the paper. Performed simulations allowed to draw the following conclusions:

- Identification based on the inverse analysis for the compression tests yielded coefficients in the model, which give good agreement between measurements and predictions of both average values and distributions of selected parameters.
- Capability to predict histograms of microstructural features instead of their average values is the main advantage of the model.
- The model was applied to simulations of the industrial hot strip rolling. The results agree with our knowledge about this process, confirming the model's capability to support the optimal rolling technology design.
- The deterministic simulation of the laminar cooling showed that the sequence of the fast/slow/fast cooling allows to obtain of a DP microstructure.
- The phase transformation model can account for the random character of the input (grain size) and boundary conditions (HTC). In consequence, the uncertainty of the predictions of the phase composition could be evaluated.
- In the hot deformation part, the model is completed and, when coupled with the finite element program, can be applied to any hot forming process. The phase transformations part is still a work in progress. In the present work we used a deterministic model with stochastic input data. In the future, we will account for the random character of the nucleation during phase transformation. The model will be validated by comparison of the predictions with measurements of distributions of various microstructural features after cooling.

ACKNOWLEDGEMENT

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