Simulation of Microstructure Evolution during Shape Rolling with the Use of Frontal Cellular Automata

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The objective of the paper is an application of the model of the microstructure evolution based on three-dimensional cellular automata (CA) for hot shape rolling simulation. A short description of frontal cellular automata (FCA) is presented. The model contains two parts: the deformation and the microstructure evolution. The CA cells do not remain as undistorted cubes, but they are deformed according to the strain tensor. The independence of the grain growing from the shape and the sizes of the cell is ensured by the so-called “virtual front tracking”. The microstructural part of the model simulates two phenomena: the nucleation and the growth of nuclei. There are three issues considered in the paper: the creation of the initial microstructure, the recrystallization and the phase transformation. When recrystallization is simulated, the nucleation and the grain boundary migration depend on the deformation parameters such as: the temperature, the strain, the strain rate, the dislocation density and the crystallographic orientation. The nucleation during the phase transformation is a function of the cooling rate and the final microstructure. These phenomena along with the deformation can be modeled over a wide range of multi-stage deformation processes. The process of shape rolling is chosen as an example. The data needed for the FCA calculations is received from the modeling by the finite element method. The results of the simulation of the microstructure evolution, during the last three passes of the round bars rolling with the consequent phase transformation, are presented in the paper.

KEY WORDS: cellular automata; microstructure; recrystallization; deformation; shape rolling.

1. Introduction

The prediction of the microstructure is one of the most important problems in materials science. There are different methods that are used for the modeling of the microstructure evolution, and among of them are the cellular automata (CA) models,¹⁾ Monte Carlo Potts models,²⁾ the finite element method (FEM) based models,³⁾ the phase field models,^{4,5)} the front tracking method^{6,7)} and the vertex models.⁸⁾ The application of the CA models, for the simulation of the different phenomena in the materials, has been significantly increased these days. The microstructure evolution is clearly a three-dimensional (3D) problem and the results obtained by the two-dimensional (2D) CA cannot always be directly transferred to a real 3D process. That is why the 3D CA has to be used in the up-to-date simulations. One of the 3D CA modifications, known as the frontal CA (FCA),⁹⁾ capable to accelerate calculations, is used for the simulation of the microstructure evolution in the paper.

The simulation of a separate phenomenon or a stage of technological processes can be carried out in the frame of simple CA models. The simulation of the same sequences of technological stages requires the combination of CA with other numerical methods, such as the finite element method, the finite differences, the discrete element method etc. The joint methods based on CA and FEM improve the accuracy

of the coupled phenomena simulation during the forming processes, and they are utilized in the paper. The problem of deformation is usually neglected during the CA modeling. Some phenomena, for example the static recrystallization, can be simulated within the space of the undistorted cells. However, the cell distortion during the modeling of the dynamic recrystallization or the multi-stage deformation cannot be neglected. The process requires the use of the deformed structure for the further modeling.

The objective of the present paper is a development of such an FCA based model which takes into account the real deformation and simulates such phenomena as the creation of the initial microstructure, the recrystallization and the phase transformation.

An example of the simulation of the microstructure evolution during the rolling of the round bars in the last three passes is also presented in the paper.

2. General Model

The accurate modeling of the microstructure evolution during the forming processes is a complex task which relies on the choice of the appropriate methods. The choice is dependent on the intended effect, the accuracy, the computation costs and so on. The cellular automata are recognized as one of the most optimal tools for the microstructure mod-

eling, in view of the computation costs and the achievable results. They can be used for the microstructure evolution simulation, both as an all-sufficient tool and in connection with other methods. In the first case, the simulations are limited by the theoretical studies for the set of deformation conditions or for the process whose parameters can be easily calculated analytically.¹⁰⁾ The use of CA combined with other methods makes it possible to obtain more accurate and more reliable results. Often, CA are jointed with the finite differences (FDM) or the finite element method (FEM). FEM is known as one of the best methods for the modeling of forming processes. The schemes of the mutual use of CA and FEM, according to their role in the model, can be divided into two groups. The first one contains a solution in which the simulations are carried out independently, without feedback. The systems with the co-operation of both components can be included in the second group. One component is primary; another is secondary, as served to deliver the parameters and variables for the proper calculations by the primary method. CA can be secondary, only provided that it is of a simple structure and does not require high calculation costs, such as the memory and calculation time. CA used for the microstructure evolution simulations, especially the tree-dimensional ones, cannot be applied as the secondary method in view of the computational requirements. Thus, CA play the primary role in the theoretical researches on uneven deformation at the level of crystals or the properties of polycrystalline structures.

The variant of independent simulations by FEM and CA, without tough feedback, is selected. The forming process is modeled by FEM in the macro-scale; the results of the FEM simulation are used by CA for the microstructure modeling in the micro-scale. It is so-called the post-processing for the obtaining of the information on the microstructure. An arbitrary FEM code or the literature data can be used in such a strategy. It is enough to meet the requirements for the coincident conditions for both methods and data for interface.

The simulation of the microstructure evolution can be conducted for arbitrary points (for which the appropriate data is available) in an arbitrary forming process, on the basis of the calculation by an arbitrary FEM code. In the paper, the shape rolling of the round bars is chosen for the presentation of the possibilities of the model based on FCA. The rolling process was simulated by Milenin with the use of his own FEM code.¹¹⁾ The simulation results were the basis for the further calculations by FCA, presented below. Because CA allows for more accurate accounting of some behaviors, for example stress-strain relations, it should be back to FEM simulation or serve for correction such relations used in FEM.

The general model of the microstructure evolution during the forming processes is based on FCA and covers such aspects of the microstructure evolution as the creation of the initial microstructure, the deformation, the recrystallization and the phase transformation. The aspects are presented below in the following sections.

2.1. The FCA Model

The use of the frontal cellular automata instead of the conventional ones makes it possible to reduce the computation time significantly, especially for the three-dimensional

models, as the significant regions are excluded from the calculations in the current time step and only the front of the changes is studied. The principles of FCA, presented in detail elsewhere,⁹⁾ are shortly reviewed here.

The base for CA is chosen as the cell c , which can be described as a set of parameters. These parameters are the following: the position p in the space, the state q and others. The definition of an automaton of the cell M consists of a set of the states Q , the alphabet Σ , the transition rules δ , the initial Q_{in} , the final Q_f states of the automaton, and can be described as $M = (Q, \Sigma, \delta, Q_{in}, Q_f)$. The cell automaton M is presented schematically in Fig. 1.

The set of the states $Q = \{q_0, q_1, q_2, q_3, q_4\}$ comprises the initial matrix state q_0 , the “frontal cell” q_1 , the “boundary cell” q_2 , the “cell inside the grain” q_3 and the transient state q_4 . The initial state can be either $Q_{in} = \{q_0\}$ for the creation of the initial microstructure, or $Q_{in} = \{q_2, q_3\}$ for other algorithms. The final state is always $Q_f = \{q_2, q_3\}$; although, if some stages of the process are not complete, the states q_0 , q_1 and q_4 can be presented in the final structure.

The cellular alphabet contains “letters” $\Sigma = \{I_0 - I_4\}$, which are treated as the conditions for the transition. Then, the transition rules δ define the current q_i , the next q_{i+1} states and the letter I_k (transition condition). Such rules δ are commonly presented either in a form of a table or by description. Shortly, the letters are of the following meanings: I_0 is the nucleation, I_1 – the time delay, I_2 and I_3 determine whether the cells are on the boundary or inside the grain and I_4 means that the mobile grain boundary reaches the current cell and involves it in the growing process.

The “language” of CA consists of some “words”, which contain several letters and mean a cell transition from the initial to the final state, for example the words $(I_0 \vee I_4)I_1(I_2 \vee I_3)$ with the initial state q_0 are responsible for the creation of the initial microstructure.

The automaton is characterized by a closed circuit of the states: $\dots q_1(q_2 \vee q_3)q_4\dots$. The states q_2 and q_3 can not only be the final states, but also the initial states for the next cycle of the modeling, and the states can be repeated for several times. This property is useful for the modeling of some processes. For example, both the nucleation and the growth of recrystallized grains are the permanent phenomena during the dynamic recrystallization and the automaton of the cell can complete several full cycles (example of such simulation presented elsewhere).⁹⁾ Another application of the model shown in the present paper is the multistage deformation with the static recrystallization, in the pauses between the rolling passes. Process with dynamic recrystallization is not

Fig. 1. Cellular automaton M (q – states, I – transition conditions).

considered in the paper.

The periodic boundary condition is mainly used for the modeling of the microstructure. In such a case, the top of the space is connected to the bottom, and also the left side is connected with the right side. The combination of the periodic and the open boundary conditions is used in the present model.

Different kinds of neighborhood are used for different parts of CA. For instance, the Moore neighborhood is used in the algorithm of the boundary motion during the simulation of the grains growth (state q_1 and condition I_4), while the unmovable grain boundaries are defined through von Neumann neighborhood (states q_2, q_3 and condition I_2, I_3).

FCA works with a varied time step, which is defined by the minimal time for passing the front through the cell. The FCA described above can be used for the simulation of the static and dynamic recrystallization, the phase transformation and the solidification.¹²⁾ Some examples of the initial microstructure and the dynamic recrystallization obtained by FCA can be found elsewhere.⁹⁾

2.2. The Deformation

The structure after the deformation demonstrates different images at the three perpendicular cross-sections. Hence, the 3D CA should be applied for the modeling of the microstructure evolution in the forming processes. The consideration of the real deformation in CA is the problem that is usually avoided. When the static recrystallization is modeled, the deformed structure can be presented in the space of the undistorted cells. Yet, when the dynamic recrystallization is considered, or the multi-stage deformation is modeled, the cell distortion cannot be neglected. The deformed structure can be used in the further modeling. Some principles of the deformation consideration in CA are described elsewhere,⁹⁾ and they also are explained below, in this section. Some results for the dynamic recrystallization can be found.^{9,10)} According to the main principle, the sizes and the shape of the cells do not remain constant. They change according to the strain tensor.

The algorithm of the consideration of the deformation is based on the idea presented by Rappaz and Gandin,¹³⁾ Beltran-Sanchez and Stefanescu¹⁴⁾ and Burbelko^{15,16)} *et al.* It is so called the “virtual front tracking”. There are two elements very important in this approach. The first one is the determination of the growing direction, and the second one is the calculation of the time required for the passing through the cell.

There are two algorithms used for the determination of the growing direction. If there is no deformation, the direction is determined by the location of the initial point (where the nucleon appears) for the spheres or ellipsoid, or by the orientation of the sides of the cubes, octahedrons or other crystals shapes. The deformation introduces some rotation for the surfaces of the growing grains and the algorithm loses its accuracy. Another algorithm calculates the direction locally, in consideration with the history of the deformation. The principle of the calculations, which can be called the increment method, is presented in Fig. 2. If the front of the changes has completely passed the cell, its color is charcoal grey; if incompletely – it is light grey; and if it has not reached the cell, it is white. Then the vector determining the

Fig. 2. Calculation of the growing direction by the increment method.

Fig. 3. Scheme to calculation of the projection of the cell on the growing direction: a – cuboid cell, b – deformed cell, c – arbitrary shape of the cell (non-uniform deformation).

growing direction for the new cell $\mathbf{r}_b$ is the sum of the vector for the previous cell $\mathbf{r}_p$ and the vector from the previous cell to the new one $\mathbf{r}_{bp}$: $\mathbf{r}_b = \mathbf{r}_p + \mathbf{r}_{bp}$. If the cellular space is undistorted, the algorithm gives the same results as the previous one, but when the shape and sizes of the cells are changed along with the deformation, in each calculation step, the results will be different.

The second part of the “virtual front tracking” algorithm presented in Fig. 3 is described below. Actually, the time needed for the front passing is calculated on the basis of the

projection L of the cell on the growing direction $\mathbf{r}$ and the grain boundary migration rate v :

$$t = \frac{L}{v} \dots\dots\dots (1)$$

There are three cases of calculation of the projection L used in the model. The first one is applied when cellular space remains undeformed (for example, during creation of initial microstructure). Then cells are cubes or cuboids. A cell-cuboid with edge lengths a_x , a_y and a_z is shown in Fig. 3(a). Some vertices of cuboid (A , B , C and D) and their projection (A' , B' , C' and D') on the growing direction $\mathbf{r}$ are marked. $\mathbf{r}$ is unit vector of the vector $\mathbf{r}_b$ determined before: $\mathbf{r} = \mathbf{r}_b / \|\mathbf{r}_b\| = (r_x, r_y, r_z)$. Then cell projection L (Fig. 3(a)) is a sum of projections of three edges of the cuboid and it is of the following form:

$$L = A'D' = A'B' + B'C' + C'D' \\ = |\overline{AB} \cdot \mathbf{r}| + |\overline{BC} \cdot \mathbf{r}| + |\overline{CD} \cdot \mathbf{r}| = a_x |r_x| + a_y |r_y| + a_z |r_z| \dots\dots (2)$$

Every projection is absolute value of dot product of $\mathbf{r}$ and appropriate edge.

The second algorithm is used when uniform deformation is applied and cellular space is small enough. Then the cell-cuboid transforms into parallelepiped cell. Deformed cell is presented in Fig. 3(b). For the cells, having the same initial shape and sizes as before, the projection L equals:

$$L = A'D' = A'B' + B'C' + C'D' = |\overline{AB} \cdot \mathbf{r}| + |\overline{BC} \cdot \mathbf{r}| + |\overline{CD} \cdot \mathbf{r}| \\ = \left| (1 + \varepsilon_x) a_x r_x + \frac{\gamma_{yx}}{2} a_y r_y + \frac{\gamma_{zx}}{2} a_z r_z \right| \\ + \left| \frac{\gamma_{xy}}{2} a_x r_x + (1 + \varepsilon_y) a_y r_y + \frac{\gamma_{zy}}{2} a_z r_z \right| \\ + \left| \frac{\gamma_{xz}}{2} a_x r_x + \frac{\gamma_{yz}}{2} a_y r_y + (1 + \varepsilon_z) a_z r_z \right| \dots\dots\dots (3)$$

where ε , γ – the components of the strain tensor. When all components of the tensor equal to 0, Eq. (3) degenerates to the previous expression (2). But if no deformation, (2) should be used in view of amount of computation. The second algorithm is mainly used in simulation that results are presented in the next sections of the paper.

The third algorithm is used for non-uniform deformation, when difference in deformation conditions on the opposite boundaries of the cellular space cannot be neglected. Then, cellular space becomes of arbitrary shape, as well as every cell. If strain tensor is used in the second algorithm, relative displacement of the vertices of initial cuboid cellular space should be calculated here. If before cuboids or parallelepipeds have three basic lengths and orientation of the edges and there is no difference to calculate the projection which parallel the edge of the four to choose from, now every twelve edges can have different length and orientation and it is a priori unknown which edges should be selected. Deformed cell is shown in Fig. 3(c). Some vertices of hexahedron and their projections are marked as in previous figures. There are two vector from the origin $0 = (0, 0, 0)$ to cell vertices A and D ($\overline{0A}$, $\overline{0D}$) shown in figure for example, as well as their projections ($\overline{0'A'}$, $\overline{0'D'}$) on the growing

direction. The projection length are calculated for each vertex as dot product appropriate vectors and unit vector of the growing direction (for example: $\overline{0A'} = \overline{0A} \cdot \mathbf{r}$) taking into account a sign. Then the projection L of the cell on the growing direction is length between the extreme points (A' and D'), i.e. difference between maximal and minimal length of all projections:

$$L = \max(\overline{0A'}, \overline{0B'}, \dots) - \min(\overline{0A'}, \overline{0B'}, \dots) \dots\dots (4)$$

The calculated time t is the basis for the time delay realized in every cell automaton through the transient state q_4 . It allows for the reduction of the original cellular space anisotropy, making it almost isotropic, for the control shape of the growing grains and its orientation in the space. The grain boundary migration rate (velocity) v is independent of the sizes of the cell, but the time of the transition of the boundary through the cell depends on the cell sizes and the growing direction. Besides, the delay allows for the introduction of the dependence of the grain boundary migration rate v on the growing direction and other process parameters, such as the temperature, the dislocation density, the disorientation angle and others.

2.3. Creation of Initial Microstructure

According to the scheme in Fig. 1, the words $(I_0 \vee I_4)I_1(I_2 \vee I_3)$ with the initial state q_0 and the final ones q_2 and q_3 are responsible for the creation of the initial structure. The transient state q_4 introduces the delay t (1). It defines the grain growth rate, which can be an arbitrary function of the growing direction, dependent on shape of growing grains.

In Fig. 4, two examples of the initial microstructure are shown. The first example of the calculations (Fig. 4(a)) is a thready structure, obtained when the growing grains are of an elongated cylindrical shape. Another example presented in Fig. 4(b) was created by the spherical grains. The last microstructure is used in the following calculations. Other examples of the initial microstructure can be found elsewhere.⁹⁾

Fig. 4. Initial structures obtained by FCA: a – elongated cylindrical grains (cubical cells), b – spherical grains (parallelepiped cells).

2.4. Recrystallization

The history of simulation of recrystallization has begun with publication Hesselbarth and Göbel.¹⁷⁾ Then Davies¹⁾ has considered influence of nucleation and growth of nuclei on recrystallization. Ding and Guo¹⁸⁾ simulated joint problem of dynamic recrystallization and flow stress calculation on the base of modeling of dislocation evolution. Reviews of cellular automata in materials science were published by Raabe¹⁹⁾ in 2002 and by Janssens²⁰⁾ in 2010. Mukhopadhyay *et al.*²¹⁾ simulated static recrystallization accounting different types of nucleation with consideration of dislocation density, temperature and misorientation on the mobility of a grain boundary.

In presented FCA the words $(I_0 \vee I_4)I_1(I_2 \vee I_3)$ (Fig. 1) with the initial states q_2 and q_3 describe the recrystallization. The FCA operates in the same way as during the creation of the initial microstructure, but uses different initial states, condition of nucleation and growth of recrystallized grains. The initial structure is created on the basis of the requirements for the microstructure; it determines the number of the grains, the nucleation conditions and the shape of the growing grains, but these parameters do not connect with any real process parameters; they are not important for the algorithm. The algorithm of recrystallization must be performed quite otherwise. Actually, there are two elements responsible for the appropriate modelling of the recrystallization. They are the nucleation (the condition for I_0) and the grain boundary migration rate (state q_4 and condition I_1).

Thus, the model of recrystallization realized in FCA consists of two parts; they are the nucleation and the growth of recrystallized grains. They work in cooperation with the dislocation model. The microstructure evolution depends on the nucleation rate and the grain boundary migration rate. The main assumptions of the model can be summarized as the following:⁹⁾

(1) The initial dislocation density of all the grains is the same and it equals the minimal value for the current thermal condition;

(2) The dislocation density ρ increases according to the dislocation theory equation. The equation takes into account both the hardening (U) and the softening (Ω): $\frac{d\rho}{d\varepsilon} = U - \Omega\rho$,

where ε is the strain;

(3) The nucleation process in the grain begins when the dislocation density in the grain reaches the critical value ρ_c ;

(4) Nuclei appear only on the grain boundaries and only during the deformation. The nucleation rate depends on the strain ε , strain rate $\dot{\varepsilon}$, temperature T and initial average grain size d_0 ;

(5) The initial dislocation density of the new grains equals the minimal value for the current thermal condition;

(6) The dislocation density of all the cells belonging to the same grain is the same, *i.e.* the dislocation density is the property of the grain themselves, not the cells;

(7) The grain boundary migration rate v is the function of the temperature T , dislocation density ρ , crystallographic orientation and others.

The models of the dislocation density, nucleation and growth of recrystallized grains are described in detail elsewhere.^{22,23)} Here, they are presented shortly.

The following model of the dislocation density is applied

for all grains. It takes into account the strain rate $\dot{\varepsilon}$, the temperature T and the dislocation density ρ , according to the following equation:

$$\dot{\rho} = a_{\rho 1} \dot{\varepsilon}^{n_{\rho 1}} \exp\left(\frac{Q_{\rho 1}}{RT}\right) - a_{\rho 2} \dot{\varepsilon}^{n_{\rho 2}} \rho^{m_{\rho}} \exp\left(\frac{Q_{\rho 2}}{RT}\right), \dots (5)$$

where R – the gas constant, $a_{\rho 1}$, $a_{\rho 2}$, $n_{\rho 1}$, $n_{\rho 2}$, m_{ρ} – the material constant, $Q_{\rho 1}$ and $Q_{\rho 2}$ – the activation energies.

The dislocation density is used for the calculation of the moment when the recrystallization begins, as well as for the calculation of the flow stress and the grain boundary migration rate. The critical value of the dislocation density for the nucleation initialization is of the following form (Roberts and B. Ahlstrom):²⁴⁾

$$\rho_c = \frac{8\gamma}{\tau l} = \sqrt[3]{\frac{20\gamma\dot{\varepsilon}}{3blM\tau^2}}, \dots (6)$$

The other application of the dislocation density in FCA is the flow stress calculation, according to equations:

$$\sigma_s = \sigma_0 + \alpha\mu b(\rho_{av})^{1/2}, \dots (7)$$

$$\sigma_0 = a_{\sigma} \dot{\varepsilon}^{n_{\sigma}} \exp\left(\frac{Q_{\sigma}}{RT}\right), \dots (8)$$

where σ_0 – the stress necessary to move the dislocation in the absence of the other dislocations, α – the constant, μ – the shear modulus, b – the Burgers vector and ρ_{av} – the average dislocation density, a_{σ} , n_{σ} and Q_{σ} – the appropriate material coefficients.

The equation describing the nucleation is of the following form:

$$\dot{N}_V = \dot{N}_{Vsrx} \left(1 - \frac{N_V}{N_{Vmd}}\right), \dots (9)$$

where $\dot{N}_{Vsrx}$ – the maximal nucleation rate corresponding to the nucleation rate during the static recrystallization, N_V – the current number of the grains, N_{Vmd} – the maximal number of the grains at the existing condition of deformation. $\dot{N}_{Vsrx}$ and N_{Vmd} determine nucleation condition. The model of nucleation is described in detail in papers.^{22,23)} The model was developed for simulation of nucleation during both dynamic and static recrystallization. The differential Eq. (9) contains two elements: $\dot{N}_{Vsrx}$ determines nucleation during the static recrystallization and N_{Vmd} , which determines number of new recrystallized grains during the dynamic recrystallization. One more element of the model is a transfer of new grains in the category of old grains; it allows for multi-stages dynamic recrystallization.

The grain boundary migration rate depends on driving force of recrystallization p and grain boundary mobility m : $v = m p$. The difference of the dislocation density of the new and old grains is the driving force and calculated on the basis of stored dislocation energy: $p = 0.5 \mu b^2 \rho$. The misorientation angle is taken into account as well. The grain boundary mobility m depends on the self-diffusion coefficient and therefore, it is defined by Arrhenius' law:

$$m = a_{Dsrx} \exp\left(\frac{Q_{Dsrx}}{RT}\right), \dots (10)$$

where a_{Dsrx} , Q_{Dsrx} – the material constants.

2.5. Phase Transformation

After the rolling and cooling, the phase transformation austenite-ferrite begins. The same words as for the previous cases, *i.e.* $(I_0 \vee I_4)I_1(I_2 \vee I_3)$, are responsible for the transformation in FCA. The initial states of the cell can be arbitrary, because the last cycle of recrystallization can not be completed, the cell can be in any possible state. The process of the phase transformation is considered as the nucleation and the growth of ferrite grains, as well. The process can be modeled with tacking into account the thermal condition, which effects on nucleation rate and growth rate of ferrite grains. Instead of that the process is considered with nucleation before grain growth. Then, nucleation or the number of the ferrite grains N_f depends mainly on the cooling rate $\dot{C}$ and the surface of the grain boundaries S . Instead of the surface of the grain boundaries, the austenite grain size D_a and the accumulated strain ε_{ret} can be introduced:

$$N_f = a_f \dot{C}^{1/2} S = \frac{1}{(1.4 + 5\dot{C}^{-1/2} + 22(1 - \exp(-0.015D_a))) \left(1 - 0.45 * (\varepsilon_{ret})^{1/2}\right)}, \quad (11)$$

As the real transformation kinetics is not the point of interest of the study, as opposed to the final results, the grain boundary migration rate is set arbitrary. Only the dependence on the disorientation angle between the paternal austenite grains and the child ferrite grains is introduced. This dependence is different from the analogous one for the recrystallization. During the recrystallization, growth is possible, when the misorientation angle of neighbouring grains is high enough, while during the phase transformation, the orientation of new ferrite grain must be the same. As a result, during the recrystallization, a new grain grows mainly in the grains other than parental, and during the phase transformation, it grows into the parental grain only.

Table 1. Rolling pass schedule.

Shape of grooves	Sizes, mm	Rolling speed, m/s	Inter-pass time, s
round	45.6 × 45.6	2.94	1.43
oval	50.4 × 35.0	3.46	1.21
round	38.5 × 38.5	3.99	1.5

Fig. 5. Points location for microstructure simulation.

3. Shape Rolling

In the present paper, the hot shape rolling process is chosen for the microstructure simulation by FCA. Multistage deformation with the static recrystallization in the pauses between the rolling passes is considered. The calculations are carried out for the continuous mill. The rolling process is simulated by the FEM code.¹¹⁾ The rolling pass schedule for the last three passes is presented in **Table 1**. The initial temperature is 900 and 1 000°C, after the cooling in the air during 1 s (for more realistic initial temperature distribution), oval bar enters into the first rolls. After the last pass bar is cooled in the air during 1.5 s. The first simulated pass is schematically presented in **Fig. 5**. The gray oval is the cross-section of the bar in the entrance to the rolls, which contours with the grooves are shown by the lines. There are three points marked 0, 1 and 2 in Fig. 5, which are chosen to simulate the microstructure evolution. Simulations are carried out on the basis of such parameters as the time, the temperature and the strain rate tensor, obtained by the FEM calculations. IF steel is chosen as the modeled material.

The FEM modeling of the rolling process was fulfilled by Milenin.¹¹⁾ Because results of FEM simulations is not main aim of the paper, only some examples are presented here, other results can be found elsewhere.^{25,26)} An efficiency of the used FEM code has been proved in²⁵⁾ by comparison with Forge3. The temperature changes for the three simulated points 0, 1, and 2 are presented in **Fig. 6**. There is the effect of cooling in contact with the rolls, the air cooling and the deformation heat on the temperature seen in the Fig. 6. An alternate of the horizontal and vertical rolls causes the alternative temperature to drop in contact with the tools. Another example²⁶⁾ (**Fig. 7**) pre-

Fig. 6. Temperature for three simulated points.

Fig. 7. Distribution of effective strain in the last pass.²⁶⁾

sents distribution of effective strain in the last pass. Shape of the bar before and after rolling as well as mesh is seen in Fig. 7. The results of the FEM calculations have been saved in the file for the further use in FCA simulation. The time, temperature and strain rate tensor in the data file are needed for the simulation by FCA. The other parameters and variables, according to (5) – (10), required for the simulation, are calculated on the basis of these data.

4. Simulation Results

The same initial microstructure (Fig. 4(b)) was used for all the simulated points. The initial FCA space contains $500 \times$

500×500 cells, with initial representative volume of $280 \times 320 \times 560 \mu\text{m}^3$ with 300 grains. It gives the initial average grain size of about $52 \mu\text{m}$. Volume of the cellular space during the whole simulation remains constant.

The simulation results (Figs. 8–14) are presented as drawings on the hexahedron's faces (Figs. 8–10, 13, 14) and as graphs showing the changes of the grain size and the flow stress (Figs. 11, 12). Litter “a” by Figs. 8–10 is correspondent to point 0, “b” – point 1, “c” – point 2. There are three time-moments for all the three points at the initial temperature of 900°C , chosen in the first set of pictures (Figs. 8–10), which are those after the first pass (Fig. 8), before the second pass (Fig. 9), and after the last (third) pass and the cool-

Fig. 8. Microstructure after the first pass; a – point 0, b – point 1, c – point 2.

Fig. 9. Microstructure before the second pass; a – point 0, b – point 1, c – point 2.

ing during the 1.5 s (Fig. 10). The deformation conditions for the three points are different and they have effect not only on the shape of the cells and the whole cellular space, but also on the shape and sizes of the grains after the deformation, as well as after the recrystallization. Because the second algorithm (Fig. 3(b)) accounting uniform deformation was applied, shape of the cells can be cuboid or parallelepiped and cellular space repeats the cells shape in larger scale. For the central point (point 0) lying in the center of symmetry of cross-section, the shear components of the strain rate equal to 0. For the other two points (1 and 2) lying in the axis of symmetry, the shear components remain

Fig. 10. Microstructure after the third pass and cooling during 1.5 s; a – point 0, b – point 1, c – point 2.

small enough, but slight deviation from the cuboid shape can be noted in Figs. 8(c), 9(c), 10(c) for the point 2. Deformation effects mainly on the sizes of cuboids (parallelepipeds). Deformation conditions are not conducive to the emergence of the dynamic recrystallization; static recrystallization appears in pauses only. The material that contacts with the tool is subject to the higher cooling, and it assists in the formation of a finer microstructure (Figs. 9(c), 10(b), 10(c)).

The conditions affect the nucleation rate as well as the grain boundary migration rate. After the first pass, a different effect of the deformation can mainly be seen, though the new small grains demonstrate some differences in their sizes for the points. The recrystallization process during the deformation begins (Fig. 8), continues during the time between the passes and completes before the next deformation (Fig. 9). It is a full static recrystallization. After the recrystallization, different grain sizes for the three points are visible in Fig. 9. The same results can be seen after all the passes. An example of such a structure after the last pass and the cooling is presented in Fig. 10.

The changes of the average grain size are calculated during the whole process in the representative points. The average grain size can be calculated as a cube root of a ratio of

Fig. 11. Average grain size: a, b, c – temperature 900°C, d – temperature 1 000°C; a, d – point 0, b – point 1, c – point 2.

Fig. 12. Flow stress during the deformation: a, b, c – temperature 900°C, d – temperature 1 000°C; a, d – point 0, b – point 1, c – point 2.

the representative volume, which is constant, to a number of the grains with a coefficient. However, another approach is applied in the paper, in which the average grain size is considered to be proportional to the ratio of the representative volume to the entire area of the surface of all the grains:

$$D \propto \frac{V}{S} = \frac{V}{(S_1 n_1 + S_2 n_2)}, \dots\dots\dots (12)$$

where V – the volume of the cellular space, μm^3 ; S – the surface area of the all the grains, μm^2 ; n_1 and n_2 – the number of the cells in state q_1 and q_2 ; S_1 and S_2 – the average boundary surfaces of the cells, μm^2 . There are several factors causing some difficulties, which influence the accuracy of the grain size calculations by FCA. They are connected with the discretization of the cellular space. The real elemental area S of the surface is less than the discrete one (S_1, S_2). The area of one cell's faces (S_1 and S_2) is not equal to the others and does not remain constant during the simulation (due to the deformation). The whole area or the surface of the single cell face is not counted, and neither is the number of the faces, as opposed to the number of the cells on the grain boundaries. Thus, the cells in the two states are counted. They are the frontal cell q_1 (n_1) and the boundary cell q_2 (n_2). However, they are determined by different neighborhoods. What is more, the frontal cells are one-sided, but the immobile boundaries are two-sided *i.e.* formed by the cells twice. The introduction of the appropriate coefficients (S_1, S_2) does not, however, allow to confirm the accuracy of the calculations being better than 10%. Nevertheless, such calculations demonstrate the changes of the average grain size, not only qualitatively, but also quantitatively, describing the microstructure evolution.

Along with the temperature increase in the point 0, the average grain size after the recrystallization rises (Fig. 11, d). The grains in the other representative points after the three passes become smaller. The analysis points to the temperature having the most influence on the grain size in the presented model. The final grain sizes after the rolling, with the initial temperature of 900°C for the point 0, 1 and 2 are 34.6 , 34.5 and $21.6\mu\text{m}$, respectively.

The flow stress, which is calculated as described above, in section 2.4, is studied, as well. The flow stress is presented as a function of the strain (Fig. 12). During the deformation, one can see the curves for the three points almost cover each other, despite a different temperature. It can be explained

by the lower strain rate accompanying the lower temperature.

Because simulations FEM and CA are almost independent, it is very important that mechanical behaviors of the material during the deformation were the same in both cases. That is why it was used the model^{22,23)} based on internal variable, which is compatible for both FEM code and CA simulation. Eqs. (5)–(8) are used in both cases, only recrystallization is taking into account in some different way. Because dynamic recrystallization does not begin, stress-strain relations in both simulations remain the same. Only several coefficients responsible for kinetics of static recrystallization have required adjustments in the FEM code.

The final microstructure in the point 0 after the last pass and the cooling during the 1.5 s at the initial temperature of 1000°C is presented in Fig. 13. It is clearly more coarse, in

Fig. 13. Final microstructure for rolling at temperature of 1000°C .

Fig. 14. Microstructure of ferrite grains in austenite after the phase transformation with different cooling rate a) $\dot{C} = 0.5$, b) $\dot{C} = 1.0$ and c) $\dot{C} = 3.0$ K/s.

comparison with the previous variant of calculations for the same point (Fig. 10(a)). These microstructures were subjected to the austenite-ferrite transformation.

After the rolling, the bars can be cooled with a different rate. The microstructure before (Fig. 13) and after the phase transformation (Fig. 14) with a different cooling rate (0.5, 1.0 and 3.0 K/s) is presented. The number of the ferrite grains is calculated according to (11). The average grain size is

computed as follows: $D = \sqrt[3]{\frac{6}{\pi} V_{av}} = \sqrt[3]{\frac{6}{\pi} \frac{V}{n}}$, where V_{av} – the

average grain volume, V – the volume of the cellular space, n – the effective number of the grains.

The average grain sizes of the austenite after the rolling at the temperature 1000°C is about 72 μm. The numbers of the ferrite grains after the transformation are 7876, 10446 and 14386. It gives the ferrite size of 23.0, 20.9 and 18.8 μm, respectively. The average numbers of the ferrite grains appearing in the austenite grain are 30.7, 40.7 and 56.0.

The average grain sizes of the austenite after the rolling at the temperature 900°C is about 35 μm. The numbers of the ferrite grains after the transformation are 18022, 26324 and 41006. It gives the ferrite size of 17.5, 15.4 and 13.3 μm, respectively. The average numbers of the ferrite grains appearing in the austenite grain are 8.0, 11.8 and 18.3.

5. Conclusions

The developed three-dimensional FCA model is discussed in the paper. In the model, the CA space, the shape and the sizes of the cells do not remain constant. Instead, they change according to the real deformation.

The frontal CA model is adapted to the simulation of the microstructure evolution during the multi-stage deformation process. The deformation, the recrystallization and the phase transformation are considered for the three passes of the shape rolling and the following cooling. The temperature and the strain rate calculated by FEM are used as the basis for the FCA simulation. The microstructure, the average grain size and the kinetics of the recrystallization can be predicted by the model.

The presented results favored the conclusion that the FCA model can be applied for the simulation of the microstructure evolution during the multi-stage deformation.

Further research will be focused on the validation of the microstructural and mechanical parameter of the cellular automata.

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