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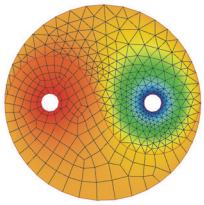

MODELING OF MICROSTRUCTURE EVOLUTION DURING THE ROLLING BY USING CELLULAR AUTOMATA

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Abstract

Prediction of microstructure evolution and properties is one of the most significant problems in materials science. The developed model contains two parts: the deformation and the microstructure. Usually, the deformation is not taken into account during the simulation by the cellular automata (CA). In the model, while strain accumulated in material is not large enough, CA cells are deforming according to the deformation, they are changing their shape and sizes. When strain reaches a preset value, CA space is reorganized to obtain the cubical shape of the cells. The microstructural part calculates the recrystallization and grains growth after the recrystallization. The model of recrystallization process includes two stages: nucleation and new grain growth. Nucleation and grain growth rate are dependent on deformation parameters such as: temperature, strain, strain rate, dislocation density and crystallographic orientation.

In the paper a description of a three-dimensional frontal CA is presented. The use of frontal cellular automata instead of conventional ones makes possible to reduce the computation time. Frontal CA model is adapted to the simulation of microstructure evolution during the flat rolling. Rolling pass schedule is used as a basis for modeling. Selected results of simulations with frontal 3D cellular automata are presented in the paper.

Key words: cellular automata, microstructure, deformation, recrystallization, rolling

1. INTRODUCTION

Prediction of microstructure evolution and properties is one of the most significant problems in materials science. Several advanced methods of analysis can be applied for this issue: vertex models [1], phase field models [2], Monte Carlo Potts [3], finite element method (FEM) [4] and cellular automata (CA) [5]. Recently an interest to applying the cellular automata for the simulation of different phenomena in materials is arising constantly. The cellular automation is used for modeling of crystallization (solidification) [6, 7], dynamic and static recrystallization [8-10], phase transformation [10], cracks propagation [11], micro-shear band and shear band propagation [12] etc. The main asset of the CA is ability for a close correlation of the microstructure with the mechanical properties in micro- and meso-scale simulation. Joining CA with the FEM undoubtedly improve accuracy of modeling of coupled phenomena during the forming processes in both micro- and macro-scale. Models for simulation of the recrystallization based on the CA are developed and recently used prevailing in two-dimensional (2D) version [13-15]. Though, three-dimensional (3D) models are also available [16]. Models based on the 2D CA are the simpler and faster, have less elements and connections, use less complicated algorithms, are simpler for design, implementation, more useful for visualization. Some problems, such as accounting of a crystallographic orientation of the grains or curvature of grains boundaries, which have

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been solved in the 2D CA, are still unsolved in the 3D CA. Microstructure evolution is pointedly theedimensional and results obtained by the 2D CA not always can be transferred to a real 3D process directly.

The objective of the paper is a development of the model of microstructure evolution during the technology with the multi-stages deformation. Then, model contains two parts: the deformation and the microstructure. In the model, the deformation is taken into account during the simulation by the CA, though usually, in the other models based on CA, it is not. The recrystallization part of the model includes two stages: nucleation and new grain growth. CA model is adapted to the simulation of microstructure evolution during the flat rolling. Selected results of simulations with frontal 3D cellular automata are presented in the last section of the paper.

2. DEFORMATION AND SPACE REORGANIZATION

Consideration of the real deformation in the CA is a problem, which is usually avoided. It is very difficult to find this topic in the publications. When static recrystallization is modeled, deformed structure can be presented in the space of undistorted cells. But when dynamic recrystallization is considered, or multi-stages deformation is modeled, cells distortion cannot be neglected. Deformed structure can be used in the further modeling. Structure after deformation demonstrates different images in three perpendicular cross-sections. That is why threedimensional CA must be applied for modeling of microstructure development including static and dynamic recrystallization. Principles of reckoning of the deformation in CA are described in [17]. Some results for dynamic recrystallization can be found in [18, 19]. Nuclei appear and new grains grow in current structure, which changes during whole deformation process. Presented model CA begin calculations with cubical cell. Then, shape of all cells is changing according to deformation while the process is proceeding. Grain growth rate is independent of the sizes of the cells, but time of the boundary movement through the cell depends on cell sizes and direction of the movement. In the present paper, hot flat rolling process is chosen for modeling. It simplifies deformation conditions and plane strain state can be applied.

In the model, while strain accumulated in material is not large enough, CA cells are deforming according to the real deformation, they are changing their shape and sizes. When strain reaches a preset value, CA space is reorganized to obtain the cubical shape of the cells. There are two variants of the reorganization possible in the model. They can be chosen manually.

The first variant is applied when deformation is accompanied with the microstructure refinement. Then, after the deformation and inter-pass time, before the next deformation, ratios of the modeled block (or cells) sizes are tested. If either ratio becomes more then two, all space is halved. The first half is remained and each cell in it is halved as well. The second half is removed from the model. That operation decreases the space and can be used if it does not lead to significant decreasing of number of the grains from cut to cut. Because periodic boundary condition is used for the more real modeling of the microstructure evolution, the halving must be taken into account. Actually, the halving in the space with periodic boundary condition means two cuts. Then, we receive two opposite sides, which cannot be connected, because they have no coincident microstructure. As a result, open boundary conditions must be applied temporarily on these sides. They are not permanent conditions but transient. Then those conditions evolve into partly-open, partly-periodic condition, and finally into the purely periodic conditions. Algorithm of such evolution is next. All grains on the both sides of the space are permanently considered as ones having open boundary condition, and can grow only inside the space. On the opposite side they cannot appear. But every other grain, which exists in the current structure or appears after the cutting, can grow not only inside space, but also outside with its appearance on the opposite side. This way boundary conditions depend on the properties of the grains, not the space.

The second variant is more complex, and can be used when volume of the space cannot be reduced. As in the first variant, after the side ratio reaches preset value (2 to 4), space is halved, but then they put together, one on the other. Such procedure supposes four cuttings and at least two bondings. If the sides are known a priori to be cut and bonded, the boundary conditions can be organized before modeling. Otherwise, at first, the modeling is carried out with the periodic conditions up to the halving, and then, the modeling is repeated with reorganized boundary conditions. For the halving and bonding, conditions must be following. For the short sides the simple periodic conditions and for the long sides the periodic conditions with displacement are used. Dis-

placement equal to a half of the space length (it is constant, measured in the number of cells). After the cutting and bonding on the former long side we obtain simple periodic conditions, and on the former short side periodic conditions with displacement. Example of this procedure is shown in figure 1. Because of that procedure can be repeated, appropriate conditions must evolve into simple periodic or periodic conditions with displacement, as it is described above for the first variant. Shape of the cells also changes. They are combined by the long sides and then are divided. Cells belonged to the different grains are combined in consideration with neighboring cells.

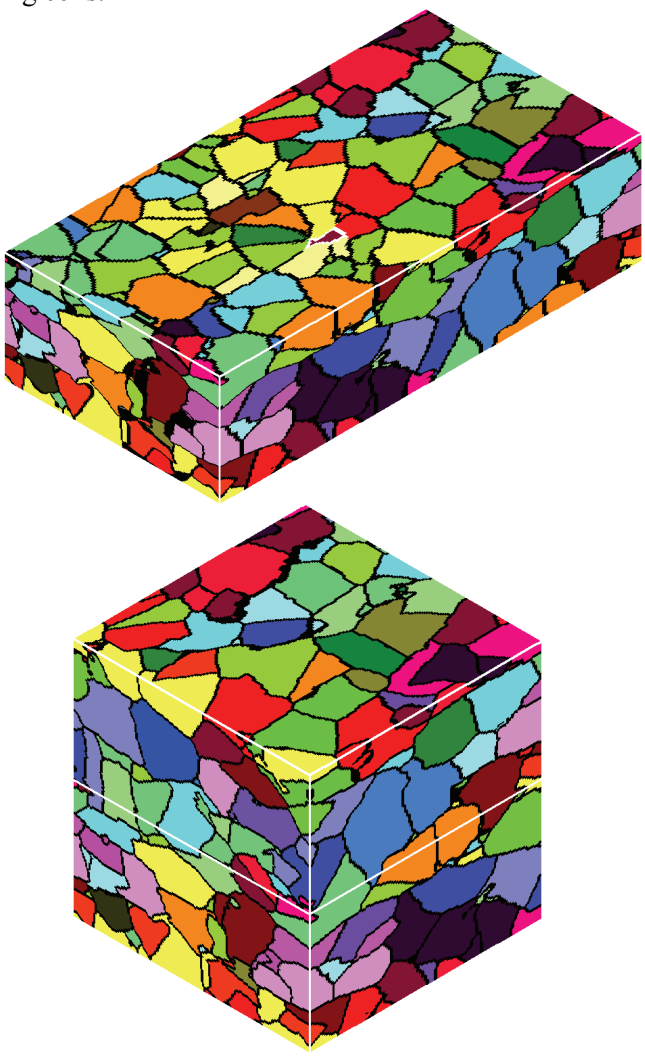

Fig. 1. *Example of cutting and bonding.*

3. FRONTAL CELLULAR AUTOMATA

The base of cellular automaton is a cell c, which can be described as a set of parameters. These parameters are position p in space, state q and others, which effect on its state or state of the neighboring cells $c = (p,q,\ldots)$. A model S based on cellular automaton designed for modeling of physical phenomena in materials can be described as following: $S = (C,N,M,G,L)$, where: C – space of the cells, N – definition of neighborhood, M – automaton of a cell, G – grains list, L –lists of the cells in the same state. A definition of the cellular automaton M consists of the set of the states Q, alphabet Σ, transition rules δ, initial Q_{in} and final Q_f states of the automaton: $M = (Q, \Sigma,\delta,Q_{in},Q_f)$.

For the modeling of the microstructure and the recrystallization is mainly used a periodic boundary condition, when the top of the space is connected with the bottom as well as the left side is connected with the right side. In presented model, a combination of the periodic and open boundary conditions is described in previous section.

For different part of the CA are used different kinds of neighborhood. In the algorithm of boundary motion during grain growth, Moore neighborhood is used. Unmovable grain boundaries are defined through von Neumann neighborhood.

In the classic CA, their behavior is based on the transition rules, which can be formulated as following. State of the cell in the next iteration depends on its current state and the current state of the cells in its neighborhood. Thus, in the classic CA, presumption of the study every cell and its neighborhood is established. It leads to necessity of the scanning whole space of cells and whole neighborhood of each cell. Let's consider cells, which are in stationary conditions. Here, stationary conditions for a cell mean that the cell and the neighboring cells do not change their state in the current iteration. Then, in the next iteration, that cell does not change its state, as well. If cell is known to be in stationary condition, it can be excluded from the study on the current iteration. Thus, for the study, cells in non-stationary condition remain only. A change of the cell state is used as indicator of non-stationary condition for whole neighborhood. It is a main idea of the frontal cellular automata. In the frontal CA, direction of information flow is changed, as well. While in the classic CA, the cells all time collect information about the state from the whole neighborhood; in the frontal ones the cell sends information to its neighborhood when it changes its state only. As a result, significant regions are excluded from the calculations and the front of the changes is studied only. The use of frontal cellular automata instead of conventional ones makes possible to reduce the computation time significantly, especially for three-dimensional models.

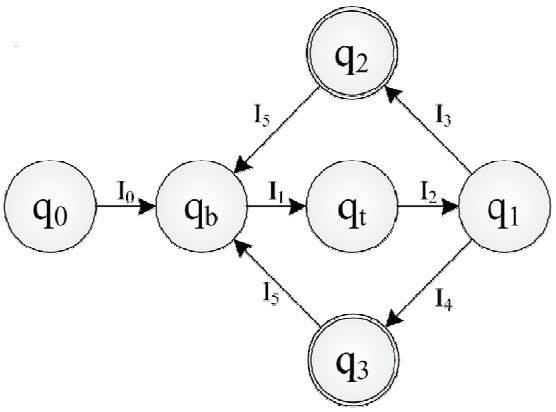

Fig. 2. *Cellular automaton M.*

Cellular automaton M used in the project is schematically presented in figure 2. Set of states $Q = \{q_0, q_1, q_2, q_3, q_b, q_t\}$ comprises initial matrix state q_0, "frontal cell" q_1, "cell on the boundary" q_2, "cell inside grain" q_3, buffer q_b and transition q_t states. The description of the model can be found in [18, 19]. Application of the presented model to the hot flat rolling is described in the next sections.

4. NUCLEATION AND GRAIN GROWTH

The model of the recrystallization consists of two stages: nucleation and new grain growth. Nucleation (figure 2) is correspondent to the transition of the cell from the state q_0 (creation of initial structure) or q_2 (recrystallization) into the states q_b, q_t and q_1 consequently. When cell reaches state q_1 its influence extends on the neighborhood. Then, neighboring cells in the state of q_2 or q_3 are involved into the process of changes – it is a grain growth process. Meanwhile, the current cell transits into the state of rest (q_2 or q_3) and remains in it until the next cycle of recrystallization begins.

Nucleation and grain growth rate are dependent on deformation parameters such as: temperature, strain, strain rate, dislocation density and crystallographic orientation. The equation describing the nucleation is of the following form:

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

where $\dot{N}_{Vsrx}$ – a maximal nucleation rate, $m^{-3}s^{-1}$, N_V – a current number of new grains, m^{-3}, N_{Vmd} – a maximal number of the grains at existing condition of the deformation, m^{-3}.

The maximal nucleation rate $\dot{N}_{Vsrx}$ is of the following form:

$$\dot{N}_{Vsrx} = a_{Nsrx}\varepsilon_{ef}^{l}\dot{\varepsilon}^{k} \tag{2}$$

where a_{Nsrx}, k, l – material constants.

The maximal number of the grains at the existing condition of the deformation N_{Vmd}, which appears in equation (1), determines a number of the grains after the whole metadynamic recrystallization following the whole dynamic recrystallization. Then, the number of grains N_{Vmd} is calculated using the equation:

$$N_{Vmd} = a_{Nmd}\dot{\varepsilon}^{n_N}\exp\left(\frac{Q_{Nmd}}{RT}\right), \tag{3}$$

where a_{Nmd}, n_N, Q_{Nmd} – material constants.

The maximal grain growth rate $\dot{D}_{srx}$ [m/s] plays an important role in the model of the microstructure evolution, it depends on the self-diffusion coefficient and therefore it is defined by an analogous expression:

$$\dot{D}_{srx} = a_{Dsrx}\exp\left(\frac{Q_{Dsrx}}{RT}\right), \tag{4}$$

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

In the present model new grains can appear during deformation only. Grain growth begins during the deformation and then lasts after the deformation.

5. THE ROLLING

The frontal CA model is adapted to the simulation of microstructure evolution during the flat rolling. The calculations are carried out for reverse mill with work rolls of 1000 mm diameter. The plate to be simulated is milled to 40.0 mm thickness and 10 m length. Rolling speed is 5 m/s. Time pauses between passes is 2.3 s. Rolling pass schedule (table 1), contained information about temperature, reduction, inter-pass time and so on, is used as a basis for modeling.

For each pass, program calculates redaction, strain, strain rate, length and time of rolling. Sizes of the cells before and after the pass are calculated in order to determine a time increment and a number of iteration during the rolling. For that, the grain growth rate is calculated according to (4). The nucleation is calculated during the deformation only. In the model the minimal number of the iteration for nucleation is established on the level of 10, as well as 10 is the minimal number of iteration for the time delay in state q_t (figure 2). Temperature is assumed to be constant during the deformation, as well as strain rate. Number of new grains calculated by the

Table 1. *Rolling schedule*

Pass number	Entrance thickness h_0, mm	Exit thickness h_1, mm	Temperature T, °C	Inter-pass time, s	Reduction r, %	Strain rate $\dot{\varepsilon}$, s^{-1}
1	40.00	27.18	1098	5.24	32	90.6
2	27.18	18.55	1087	6.6	31.7	90.1
3	18.55	12.75	1061	8.7	31.3	89.4
4	12.75	8.95	1010	11.2	29.8	87.3
5	8.95	6.49	928	14.6	27.5	83.6
6	6.49	5.00	825	5.0	22.9	76.1

end of iteration is used for the nucleation as an increment between current number and its number after the previous iteration.

After the deformation grain growth is simulated without the nucleation. Temperature changes are linearly approximated from pass to pass. Whole inter-pass time is a sum of the pauses between passes and time of the rolling calculated on the basis of length of the plate and the rolling speed. After the last pass material is cooled with the cooling rate of 10°C/s during the time of 5 s.

6. CA SIMULATION

Material constants are set for IF steel. Initial average grain size is 120 μm. Initial CA space is 200x200x200 cells or a cube with the side of 0.5 mm. Initial microstructure is presented in figure 3. Axis x is a rolling direction, y is lateral direction, z is an axis along the thickness of the plate. Size y of the CA space remains constant, x is elongated and z is reduced. Forty five colours are chosen for representation of crystallographic orientation. Grain boundaries are black; boundaries of the new growing grain are white.

Next figures 4-6 demonstrate some results of the simulation of the microstructure development. Complete recrystallization after the passes, except the two last, is observed as a consequence of relatively high temperature in the first passes and long inter-pass time. Before the last pass (figure 5), white boundaries of growing grains mean that recrystallization is not finished. After the last pass and cooling, as a result of low temperature and high cooling rate, recrystallization is stopped at the every beginning. Only a few little new grains can be seen in figure 6. Grain size is calculated according to: $D = c\sqrt[3]{V/N_g}$, where V – representative volume, m^3, N_g – number of grains, c – geometrical factor.

There are results of three variants, which differ by initial grain size (185 or 230 μm) or by grain growth rate, presented in figure 7. Flow stress is shown as a function of strain and time. The first one (figure 7a) allows to observe changes of the strain in the each pass; meanwhile dependence on time shows kinetics of recrystallization (figure 7b). Last graph (figure 7c) demonstrates changes of grain size D, which is calculated according to equation: $D = kV/N_b$, where V – representative volume, m^3, N_b – number of boundary cells, k – coefficient, m^{-2}. Stress arises from pass to pass because of temperature decrease. Due to high strain rate there are static recrystallization observed only. Interpass time increases, as well as time of recrystallization.

Fig. 3. *Initial structure on the planes 0XY, 0XZ and 0YZ respectively, average grain size D = 120 μm. Representative volume V = 0.125 mm³.*

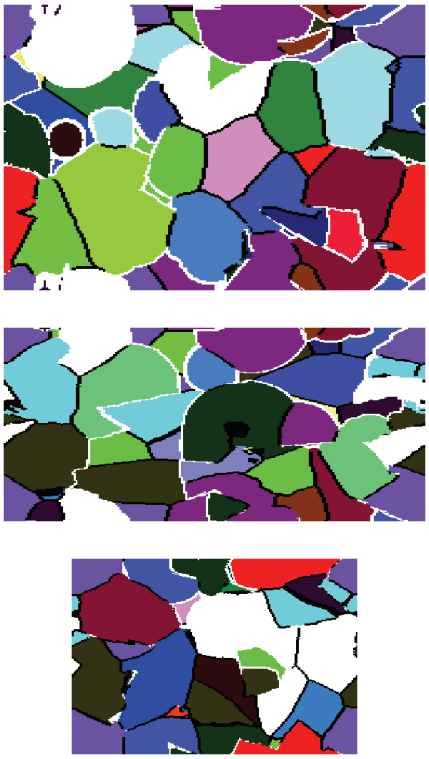

Fig. 4. *Microstructure before the 2nd pass, average grain size D = 116 μm. V = 0.125 mm³.*

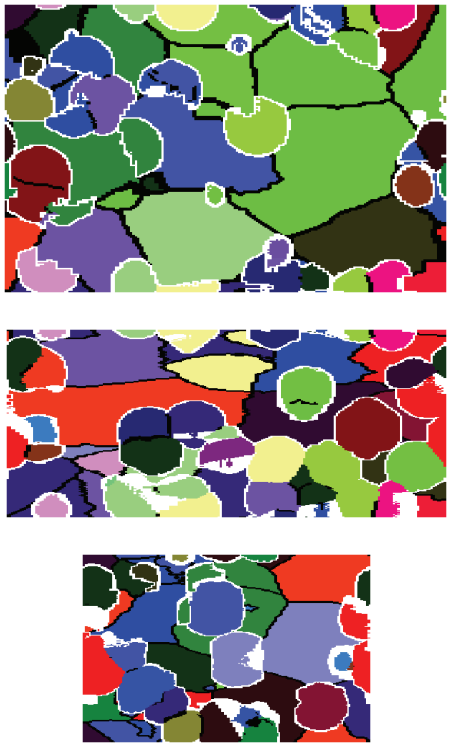

Fig. 5. *Microstructure before the 6th pass, average grain size D = 27 μm. V = 0.00195 mm³.*

After the first four passes static recrystallization is completed and then after the fifth pass grain growth is severely decelerated and material is recrystallized partly. After deformation, it is possible to simulate phase transformation. There are two variants of cooling presented on figure 8. Low cooling rate allows to obtain usual ferrite structure (figure 8b), while high cooling rate leads to lamellar structure (figure 8c).

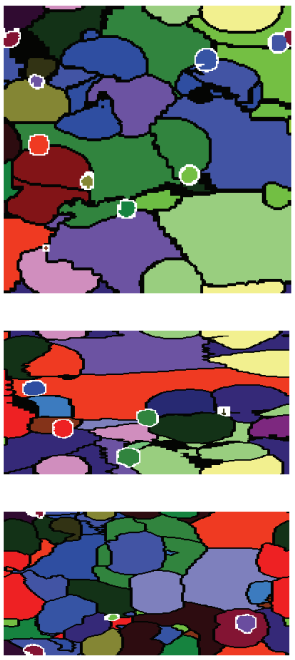

Fig. 6. *Microstructure after the cooling, average grain size D = 18 μm. V = 0.00098 mm³.*

CONCLUSSION

In the paper a description of a three-dimensional frontal CA is presented. The use of the frontal cellular automata instead of conventional ones makes possible to reduce the computation time. The frontal CA model is adapted to the simulation of microstructure evolution during the flat rolling. Rolling pass schedule is used as a basis for modeling. Selected results of the simulations with the frontal 3D cellular automata presented in the paper demonstrate possibility of the developed model.

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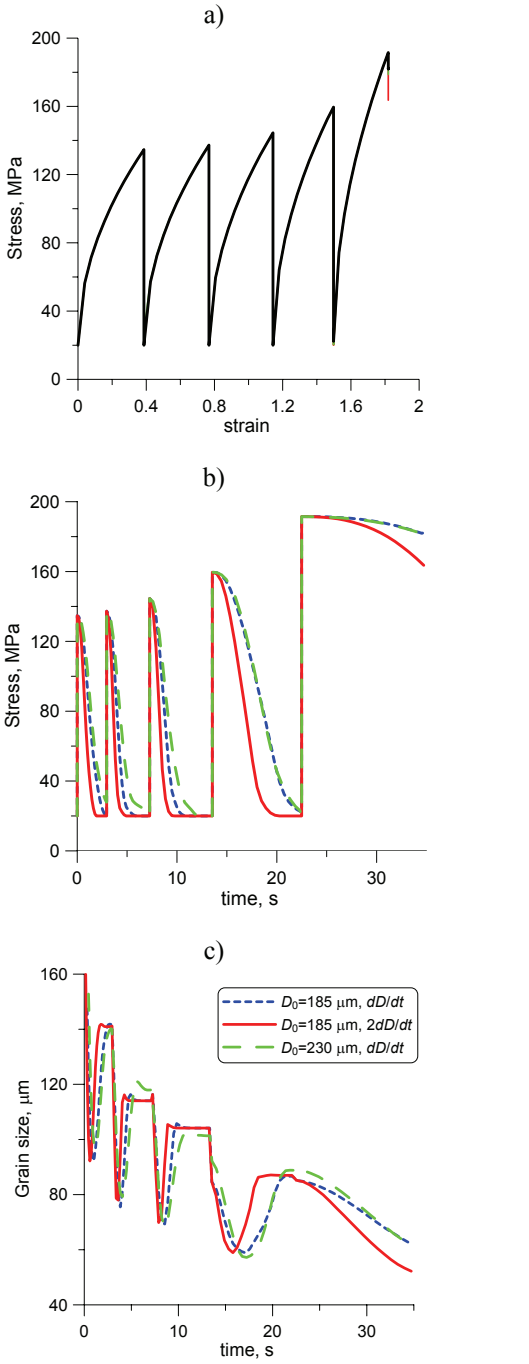

Fig. 7. *Flow stress (a, b) and average grain size (c) during the rolling.*

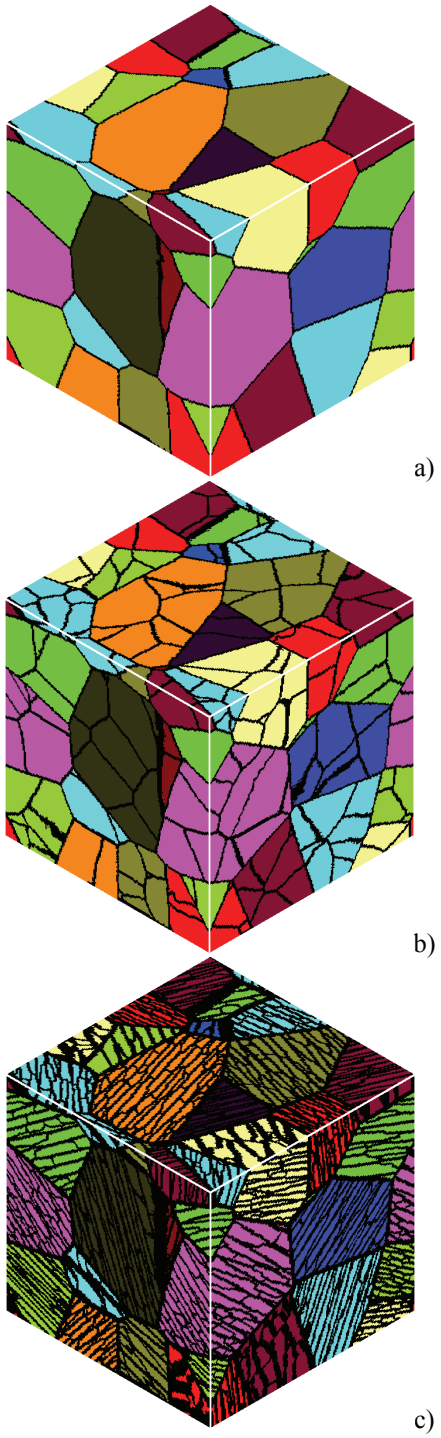

Fig. 8. *Microstructure: a) before phase transformation; b), c) after transformation with low (b) and high (c) cooling rate.*

REFERENCES

1. Weygand, D., Brechet,Y., Lepinoux, J., 2001, A Vertex Simulation of Grain Growth in 2D and 3D, Adv. Eng. Mater., 3, 67-71.
2. Fan, D., Chen, L.Q., 1997, Computer simulation of grain growth using a continuum field model, Acta Mat., 44, 611-622.
3. Holm, E.A., Hassold, G.N., Miodownik, M.A., 2001, On misorientation distribution evolution during anisotropic grain growth, Acta Mat., 49, 2981-2991.
4. Bernacki, M., Chastel, Y., Digonnet, H., Resk, H., Coupez, T., Loge, R.E., 2007, Development of numerical tools for the multiscale modeling of recrystallization in metals, based on a digital material framework, Comp. Meth. Mat. Sci., 7, 142-149.
5. Davies, C.H.J., 1997, Growth of Nuclei in a Cellular Automation Simulation of Recrystallization, Scr. Mater., 36, 35-40.
6. Rappaz, M., Gandin, C.-A., 1993, Probabilistic Modelling of Microstructure Formation in Solidification Processes, Acta Metal. Mater., 41, 345-360.
7. Raabe, D., 2004, Mesoscale simulation of spherulite growth during polymer crystallization by use of a cellular automaton, Acta Mater., 52, 2653-2664.

8. Hurley, P.J., Humphreys, F.J., 2003, Modelling the Recrystallization of Single-Phase Aluminium, Acta mater., 51, 3779-3793.
9. Qian, M., Guo, Z.X., 2004, Cellular Automata Simulation of Microstructural Evolution during Dynamic Recrystallization of an HY-100 Steel, Mater. Sci. Eng. A, A365, 180-185.
10. Kumar, M., Sasikumar, R., Kesavan Nair, P., 1998, Competition between nucleation and early growth of ferrite from austenite – studies using cellular automation simulations, Acta Mater., 46, 6291-6303.
11. Das, S., Palmiere, E.J., Howard, I.C., 2002, CAFE: a Tool for Modeling Thermomechanical Processes, Proc. Thermomech. Processing: Mechanics, Microstructure & Control, eds. Palmiere, E.J., Mahfouf, M., Pinna, C., Sheffield, 296-301.
12. Makarov, P.V., Romanova, V.A., 2000, Mesoscale plastic flow generation and development for polycrystals, Theor. Appl. Fracture Mech., 37, 1-7.
13. Kugler, G., Turk, R., 2006, Study of the influence of initial microstructure topology on the kinetics of static recrystallization using a cellular automata model, Comp. Mater. Sci., 37, 284-291.
14. He, Y., Ding, H., Liu, L., Shin, K., 2006, Computer simulation of 2D grain growth using a cellular automata model based on the lowest energy principle, Mater. Sci. Eng. A, A429, 236-246.
15. Raabe, D., Hantcherli, L., 2005, 2D cellular automaton simulation of the recrystallization texture of an IF sheet steel under consideration of Zener pinning, Comp. Mater. Sci., 34, 299-313.
16. Ding, H.L., He, Y.Z., Liu, L.F., Ding, W.J., 2006, Cellular automata simulation of grain growth in three dimensions based on the lowest-energy principle, J. Crystal Growth, 293, 489-497.
17. Svyetlichnyy, D.S., 2006, Consideration of Deformation during the Automata Cellular Simulation, Nowe Technologie i osiągnięcia w metalurgii i inżynierii materiałowej, eds. Dyja, H., Szecówka, L., Conference Proceedings, Częstochowa, 533-536 (in Polish).
18. Svyetlichnyy, D., 2007, Three-dimensional cellular automata for simulation of microstructure evolution, Proc. Conf COMPLAS IX , eds. Oñate, E., Owen, R., Suárez, B., Barcelona, 983-986.
19. Svyetlichnyy, D., Matachowski, J., 2007, Three-dimensional cellular automata for simulation of microstructure evolution during recrystallization, Proc. 9th Int. Conf. on Numerical Methods in Industrial Forming Processes, NUMIFORM 2007, eds. César de Sá, J. M. A., Santos Abel, D., Porto, 1357-1362.

ZASTOSOWANIE AUTOMATÓW KOMÓRKOWYCH DO MODELOWANIA ROZWOJU MIKROSTRUKTURY PODCZAS WALCOWANIA

Streszczenie

Jednym z najważniejszych problemów nauki o materiałach jest przewidywanie rozwoju mikrostruktury i własności mechanicznych. Opracowany w niniejszej pracy model składa się z dwóch części, które uwzględniają odkształcenie i zmiany mikrostruktury. Zwykle odkształcenie nie jest uwzględniane podczas symulacji za pomocą automatów komórkowych. Natomiast, w przedstawionym modelu, dopóki zakumulowane w materiale odkształcenie nie jest wystarczająco duże, dotąd komórki w przestrzeni automatów odkształcają się zgodnie z tensorem odkształcenia, zmieniając swój kształt i rozmiary. Natomiast gdy odkształcenie osiągnie pewną ustaloną dużą wartość, która spowoduje znaczne zniekształcenie początkowego kształtu komórek, przestrzeń automatów zostaje przebudowana tak aby komórki wróciły do kształtu zbliżonego do sześcianu foremnego. Druga część modelu związana z rozwojem mikrostruktury, służy do symulacji rekrystalizacji i rozrostu ziarna. Algorytm procesu rekrystalizacji składa się z dwóch etapów: zarodkowania i rozrostu nowych ziaren. Prędkość zarodkowania i rozrostu ziaren uzależniono od takich parametrów procesu jak temperatura, odkształcenie, prędkość odkształcenia, gęstość dyslokacji i krystalograficzna orientacja ziaren.

W pracy opisano trójwymiarowe frontalne automaty komórkowe. Zastosowanie takich automatów w miejsce konwencjonalnych pozwala na znaczące zmniejszenie czasu obliczeń. Frontalne automaty komórkowe przystosowano do symulacji rozwoju mikrostruktury podczas walcowania wyrobów płaskich. Plan gniotów wykorzystano jako dane wejściowe do modelowania. W publikacji przedstawiono wybrane wyniki symulacji za pomocą frontalnych automatów komórkowych.

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