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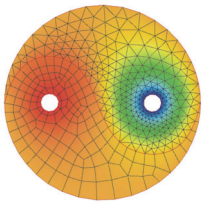

IDENTIFICATION OF THE STATIC RECRYSTALLIZATION CELLULAR AUTOMATA MODEL PARAMETERS BASED ON INVERSE ANALYSIS

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Abstract

Development of the inverse algorithm for identification of the discrete cellular automata model of the static recrystallization based on the particle swarm optimization method is the main aim of the work. First, the idea of the inverse analysis approach is presented. Then subsequent modules of the algorithm are discussed, namely: direct problem model, experimental setup and optimization algorithm. The optimization part is realized by the basic variant of particle swarm optimization (PSO) method. Finally, examples of identified model parameters are presented and obtained results of recrystallized microstructures are compared with the experimental data.

Key words: Inverse Analysis, Cellular Automata, Particle Swarm Optimization, Static Recrystallization

1. INTRODUCTION

Complex numerical models to simulate microstructure development in metallic materials based on the cellular automata (CA) method are recently more frequently published in the scientific literature (Das, 2010; Hallberg et al., 2010; Kugler & Turk, 2006; Popova et al., 2014; Madej et al., 2011; Madej et al., 2013; Raghavan & Satyam, 2009; Seyed Salehi & Serajzadeh, 2012; Sieradzki & Madej, 2013; Sukhopar & Gottstein, 2012; Svyetlichnyy, 2013; Zheng et al., 2012). However, numerical simulations of thermo-mechanical processing with these CA models require accurate information about proper model parameters adjusted to particular investigated material. Precise determination of these parameters (such as yield stress, activation energies, diffusion coefficients, critical dislocation densities etc.) is a major challenge for researchers for the last three decades. Unfortunately, proper determination of material parameters that are insensitive to the processing conditions is extremely time consuming as it requires a series of experimental and numerical investigations. However, the computational power of modern computers has significantly increased in recent years and currently it is possible to perform even large number of calculations in an acceptable computational time. In the past, computation of e.g. 1000 simulations of recrystallization or phase transformation took weeks if not months and now it can be done in only few hours. As a result, mentioned progress created new possibilities for practical use of time consuming optimization procedure in application for fast and efficient identification of model parameters based on the e.g. inverse approach (Szeliga et al., 2004; Szeliga et al., 2006). One of commonly used optimization methods is the nature inspired Particle Swarm Optimization method (PSO) (Gao et al., 2012, Wang et al., 2008; Yu-Zhen et al.,

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2012; Zhiwen et al., 2013). The PSO algorithm is an efficient solution in optimization of problems with multiple local minima. Thus, the approach based on basic variant of PSO is used in the present research to accurately identify parameters of the developed cellular automata static recrystallization model.

2. INVERSE APPROACH

As mentioned, the model parameters identification procedure can be defined as the inverse problem. Inverse algorithm operates on relation between three different vectors. The first, contains material parameters that have to be identified e.g. activation energy for different phenomena, diffusion coefficients, rheological model variables, etc. The second is known and well defined, it contains process conditions e.g. temperature, strain rate, time etc. The third, stores information obtained from experimental investigation e.g. process kinetics, flow stress values, final grain size, etc. Thus, the inverse problem can be defined in the mathematical form as:

$$d = f(x, p), \tag{1}$$

where: x – unknown vector, d – results obtain from experiment, p – process conditions.

The typical inverse analysis algorithm consists of three parts (figure 1):

- Numerical simulation. Direct problem solution can be based on many different numerical methods e.g. finite element method or discrete models e.g. cellular automata approach, however it always replicates the experimental set up.
- Experiment. The results of measurements of e.g. loads, temperatures, grain sizes, recrystallization volume fractions, volume fraction of particular phases, process kinetics are considered as input to evaluate the objective function to solve the inverse problem and identify model parameters.
- Optimization algorithm. These procedures are used to minimize the goal function $\varphi(x)$, which in general presents the discrepancies between experimental and numerical results. The choice of optimization method is important for the efficiency of the inverse solution.

Data buffer in (figure 1) represents implemented parser that transforms data from the text files containing relevant information into the object in c++ language. Subsequent elements of the inverse algorithm applied to the static recrystallization cellular automata model identification process are described in the following sections.

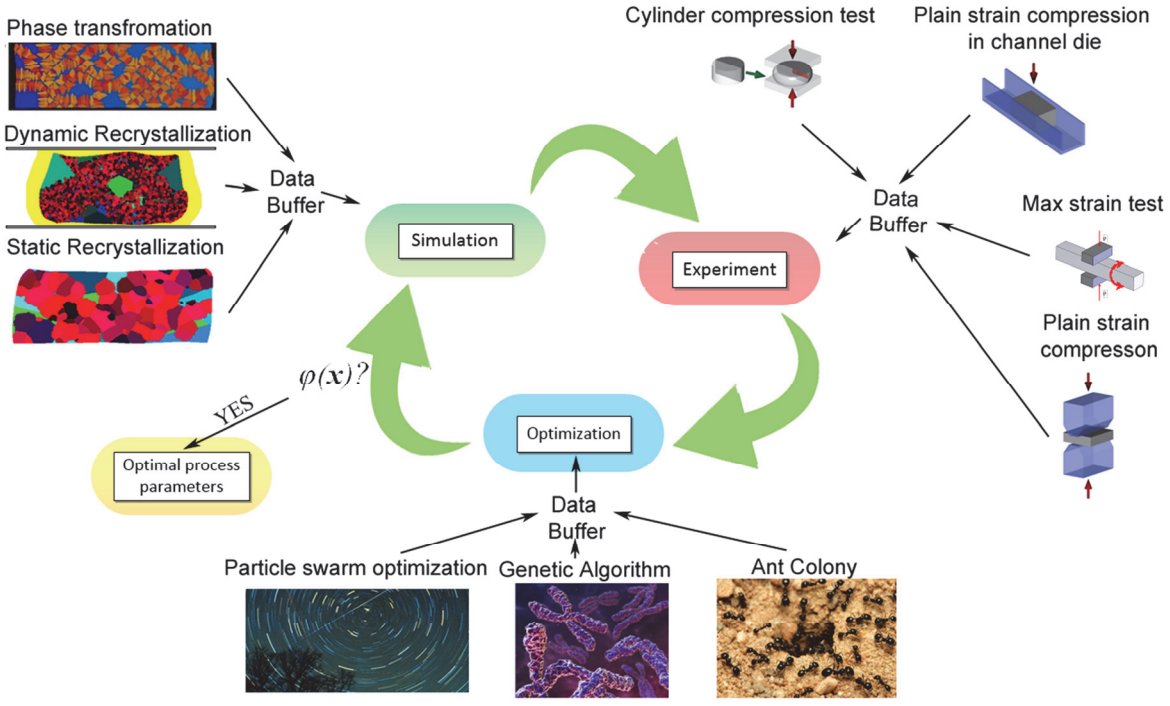

Fig. 1. *General concept of the inverse analysis algorithm.*

3. NUMERICAL SIMULATION - CELLULAR AUTOMATA STATIC RECRYSTALLIZATION MODEL

The main idea of the CA technique is to divide a specific part of the material into one-, two-, or three-dimensional lattices of finite cells, where cells have clearly defined interaction rules between each other. Each cell in this space is called a cellular automaton, while the lattice of cells is known as cellular automata space. The CA major components are:

- CA space – finite set of cells, where each cell is described by a set of internal and state variables describing the state of a cell.
- Neighborhood – describes the closest neighbors of a particular cell. It can be in 1D, 2D and 3D space. Example of neighborhoods definition are presented in figure 2.
- Transition rules *f* – the state of each cell in the lattice is determined by the previous states of its neighbors and the cell itself by the transition function *f*.

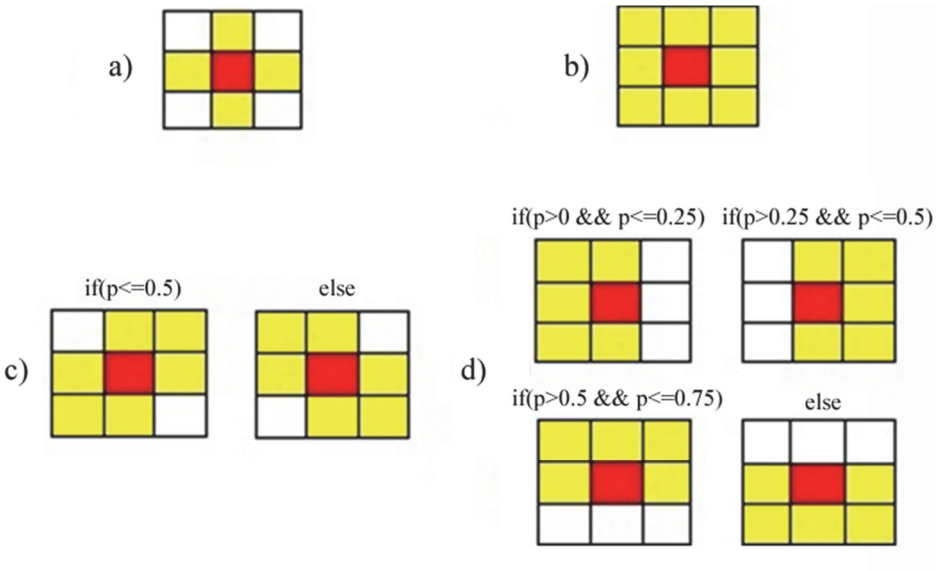

Fig. 2. *Neighborhood definition in the CA method a) von Neumann, b) Moore, c) hexagonal random (p from <0,1>), d) pentagonal random (p from <0,1>).*

The most important part of the cellular automata model is the third component - the set of transition rules; as the dynamics of the system is introduced into the model by these rules. The stochastic properties of the system, can be incorporated into the CA microstructure evolution models mainly through the introduction of non-deterministic transition rules and the definition of the neighborhood.

Due to the fact, that all models based on the cellular automata method, have some common elements e.g. solution space, type of neighborhood, strictly defined state boundary conditions or general transition rules, there is a possibility of encapsulation of those elements in the form of an universal software – framework developed by the authors (Gołąb et al., 2014). Such an application provides a possibility to define the parameters that are common to various material models, as well as to define particular transition rules releasing the end-user from implementation issues in an easy and efficient way.

The developed framework was used to implement the CA model for static recrystallization (SRX), which is used as a direct problem model in the present paper.

The developed SRX CA model generally is composed of the tree main steps: preparation of initial microstructure, nucleation and subsequent grain growth.

During the first stage, the initial microstructure is preprocessed in order to transfer it into the digital material representation (DMR) form. The DMR can be obtained on the basis of the photography of the real microstructure before the deformation process, or generated using different numerical techniques (Madej et al., 2013).

The nucleation in the CA model is based on physical rules and takes into account the influence of real temperature. The number of nuclei that can appear in the material volume per unit of time is controlled by the equation:

$$N = M_N \exp\left(-\frac{Q_a}{RT}\right), \qquad (2)$$

where: Q_a – activation energy for nucleation, R – universal gas constant, T – temperature, M_N – coefficient computed using the formula:

$$M_N = C_0(H_i - H^C), \tag{3}$$

where: C_0 – scaling parameter, H_i – amount of accumulated energy in the particular cell obtained from simulation of deformation process in Abaqus software (Madej et al., 2011), H^C – critical amount of energy, which is necessary to trigger nucleation. H^C is calculated from the following formula:

$$H^C = \frac{\varepsilon_c}{a\varepsilon_c + b}\gamma_{lagb}, \tag{4}$$

where: ε_c – critical plastic strain, a, b – parameters which are fitted during the experimental analysis, γ_{lagb} – low angle grain boundary energy.

The probability of nucleation in the unit of time is computed as:

$$P = N\, S_N\, t_{step}, \tag{5}$$

where: S_N – the volume in which the nucleus can appear, t_{step} – the length of time step in each CA iteration.

Influence of the recovery process on the amount of accumulated energy is considered in the present research and results in lowering the value of the accumulated energy in particular cell:

$$H_i = \left[H_{i0}^{1/2} - C_1 \mu^{-1/2} kT \ln\left(1 + \frac{t}{\tau_0}\right)\right]^2, \tag{6}$$

where H_{i0} –initial stored energy at the end of deformation, C_1 – parameter, k – Boltzmann constant, τ_0 – time constant, which is set as 1s, t – time.

Recovery is assumed to occur from the beginning of the heating process and influences the kinetics of the grain growth. The velocity of the grain growth is described by the standard equation:

$$v = M \cdot P, \tag{7}$$

where: M – grain boundary mobility, P – the driving pressure.

The value of M is computed as:

$$M = \frac{D_0 b_B^{\,2}}{kT}\exp\left(-\frac{Q_b}{RT}\right), \tag{8}$$

where: D_0 – diffusion constant, b_B – Burger's vector, Q_b – activation energy for grain boundary motion.

The level of coverage of the particular cell by the recrystallization front in the t-th time step can be computed by means of the equation:

$$RX_{i,j,t}^{fraction} = RX_{i,j,t-1}^{fraction} + \sum_{k=1}^{rx}\left(\frac{v_k t_{step}}{c_s}\right), \tag{9}$$

where: $RX_{i,j,t-1}^{fraction}$ – level of coverage in the t-1-th time step, rx – number of recrystallized neighbors, v_k – velocity of the recrystallization front in k-th cell (7).

Thus, based on the above equations a governing transition rule describing the changes in the unrecrystallized (*uSRX*) to recrystallized (*SRX*) state is defined as:

$$\mathbf{Y}_{i,j}^{t+1} = \begin{cases} SRX \Leftrightarrow RXF_{i,j}^{t} > 1.0 \\ \mathbf{Y}_{i,j}^{t} \end{cases}, \tag{10}$$

where: $\mathbf{Y}_{i,j}^{t}$ – state of the neighboring cell (i, j) in a particular time step t.

More details about the developed model are presented in earlier authors paper (Madej et al., 2013).

Four most important parameters from the SRX model were selected for the identification stage in the present research, namely:

- Q_a – activation energy for nucleation,
- ε_c – critical plastic strain,
- C_1 – parameter in the recovery module,
- Q_b – activation energy for grain boundary motion.

4. EXPERIMENT

Experimentally, the recrystallization process was investigated using the dilatometer DIL 805A/D. Samples with dimension 1mm × 7mm were cut from the 65% cold rolled ferritic-perlitic steel parallel to the rolling direction. Heating conditions were adopted as presented in figure 3 and involved heating with constant heating rate to five different temperatures followed by immediate quenching to freeze the microstructure. To examine the state of the samples subjected to annealing, EBSD (Electron Back Scattered Diffraction) analysis was conducted with SEM/FEG. The EBSD analysis can effectively distinguish the recrystallized grains since they do not contain the deformation substructure composed of dislocation arrangements and are surrounded by high-angle grain boundaries. Obtained morphologies with clearly visible grains and subgrain structures are shown in figure 4 (at the temperature 750°C, 100% of material was fully recrystallized and phase transformation started, so the morphology is not presented).

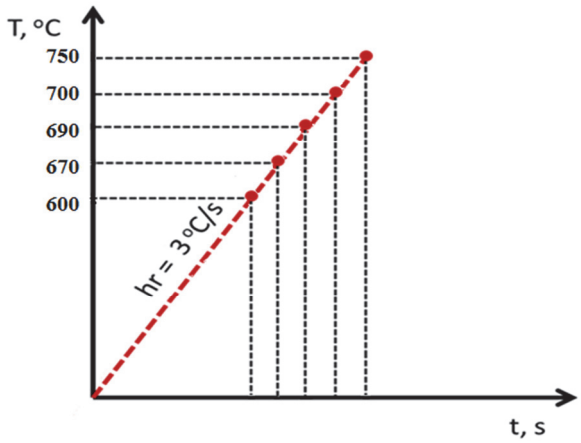

Fig. 3. Process temperature conditions.

5. OPTIMIZATION ALGORITHM

The nature inspired particle swarm optimization (PSO) algorithm was selected for the optimization stage in the inverse analysis. The PSO is an iterative optimization method based on population of particle, each particle represent one particular solution. A lot of modifications of the PSO algorithm can be found in the literature (Muhammad et al., 2013). Authors decided to use a basic variant, with only one modification introducing the *w* parameter, which determinates the change of particles velocity. Each particle in the algorithm is moving across the search-space and their current positions are calculated from previous time step using the position and particle velocity:

$$x_{i,d}(t+1) = x_{i,d}(t) + v_{i,d}(t+1), \qquad (11)$$

where i – particle number, d – problem dimension, $v_{i,d}(t+1)$ – magnitude of particle position change:

$$v_{i,d}(t+1) = (w \cdot v_{i,d}(t) + (c_1 \cdot r_1 \cdot (p_{i,d}(t) - x_{i,d}(t))) + (c_2 \cdot r_2 \cdot (g_{i,d}(t) - x_{i,d}(t))) \qquad (12)$$

where: w – inertia weight parameter, $v_{i,d}(t)$ – i-th particle velocity from previous time step, c_1 – cognitive weight equal 1.4, c_2 – social weight equal 1.4, r_1, r_2 – random number <0,1>, $p_{i,d}(t)$ – best known

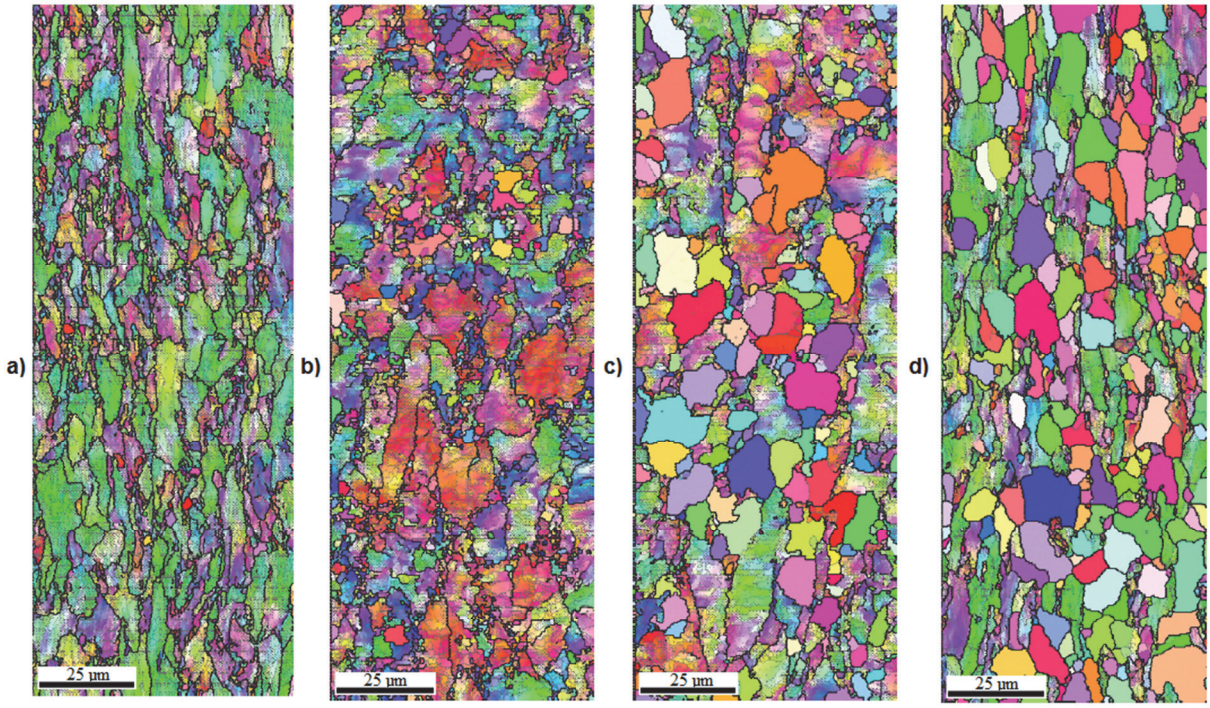

Fig. 4. Morphology of material after heating to temperatures a) 600°C, b) 670°C, c) 690°C, d) 700°C.

Based on laboratory experiments presented in figure 4, experimental data used to create a goal function for the inverse analysis were obtained: average grain size and recrystallized volume fraction (table 1).

Table 1. *Parameters obtain from experimental investigation of SRX.*

Temperature	600°C	670°C	690°C	700°C	750°C
Grain Size	1.67	2.70	4.90	5	6
SRX volume fraction	0.176871	0.217687	0.544218	0.605442	1

position of i-th particle, $x_{i,d}(t)$ – particle position form previous time step, $g_{i,d}(t)$ – best known position in swarm, d – in lower index determinate problem dimension.

Particle movement is determined by particle local best known position and the best known positions in the search-space called swarm. Diagram of the PSO adapted to the Cellular Automata method is presented in figure 5.

ments, $RX_{fraction}$ – recrystallization volume fraction obtain in particular simulation, ms – number of experiments ($ms = 5$).

As seen in figure 5, first initial model conditions namely material morphology, energy distribution after deformation and the temperature after deformation are introduced. All these parameters are taken from Abaqus Software simulation of plastic deformation process (Madej et al., 2013). Then to each

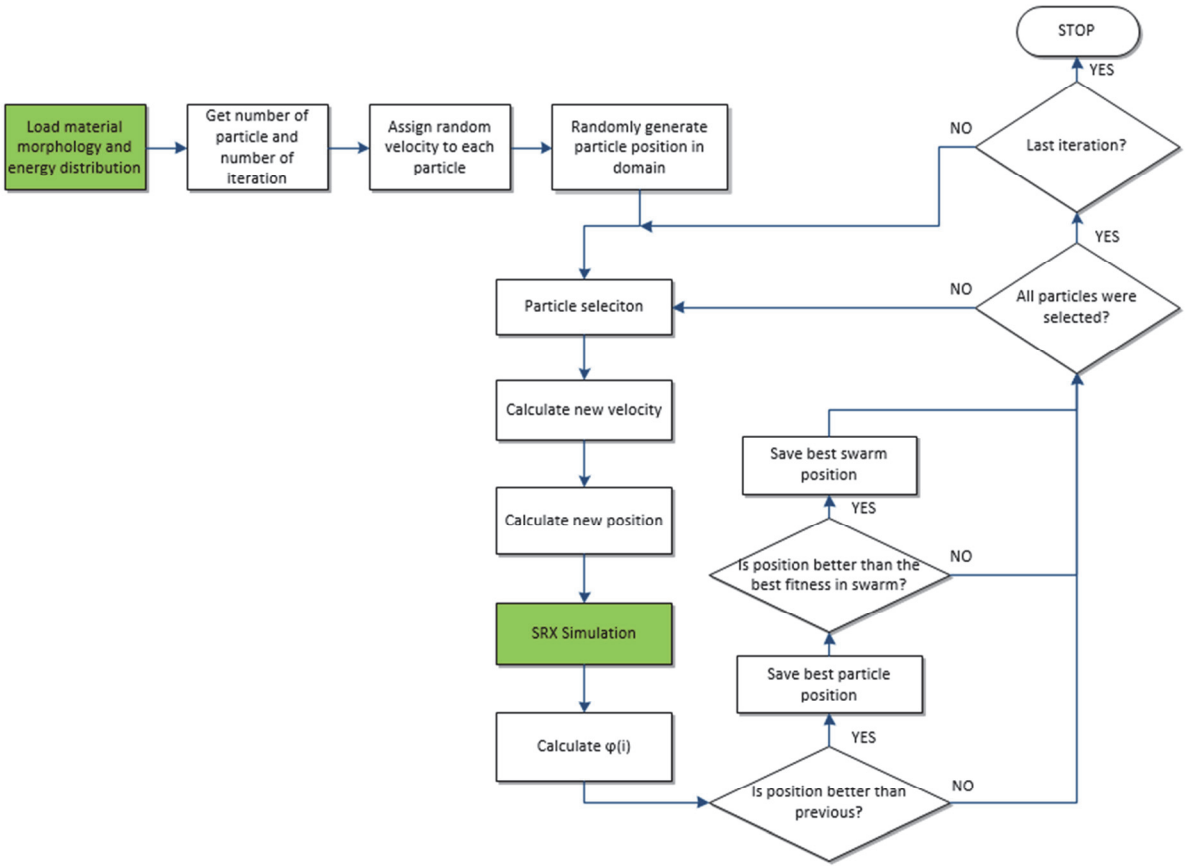

Fig. 5. *Diagram of Particle Swarm Optimization method adapted to the Cellular Automata method.*

The goal function for the identification of the static recrystallization model was defined by the following formula composed of the two components: grain size and kinetics errors, respectively:

$$\varphi(x) = w_0 \sqrt{\sum_{k=1}^{ms} (D_{init} - D_{gr})^2} + w_1 \sqrt{\sum_{k=1}^{ms} (RX_{init} - RX_{fraction})^2} \tag{13}$$

where: w_0, w_1 – scaling parameter that guarantee the same weigh of grain size and recrystallization volume fraction on final result ($w_0 = 1/7$, $w_1 = 1$), D_{init} – initial grain size from measurements, D_{gr} – grain size calculated in particular simulation, RX_{init} – initial recrystallization volume fraction from measure-

particle in the swarm an initial position, velocity and best known position of particle in the solution domain are assigned. After that, following steps of the PSO algorithm are performed for each particle located in solution space:

- Select random numbers r_1, r_2 and update velocity value using (12).
- Update particle position from (11).
- Simulate direct problem for new defined model parameters.
- Evaluate new goal function value calculated from (13).
- Updated the particle best known position if goal function has improved.

– Update the best known position in swarm if goal function is better than the best goal function value in the entire swarm.

After given number of iterations algorithm will finish the identification process and model parameters for subsequent calculations will be provided.

6. RESULTS OBTAINED FROM THE INVERSE ANALYSIS

During the identification based on the PSO algorithm 50 particle swarm was used. Inertia weight parameter w was set to 0.9 and after each 20 algorithm iterations it is assumed that the value decreases by 0.05, to provide large change in particle position and give the possibility to investigate more locations in the space solution.

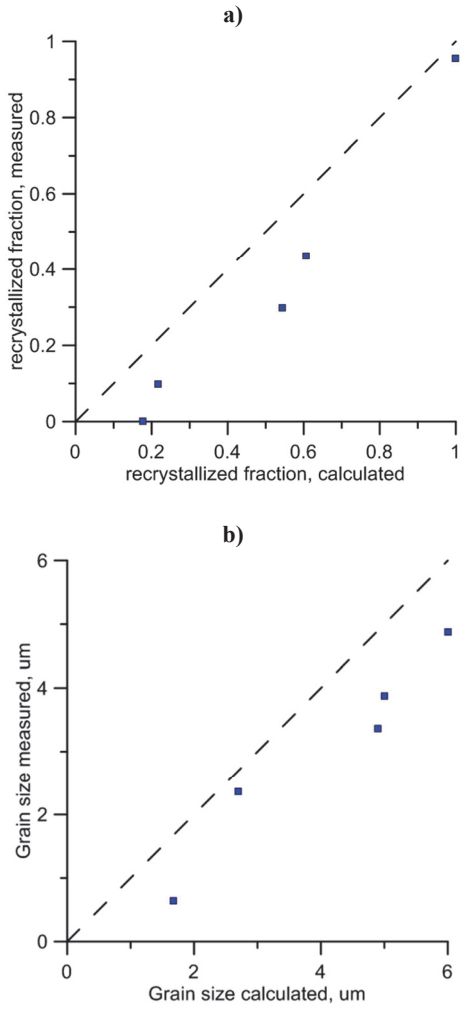

Fig. 6. *Comparison of the results obtain after 10 iteration of PSO algorithm: a) recrystallization volume fraction, b) grain size.*

The stop criterion was defined twofold: number of iterations larger than 400 or goal function value lower than 0.2 (swarm of 50 particle with 400 iterations results in maximum 20000 simulations of the SRX model). Results obtained from realized simulations with the following parameters are presented in figure 6, 7.

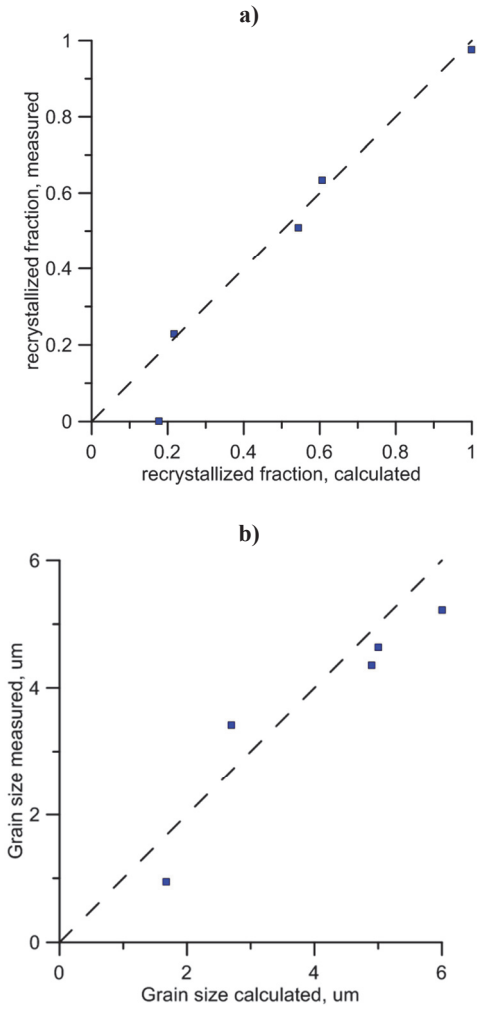

Fig. 7. *Comparison of the results obtain after 100 iteration of PSO algorithm: a) recrystallization volume fraction, b) grain size.*

Final values of errors obtained for the grain size and recrystallized volume fraction (kinetics) were equal to 0.134782 and 0.0546275, respectively (figure 8a) while the final goal function value dropped below 0.2 (figure 8b). Subsequent iterations of the algorithm do not provided significant improvement of the obtained results, so authors decided to show only 100 PSO iterations, which correspond to 5000 SRX simulations.

Parameters obtained after the identification stage based on the inverse approach are collected in table 2.

Algorithm finds optimum solution for parameters presented in table 2, however not all cases have good agreement with measurements. As can be noticed in figure 7a, for the lower volume fractions,

there is a large discrepancy between measurements and calculations. It can be caused by measurement inaccuracy due to initial stages of SRX or size of one cellular automata cell (CA model resolution).

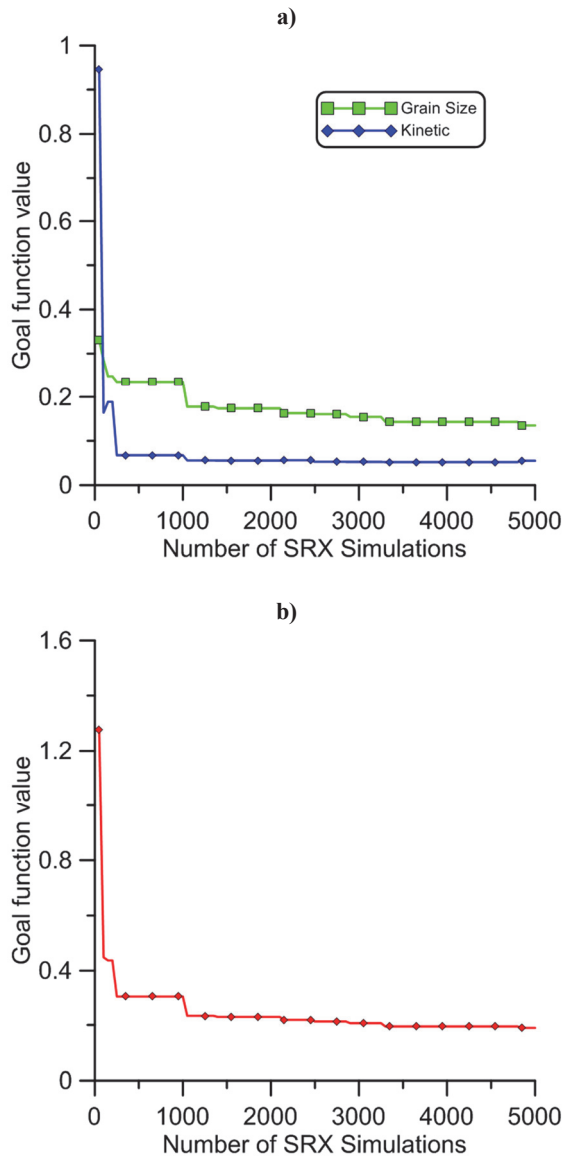

***Fig. 8**. Goal function value for simulation of 50 particle: a) function divided into grain growth and kinetic components, b) overall value of goal function -φ(x).*

***Table 2.** The parameters obtained after 100 PSO iterations.*

Parameter	Q_a [kJ/mol]	ε_c	C_1	Q_b [kJ/mol]
Value	170.08	0.12	1e27	136.96

7. CONCLUSIONS

Based on the presented investigation it can be conducted that:

- PSO method can be successfully applied for the identification of discrete cellular automata models.
- PSO algorithm finds optimum with goal function value lower than assumed.
- Algorithm is sensitive for measurement inaccuracy in the initial stages of the SRX phenomenon what influences accuracy of the solution. This is attributed with the resolution of the EBSD maps and corresponding CA space.

Obtained parameters will be used in the future work to investigate kinetics of the SRX for various process conditions.

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IDENTYFIKACJA PARAMETRÓW MODELU AUTOMATÓW KOMÓRKOWYCH DO SYMULACJI REKRYSTALIZACJI STATYCZNEJ Z WYKORZYSTANIEM ANALIZY ODWROTNEJ

Streszczenie

W artykule omówiono identyfikację parametrów modelu automatów komórkowych (Cellular Automata - CA) do symulacji rekrystalizacji statycznej z wykorzystaniem metody roju cząstek (Particle Swarm Optimization). W pierwszej części pracy przedstawiono główne założenia wykorzystanej do identyfikacji metody analizy odwrotnej. Następnie przedstawiono opracowany model automatów komórkowych, inspirowaną naturą metodę optymalizacji oraz omówiono uzyskane dane eksperymentalne. W ostatniej części przedstawione zostały wyniki przeprowadzonego procesu identyfikacji.

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