Multiscale model of dynamic recrystallization in hot rolling

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ABSTRACT: The paper is focused on development of multi-scale CAFE approach, which combines cellular automata (CA) and finite element (FE) methods. The CA model of dynamic recrystallization (DRX) was implemented into the thermal-mechanical FE code, which simulates rolling process using steady state Eulerian approach. Several CA spaces were created at the cross section of the sample and their state was calculated using changes of the external variables along the flow lines. Current local values of temperature, strain, strain rate and stress are calculated by the macro-scale FE model and then passed to micro-scale CA simulations. Improvements in analysing of average grain size in CA simulation were introduced. The CAFE calculations were performed for hot rolling of the carbon-manganese steel. The resulting grain sizes after the process were compared with the experimental data, achieving satisfactory consistency.

Key words: Dynamic recrystallization, Hot rolling, Multiscale model, Cellular automata, CAFE

1 INTRODUCTION

The work is focused on development of the model, which allows connection between phenomena occurring in materials in various scales. Multiscale CAFE approach, which combines cellular automata (CA) and finite element (FE) methods, is used. In this approach FE method describes material in the macro scale, while CA method simulates micro and mezo scale phenomena. In consequence, the models operating at different scales contribute to the local evolution of microstructure. Earlier research proved qualitatively exceptional predictive capabilities of the CAFE method in modelling strain localization [1] and dynamic recrystallization (DRX) [2]. In this paper, the effort was made to improve the transition rules, which were developed in [2], and which describe the state of the material at the micro scale. The second aim of the study is to assess the capabilities of the model in qualitative prediction of microstructure development during DRX. It was done by comparison of the CAFE model predictions with the experimental data for hot rolling in the laboratory mill.

2 MODEL

2.1 Finite element solution

The FE program developed by the authors and based on rigid-plastic thermomechanical solution is used. Details of the model are given in [3] and are not repeated here. Flow stress is the material parameter in this model and can be calculated by the CA model.

2.2 CAFE model

The CA model accounts for the evolution of microstructure and dislocation density. The 2D CA lattice with neighbourhood described in [2] and with periodic boundary conditions is used. The lattice of cells represents the image of microstructure and reproduces topological relations between grains. The state of each cell is described by four state variables: 1) local dislocation density ρ, 2) orientation ϕ, 3) distance variable x that controls migration of GB, 4) assignment to a grain. The grains in the model are represented by instances of *Distant Neighbourhoods*

(DN), as described in [2].
The increment of average dislocation density is calculated at grain level, separately for every grain, using differential equation [4]:

$$\frac{d\rho_{gr}}{dt} = k_1 \frac{\dot{\varepsilon}}{bl} - k_2 \dot{\varepsilon}^m \exp\left(\frac{Q_s}{RT}\right)\rho_{gr} \quad (1)$$

where t – time, ρ_{gr} – average dislocation density in a grain, b – Burgers vector, l - mean free path of dislocation, $\dot{\varepsilon}$ - strain rate, Q_s - activation energy of self-diffusion, T – temperature, R – gas constant, k_1, k_2, m - parameters. It is assumed in the model that for the small recrystallized grains, the mean free path of dislocations is comparable with grain size, calculated according to the formula:

$$D = 2\sqrt{\frac{n_{gr} S_c}{\pi}} \quad (2)$$

where D - substitute grain size, S_c – area of CA cell, n_{gr} – number of CA cells belonging to the grain.
The solution of equation (1) is done using Runge-Kutta (RK4) method. The average dislocation density calculated in previous time step is used as an initial condition for the following step. Non-uniform distribution of dislocation density is imposed by nondeterministic algorithm controlling the incremental updates of ρ variable in the CA cells. It should be noted, however, that all interactions between the cells remain local, i.e. there is no global data required for the updating algorithm.
The structure of the transition rules is decisive for the CA method. These rules enable simulation of nucleation and subsequent grain growth. Despite the rules itself are deterministic, the result of their application is not deterministic, due to quasi-random neighbourhood definition and dislocation density distribution within the CA lattice. The rule describing the nucleation of new grains is based on critical dislocation density criterion. The nucleus appears if the cell is located at the GB and the dislocation density in the cell reaches critical value ρ_c, given by the following equation [5]:

$$\rho_c = \left(\frac{20\gamma\dot{\varepsilon}}{3blM\tau^2}\right)^{1/3} \quad (3)$$

where γ - GB energy, M – GB mobility, τ - average energy of dislocation line.
Due to nonuniform distribution of dislocation density within grains, the value of ρ at the GB is also nonuniform. Thus, it is possible to select the subset of the sites in the CA lattice, in which the nuclei appear. Such formulation requires neither calculation of the nucleation probability nor nucleation rate, which seems to be an advantage in comparison to the previously published approaches, e.g. [6]. The current model allows the nuclei to appear rather due to actual process conditions than due to premise on the a priori known nucleation rate. However, as it will be indicated in the further part of article, this is an obstacle in interpreting the average grain size, particularly in conditions of fast nucleation of new grains.
Once the CA cell is selected as a nucleus, the dislocation density in the cell is set to ρ_{DRX}. The random orientation is assigned to newly created grain. Since each grain is identified with a distant neighbourhood, new DN is also created and the list of grains is updated.
The further growth of recrystallized grains is described by the second rule, which is based on the GB velocity, which depends on the GB mobility M and on the driving force for growth F:

$$v = \alpha M F \quad (4)$$

where α is the scaling factor. The GB mobility is related to misorientation angle θ [7] combined with temperature dependence [8] describing mobility of high angle GB:

$$M = M_0 \exp\left(\frac{-Q}{kT}\right)\left[1 - \exp\left(-B\frac{\theta}{\theta_m}\right)^n\right] \quad (5)$$

where M_0 – pre-exponential factor, Q - activation enthalpy for GB motion, k – Boltzmann constant, T – temperature, θ_m - misorientation angle, θ_m - misorientation angle for high angle GB, B, n – coefficients. GB energy γ is calculated from the Read–Shockley equation [8]:

$$\gamma = \gamma_m \frac{\theta}{\theta_m}\left(1 - \ln\frac{\theta}{\theta_m}\right) \quad (7)$$

where γ_m - GB energy for high misorientation θ_m.
The relationship describing driving force for grain growth is similar to those used in [6]. The main part of driving force is connected with difference of dislocation density between the current CA cell belonging to the recrystallized grain and the i^{th} neighbouring cell belonging to the deformed matrix:

$$F_i = \pi D^2 \tau\left(\rho_i - \rho\right) - 4\pi D\gamma_i \quad (8)$$

Total driving force in the cell is the average of F_i. The substitute grain size D is calculated from equation (2). The increment of the distance variable x is evaluated from the GB velocity:

$$\Delta x = \frac{v\Delta t}{\sqrt{S}} \tag{9}$$

where Δt - length of the time step, S – area of the 2D CA cell. The distance variable is updated by Δx using threshold function, which ensures $0 \le x \le 1$. The average and the largest Δx are used for estimation of the time step during CA simulation.

The model predicts both the average grain size and distribution of grain size. The list of DN is analyzed regarding the grain size. As a result the frequency of occurrence is calculated for every class of size. However, the difficulty in the interpretation arises from the formulation of nucleation criterion, which implies the fast nucleation of new grains in consecutive time steps. Even though only the small fraction of these nuclei are successful and grow, the total number of grains in CA lattice increases. Thus, the calculated average grain size decreases substantially faster than it is observed experimentally. In order to limit the influence of this factor, the smallest grains of size comparable to single CA cell are neglected in calculation of average grain size.

The CA model was implemented into the FE code. The idea of the current CAFE model for the DRX is shown in figure 1. Several CA spaces are created at the cross section of the rolled sample and their state is calculated using changes of the external variables along the flow lines. In consequence, the local development of individual microstructure components is computed through models operating at different scales. The current, local values of temperature, strain, strain rate and stress are calculated by the macro-scale finite element model. Nucleation of new grains and GB motion, which are fundamental for the recrystallization model, are calculated at the micro scale by the CA model.

3 EXPERIMENT

The material was carbon-manganese steel containing 0.142%C, 0.29%Si, 0.50%Mn, <0.002%S, 0.008%P, 3.10%Ni, 0.98%Cr, 0.28%Mo, 0.04%Cu. Hot rolling was performed on the two-high rolling mill. Main parameters of the experiment are given in Table 1. The samples were preheated in the furnace at the test temperature for 15 min, rolled and quenched immediately after rolling. Microstructure at the cross section of the samples after rolling was investigated using light microscopy. Both average grain size and distribution of grain size were measured.

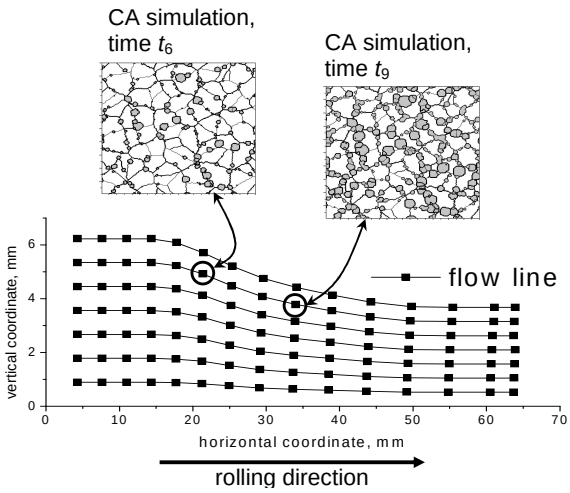

Fig. 1. The idea of the CAFE model – local values of macroscopic thermal and mechanical parameters are passed to micro-scale CA model predicting evolution of microstructure

Table1. Parameters of the experiments

Parameter	Values
sample	17.8x25.4x100 mm
roll diameter	200 mm
temperatures	950°C, 1150°C
roll velocities	35 rpm

4 RESULTS

The initial image of microstructure, which is a starting point for CA calculations, was generated using CA algorithm of a normal grain growth. It enables various distributions of size and orientation of the grains in the CA lattice. The lattice size was 200x200 cells. In order to ensure that digital representation of microstructure conforms the measured grain size, the area of each cell was selected 1.68×10^{-12} m^2 for $T = 950^oC$ and 1.16×10^{-11} m^2 for $T = 1150^oC$. Initial time step for CA simulation was chosen 2×10^{-3} s. The parameters of CA model were determined using optimization technique [9] aimed at minimization of differences between experiment and results of computations.

The result of CAFE calculations performed for $T = 950^oC$ is shown in figure 2. The measured grain size at the centre of sample after the rolling was 12 μm, which is in good agreement with the model. As it can be expected, the DRX process occurs the most

rapidly in the upper region of the sample, due to highest local values of $\dot{\varepsilon}$ and ε.

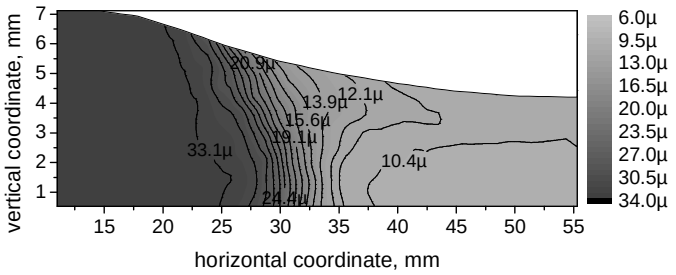

Fig. 2. Distribution of average grain size [m] at the cross section of the rolled sample calculated by CAFE model for T = 950°C;

The results for T = 1150°C are shown in figure 3. Distribution of grain size at the cross-section of the sample is presented in figure 3a. A satisfactory qualitative agreement between CAFE prediction and result of measurement (29μm) is observed.

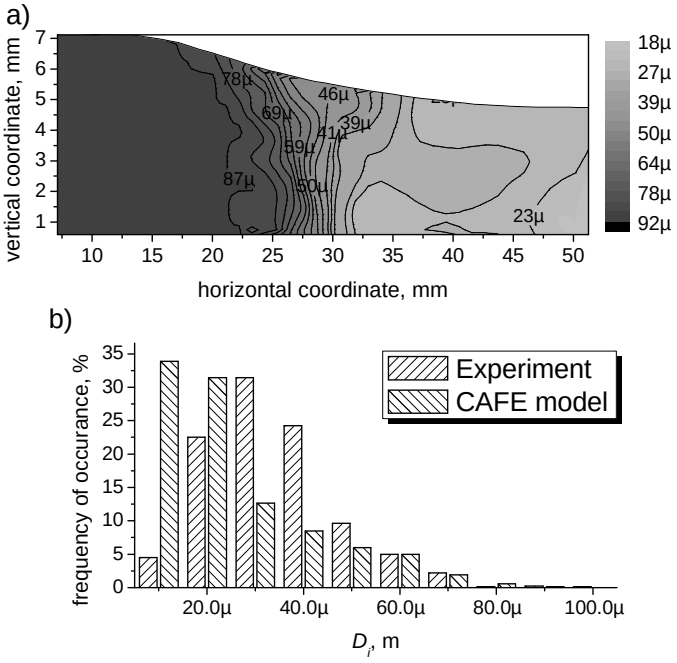

Fig. 3. Results of CAFE model, T = 1150 °C: a) distribution of average grain size [m] at the cross section of the rolled sample, b) comparison of grain size distribution calculated by CAFE model and measured at the centre of the sample.

The model is capable of classifying the grains according to its size at the given points in the sample. The comparison of measured distribution of grain size at the centre of deformed sample and corresponding result of CAFE model are shown in figure 3b. There are differences observed for almost every class of size, the most remarkably for very small grains. Nevertheless, the very small nuclei are possibly not revealed by light microscopy, so it turns out that the reason of this discrepancy is ambiguous.

5 CONCLUSIONS

The CAFE model accounting for DRX was applied to hot rolling process. The model is capable to predict distribution of grain size at the cross-section of the sample. In this work the grains of size comparable with a single CA cell, which are not revealed by light microscopy due to limited resolution of the method, were neglected in calculation of average grain size. As a result, the discrepancies between experiment and calculation were reduced.

It is proved that applying CAFE model to simulation of hot rolling supplies new quality of information regarding microstructure. Beyond this, feedback from the CA to the FE allows to account for the microstructure in the flow stress model. An increase of the computing time, about 150% comparing to the conventional model, is the drawback of the method.

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