Modelling of phase transformations in steels accounting for a stochastic character of the austenite grain size after hot forming

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1. Introduction

Exploring a possibility of a stochastic modelling of thermomechanical processing is the objective of our research. Motivations for these research were twofold. Firstly, the continuous development of the industry is associated with the search for construction materials with exceptional properties. Heterogeneous materials meet these requirements and they are now widely used in forms of metallic alloys, among which multiphase steels are a leading example [1]. Secondly, a problem of the uncertainty of predictions of product microstructure and properties is important today [2]. Knowledge of the possible spread of the predicted target values, such as microstructural parameters, is needed for a reliable process design. Investigation of both these aspects requires advanced models, which can predict distribution of microstructural features instead of their average values. Although a number of material models with various complexity and predictive capabilities has been recently developed [3], mean-field models are still commonly used in the design of processes. It is due to low computing costs of these models. On the other hand, predictive capabilities of the mean-field models are limited and it leads to limitations of the design methodologies. Therefore, we focused on a search for a possibility to extend predictive capabilities of the mean-field model while the computing costs are kept on a reasonably low level. It has been shown in [4], that the model with internal stochastic variables allows description of the heterogeneous microstructure of metals accounting for distributions of various features. Following this, we developed the stochastic model, which describes evolution of the dislocation density and the grain size during hot deformation. Analysis and optimization of the numerical parameters of this model are described in [5] while its identification, validation and application to the hot rolling is presented in [6]. It should be pointed out, however, that properties of product are obtained by a control of phase transformations during cooling after hot forming. In our first approach to this process the deterministic phase transformation model was used with the stochastic initial conditions in the form of dislocation density and grain size histograms calculated by the hot deformation model.

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2. Model and results

Details of the stochastic hot deformation model are described in [5,6]. In this model, the critical time for dynamic recrystallization in the deterministic model [7], which is not a physical quantity, was replaced by the stochastic variable $\xi(t_i)$. After discretization in time, the evolution of the dislocation density in function of time is governed by the following equation [5]:

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

where: t – time, ρ – dislocation density, A_1, A_2 – coefficients responsible for hardening and recovery and defined in [5], a_7 – a coefficient responsible for the strain rate sensitivity of the recovery.

The parameter $\xi(t_i)$, accounts for a random character of the recrystallization and its distribution is described by the conditions:

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

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

where: D – grain size, R – gas constant, T – temperature in K, τ – energy per unit dislocation length, γ – a mobile fraction of the recrystallized grain boundary, a_4, a_5, a_6 – coefficients.

Presented model calculates distributions of the dislocation density and the grain size during hot deformation. This model was used to supply the input data for the simulations of phase transformations. The kinetics of transformations was calculated from the upgrade of the JMAK equation described in [3]. This upgrade accounts for the influence of the state of the austenite (grain size, dislocation density) on the transformations. All calculations were performed for the multiphase CP steel. The hot strip rolling process in the 6-stand finishing mill was considered as an example. The slab thickness was 66 mm and the pass schedule 66 → 40.6 → 19.1 → 9.4 → 5.43 → 3.58 → 2.9 mm was investigated, see [6] for details. The entry temperature to the finishing mill was 1010°C and the rolling velocity in the last stand was 5 m/s. The innovative route for the multiphase steel strips, which assumes ultra-fast cooling (UFC) after stands 4 and 5, was simulated. In consequence, rolling in the stands 5 and 6 was below the recrystallization temperature. Typical results for these two passes are shown in Figure 1. The distributions of the dislocation density and the grain size at the temperature A_{e3} were used as an input data for simulations of phase transformations.

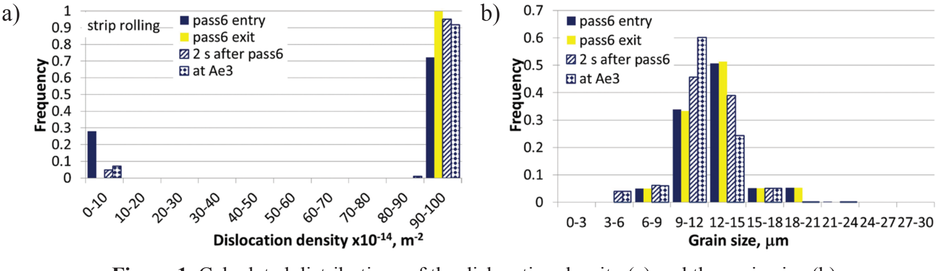

Figure 1. Calculated distributions of the dislocation density (a) and the grain size (b) at various stages of the process.

A typical system of laminar cooling after hot rolling [8] was considered as an example of a practical application of the model. The system is composed of two sections each divided into 4 zones. Cooling conditions, which compose water fluxes and corresponding heat transfer coefficients, are given in [8]. Rolling velocity, strip thickness and entry temperature, as well as histograms of the grain size and the dislocation density (Figure 1) at the beginning of phase transformations, were an input data for the simulations. The optimal cooling sequence, which should give 42% of ferrite, 44% of bainite and 14% of martensite for the strip thickness 2.9 mm, strip velocity 5 m/s and average grain size 15 μm, was considered. The effect of the dislocation density on the phase transformations was accounted for following the data published in [9]. Beyond the grain size, a stochastic character of the temperatures was accounted for. This was done in a qualitative manner only. Due to a lack of the large data set necessary for the statistical analysis, a Gauss distribution of the entry temperature with the standard deviation of 12°C was assumed on the basis of measurements in one of the hot strip mills. Time-temperature profile during cooling for the optimal cooling conditions was calculated by the FE program. The stochastic model predicted distributions (histograms) of such parameters as volume fractions of phases and size of ferrite grains. Selected result of calculations for the volume fractions is shown in Figure 2.

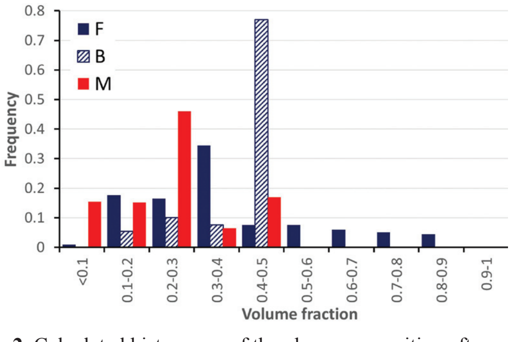

Figure 2. Calculated histograms of the phase composition after cooling.

It is seen that the heterogeneity of the microstructure prior to transformations and uncertainty of the temperatures result in heterogeneity of the phase composition. Although the volume fraction of the bainite is reasonably stable, the fractions of the ferrite and the martensite are more sensitive to variations of the parameters. On the basis of all simulations it was concluded that: i) Heterogeneity of the dislocation density and the grain size results in the heterogeneity of the phase composition in the final product. When the cooling rate increases, the heterogeneity of the microstructure increases; ii) Increase of the dislocation density prior to phase transformations accelerates ferritic transformation. In consequence, the volume fractions of bainite and martensite are lower. This effect is stronger for larger cooling rates; iii) In simulations we assumed stochastic character of the temperatures during cooling. It allowed to show the capability of the model to account for the uncertainty of the boundary conditions. Large number of the temperate measurements, which will allow statistical analysis of the data, is necessary for the reliable prediction of the uncertainty of the simulations.

In the presented solution deterministic model of phase transformations was used. Randomness was introduced in the solution by a stochastic character of the input data and the boundary conditions. Accounting for the stochastic character of the nucleation of the new phase during phase transformations should improve the reliability of the solution, what will be an objective of our future works.

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