Computer Modeling of Microstructures with Probabilistic Cellular Automata Method Using Different Nucleation Rate Functions

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Abstract. Computer modelling widely uses cellular automata method for simulation of the microstructure of various materials. This work deals with the modification of cellular automata method – probabilistic cellular automata. The software for the synthetic generation of microstructures of polycrystalline materials has been developed. Using the software, the coefficient of the form, the normalized grain area, the scale factor and the angle of grain orientation are determined. For the obtained data, statistical processing and probability density functions have been obtained. According to statistical parameters, the comparison of the obtained results with the parameters of the microstructure of pure iron and H62 copper alloy has been performed. Modelling has been performed with different nucleation rate models.

Keywords: microstructure, probability cellular automata, microstructure quantitative characteristics, nucleation rate

1 Introduction

Computer simulation is a powerful tool in reproducing microstructures of different materials. It is the use of computer simulation to reproduce various microstructures quickly and efficiently. For practical purposes, it is important to reproduce microstructures that are statistically equivalent to real materials. They have the greatest influence on the mechanical properties of materials.

One common method for modelling the microstructure of polycrystalline materials is the method of cellular automata. Cellular automata began to be used in the middle of the XX century [1–3]. The term "cellular automaton" means a set of dependent elements with given states and rules. These rules determine the states of these elements and dependencies between them vary in time. Time and states are discrete. The use of the described models for the formal modelling of self-reproductive organisms was first proposed in the work of von Neumann [2]. Elements of cellular automata are proposed to be represented by one-dimensional, two-dimensional or multidimensional infinite rectangular tables. The state of the element varies depending on its state and state of its closest neighbours.

Cell-based models are widely used to predict behaviour in various industries. Cellular automata method widely uses in cryptography [4, 5], image processing [6–9], biology [10–12], physics [13, 14]. All these works cover a lot of possibilities of using the method of cellular automata. However, one of the most successful applications of the method is in the field of material science and engineering [15]. A lot of modifications of the method have been developed for the simulation of crystallization, recrystallization and evolution of the internal structure of materials [15–25]. Papers [16, 18, 19] deals with recrystallization in metals and alloys. In [17] authors reconstructs deformed microstructure using a cellular automaton. Irregular cellular automaton modification introduced in [20]. Microstructure and grain structure evolution during recrystallization [21, 23], additive manufacturing [22] and welding process [25] are also modelled.

In most works, the method of cellular automata is used to synthetically reproduce the microstructure of materials. However, the mentioned works almost do not investigate the influence of cellular automaton parameters on the quality of the created microstructures. Also, to increase the possibilities of modelling processes with stochastic nature, the modification of the method has been developed. Probabilistic method of cellular automata also uses in material internal structure simulation [16, 17, 19]**.** There are other ways to material modelling [26–28] and simulation planning [29, 30].

It should be noted work [17]. In the work partially investigated the distribution of grain size. However, the simulation is performed on a hexagonal grid. Thus, almost completely absent works devoted to the study of the quality of synthetically created microstructures and their statistical correspondence with real microstructures.

The scientific novelty of this paper is to develop a modification of the method of cellular automata, which uses probabilistic neighbours, as well as to determine the most successful parameters of the method by comparing the results with real microstructures. The practical value of developing such a modification of the method is to improve the quality of synthetic microstructures that can be used to model the mechanical behaviour of materials in multilevel modelling.

2 Problem statement

It is proposed to develop software that allows simulating the microstructure of metals using the probabilistic method of cellular automata. To do this the following tasks have been formulated:

- To study the developed modifications of the method of cellular automata for the simulation of microstructures;
- To develop software that allows simulating the microstructure of metals according to randomly assigned centres of grains and various of nucleation rate functions;
- Test the work of the software, determine the statistical characteristics of the size, shape and orientation of the grains;
- Compare the results with real microstructures.

3 Modelling with cellular automata

The cellular automaton K from a mathematical point of view [31–33] is an ordered set of four components:

$$K = < z^d, \nu, A, \varphi > \tag{1}$$

where z^d is set of d-dimensional vectors with integer coordinates (cell space);

$\nu = \{\nu_i \mid \nu_i = (x_{1i}, ..., x_{di}), \exists \nu_i = 0\}, i = 1, ..., m$ is a finite set of power m of vectors with zero vector (cell neighbourhood template);

A is the finite set of power k states of the cell with a dedicated state of rest $\emptyset$ (the alphabet of the cellular automaton);

φ is the local function of the transitions, defined in the discrete-time, which changes the states of the cell, which is a zero element in the template, depending on the state of the cells that form the neighbourhood pattern $\varphi: A^m \to A$; with $\varphi(\varnothing, \varnothing, ..., \varnothing) = \varnothing$. The state of all cells at the time t creates the current configuration $c^t : z^d \to A$.

All cells form a cellular automaton grid. Grids can be different types, differing in size and shape of cells. Each cell is a finite automaton which states are determined by the states of neighbouring cells and its states.

Cellular machines, in general, are characterized by the following properties:

- Changing the values of all cells occurs simultaneously after calculating the new state of each grid cell.
- The grid is homogeneous. It is impossible to distinguish any two places on the grid over the landscape.
- Interactions are local. Only the surrounding cells (usually neighbouring ones) can affect this cell.
- The set of states of the cell is finite.

In a two-dimensional (planar) case, the grid is implemented by a two-dimensional array. Each cell has eight neighbours. To eliminate boundary effects, the grid can be wrapped in a torus. It allows to use the following ratio for all automaton cells:

$$\begin{aligned} a'_{i,j} = \varphi(&a_{i,j}, a_{i-1,j}, a_{i-1,j+1}, \\ &a_{i,j+1}, a_{i+1,j+1}, a_{i+1,j}, a_{i+1,j-1}, a_{i,j-1}, a_{i-1,j-1}) \end{aligned} \tag{2}$$

In this work, for modelling the crystallization process, the cell can be in two states: the melt and the crystal.

To move from the deterministic to the probabilistic method of cellular automata, the following idea is used. Rules for switching from one state become non-deterministic. Thus, the transition from state to state occurs with a certain probability. Figure 1 shows typical transfer rules φ for the probabilistic method.

The application of this probabilistic approach allows creating more complicated rules of transition from state to state and reducing the effect of discreteness on the results of the algorithm.

From a physical point of view, the crystallization process should be uniform in all directions. Due to local fluctuations and temperature gradients, the uniformity of the chemical composition of the melt, crystallization occurs nonuniformly in different directions. To simulate this effect, it is proposed to set the crystallization rate in the form of an ellipse. The ellipse radii correspond to the crystallization rate in the corresponding directions. To determine the transition probability, an ellipse has been projected onto field cells. The shaded area indicates the probability of the transition of neighbouring cells to a solid-state. A more detailed description of the algorithm is given in [34].

Fig. 1. Cell neighbours: a – von Neumann; b – Moore; c – probabilistic neighbour

4 Nucleation rate models

One of the characteristics affecting the microstructure of the material is the nucleation rate (*J(n)*). Researchers in their papers [35–38] note that the nucleation rate depends on the Gibbs free energy. But it is difficult to introduce these models in discrete space and time of cellular automatons. Therefore, to evaluate the influence of crystallization parameters on the geometric characteristics of the formed microstructures, it is proposed to use the generalized models given [35–38] as the following models (3) – (7). These models are based on the assumption that the number of crystallization centres N_{gr} for all models has the same value at N_p iteration of the algorithm. The nucleation rate is defined as a derivative of the number of grains *N(n)* function, *n* is the iteration number of the algorithm. The visualization of the proposed models is shown in Fig. 2.

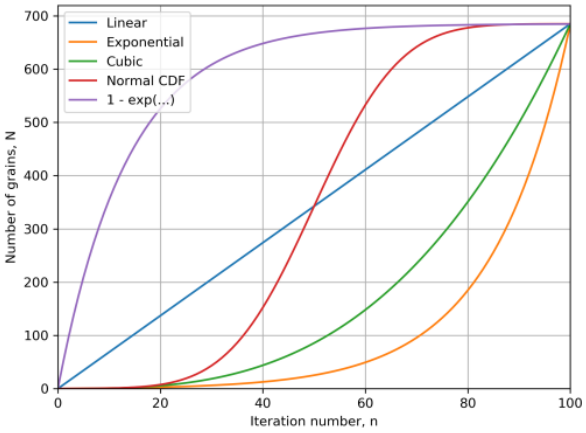
$$N(n) = \frac{N_{gr}}{N_p^3} n^3, \qquad J(n) = \frac{3N_{gr}}{N_p^3} n^2, \tag{3}$$

$$N(n) = \frac{N_{gr}}{N_p} n, \qquad J(n) = \frac{N_{gr}}{N_p}, \tag{4}$$

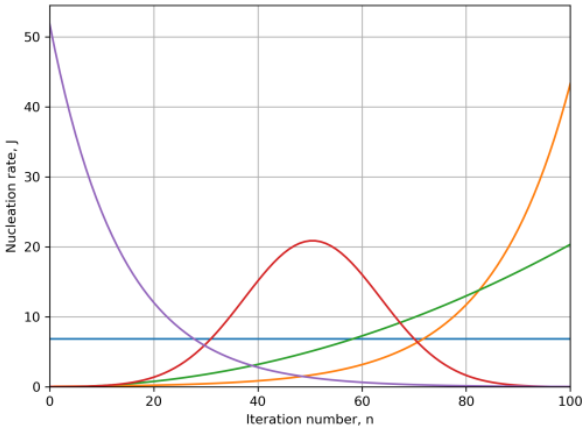
$$N(n) = \exp\left(\frac{\ln(N_{gr})}{N_p} n\right), \qquad J(n) = \frac{\ln(N_{gr})}{N_p} \exp\left(\frac{\ln(N_{gr})}{N_p} n\right), \tag{5}$$

$$N(n) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{n - N_p/2}{\sqrt{N_g}}\right)\right], \; J(n) = \frac{1}{\sqrt{N_{gr}\pi}} \exp\left(\frac{N_p/2 - n}{\sqrt{N_{gr}}}\right), \tag{6}$$

$$N(n) = N_{gr}\left[1 - \exp\left(-\frac{N_p}{2N_{gr}} n\right)\right], J(n) = \frac{N_p}{2} \exp\left(-\frac{N_p}{2N_{gr}} n\right). \tag{7}$$



a



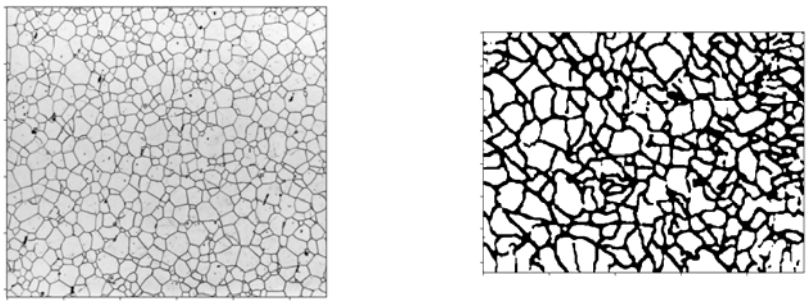
b

Fig. 2. Number of grains (a) and nucleation rate (b)

5 Simulation results

The following parameters for the test calculations have been chosen. The image size is 513 × 565 pixels and contains from $N_{gr} = 693$ grains, $N_p = 100$. These parameters are used for modelling by the method of cellular automata. Figure 4 shows the results of microstructure generation with different nucleation rates using the probabilistic neighbour from fig. 1c. To compare results with real microstructures two images have been selected. The first one –is pure iron microstructure, the second one is H62 copper alloy [39] (Fig. 3). For these images, geometric parameters have also been calculated. For assessing the uniformity of nuclei centre occurrence side histogram has been plotted. It allows estimating the probability density function of nucleation centres.

All simulations have been performed using the original program. It is written using python language with numpy library. This program allows modelling cellular microstructures according to specified parameters.



a b

Fig. 3. Microstructures: a – pure iron; b – copper alloy H62 copper alloy [39]

For the quantitative analysis of the similarity between microstructures, the following features have been chosen. The form factor C_s. This coefficient is defined as the normalized ratio of the grain area A_{gr} to the square of the grain perimeter P_{gr}. If the grain has a perfect circle shape, then $C_s = 1$. For all other cases $0 < C_s < 1$. For example, for the square $C_s = \pi / 4 = 0.7853$.

$$C_s = 4\pi \frac{A_{gr}}{P_{gr}^2}. \tag{8}$$

Also the normalized grain area A_n is used as the ratio of the A_{gr} grain area to the total area of the image A.

$$A_n = \frac{A_{gr}}{A} \tag{9}$$

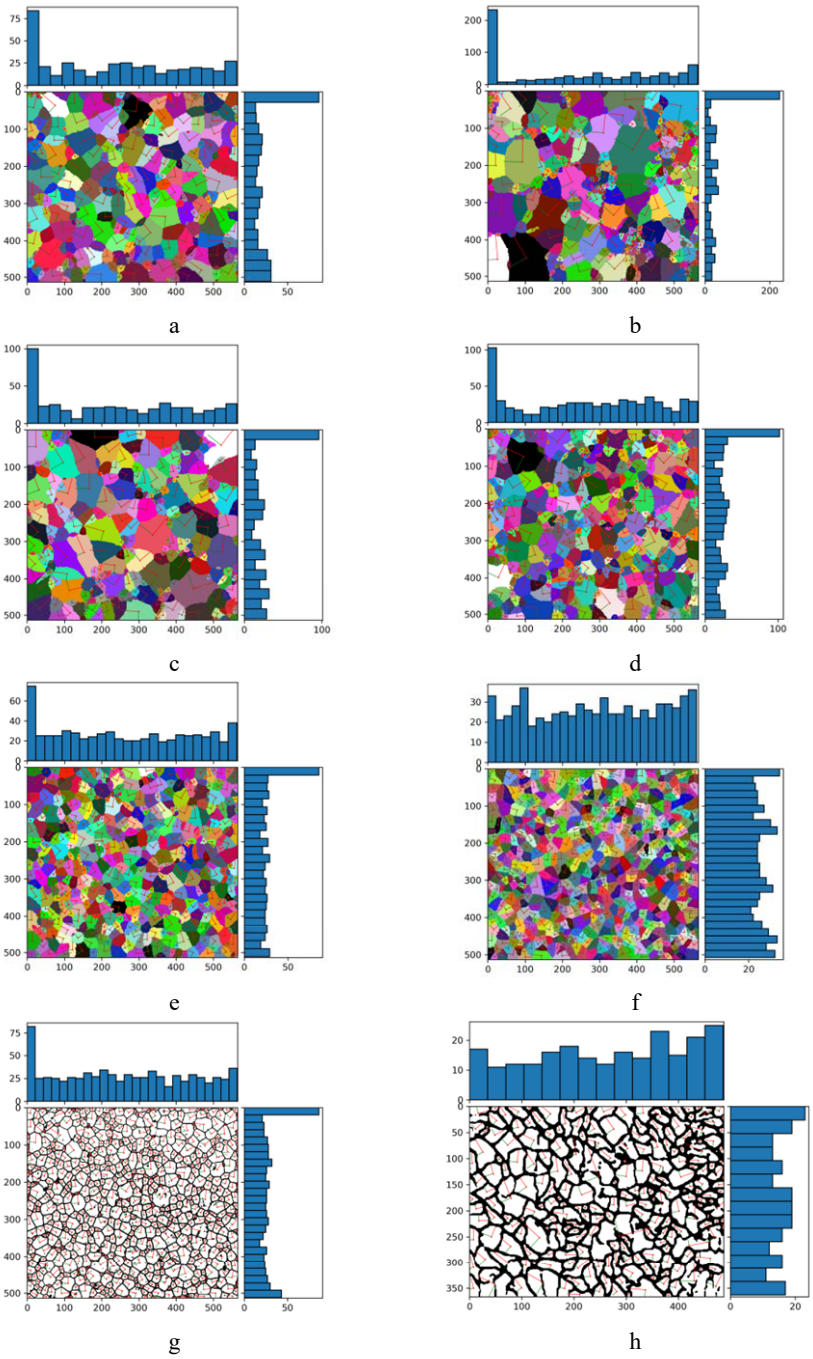


Fig. 4. Microstructures generated by cellular automata method (a-f), pure iron (g), H62 copper alloy (h)

Often, a scale factor S_c is used to compare grain parameters. It is introduced as a ratio of a larger characteristic (S_x) grain size to lesser (S_y) (fig. 5).

$$S_c = \frac{S_x}{S_y} \tag{10}$$

To determine the angle of grain orientation, the angle ψ is introduced, as is the angle between the horizontal and the largest characteristic diameter of the grain (fig. 5).

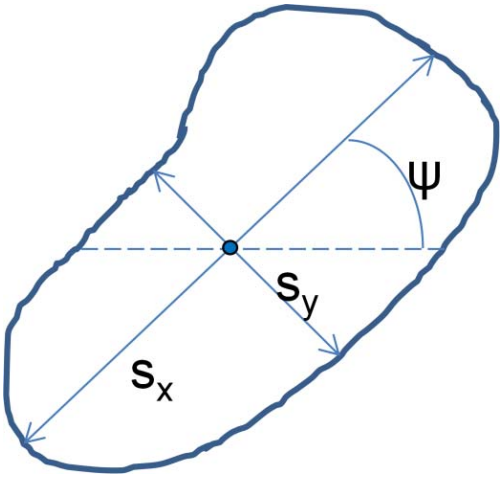


Fig. 5. Sketch of one cell parameters

For the comparison of microstructures for each grain of the generated microstructure, the values of four coefficients have been calculated. These values have been statistically processed and histograms have been constructed. These histograms have been approximated by the kernel density estimation method [40]. The approximated probability densities for the coefficients are shown in Figure 5. Descriptive statistic parameters are collected in table 1.

Table 1. The mean and standard deviation of microstructure parameters

Nucleation rate model	N_{gr}	A_n, $\times 10^{-3}$		C_s, $\times 10^{-1}$		S_c		ψ, rad	
		mean	***std. dev***	***mean***	***std. dev.***	***mean***	***std. dev.***	***mean***	***std. dev.***
CDF (6)	580	1.72	2.52	5.87	0.87	1.65	0.51	1.61	0.87
Constant	679	1.47	0.77	6.05	0.80	1.71	0.52	1.55	0.86
Cubic (3)	364	2.74	4.46	6.04	0.78	1.60	0.44	1.50	0.81
Exponential (5)	513	1.94	4.64	5.93	0.79	1.60	0.48	1.56	0.85
H62 Copper Al.	223	2.82	3.10	5.70	1.48	1.94	0.72	1.73	0.90
Linear (4)	346	2.89	3.40	6.02	0.90	1.64	0.56	1.58	0.85
Pure Iron	693	1.10	1.06	5.84	1.31	1.73	0.94	1.57	0.85
Reverse Exp (7)	590	1.69	1.38	6.08	0.79	1.63	0.47	1.64	0.83

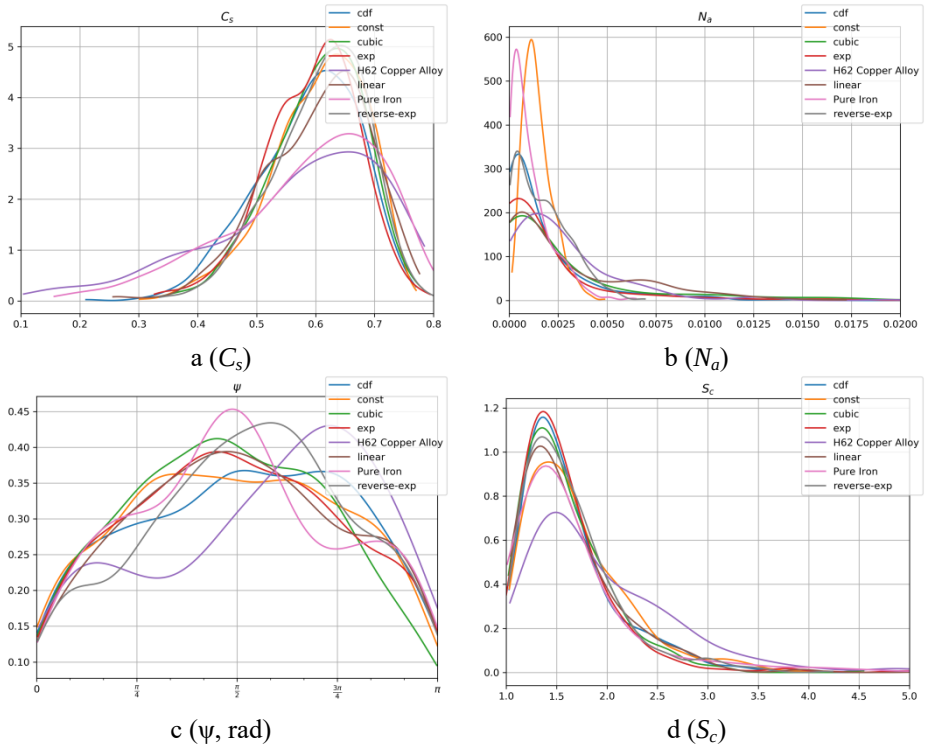


Fig. 6. The probability density function of microstructure parameters: a - C_s; b - N_a, c - ψ, d - S_c

As can be seen from the figures, the distribution of parameters is very similar. However, there are some differences. The probability density distribution of the parameter C_s for all microstructures which is created using the cellular automata method has a similar structure. Microstructures of pure iron and copper H62 alloy stand out from the total number. They have a heavier left edge of the distribution. This suggests that more elongated grains are more common in these microstructures than is obtained as a result of modelling.

The distribution of the parameter A_n also has significant similarities. However, for the case of pure iron, the best match is shown by the constant model, and in the case of copper alloy – exponential or cubic.

The probabilistic neighbourhood was initially tuned to obtain the expected orientation $\psi = \pi / 2$. This is confirmed by the obtained probability densities. The copper alloy has another preferred grain orientation $\psi = 3\pi / 4$, which is confirmed by the obtained values. According to S_c scales, there is the best coincidence of results.

Acknowledgement

This work has been supported by the Ministry of Education and Science of Ukraine in the framework of the realization of the research project "Development of methods

for mathematical modelling of the behavior of new and composite materials aims to structural elements lifetime estimation and prediction of engineering designs reliability" (State Reg. Num. 0117U004969).

Conclusions

In this work, the implementation of the method of cellular automata probabilistic neighbours is developed. The developed method shows the results of the generation of the microstructure of the material.

A comparison of the obtained microstructure of pure iron and H62 copper alloy with synthetic microstructures has been made on the coefficient of the form, the normalized grain area, the scale factor and the angle of the grain orientation.

The results of the comparison showed that the probability densities of the corresponding parameters have a qualitative similarity. However, by the parameter of the normalized grain area, the distribution for pure microstructure has differences.

However, identifying the best way to reproduce microstructures is problematic. For some situations, better results can be achieved by one criterion, but this results in worse performance by another.

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