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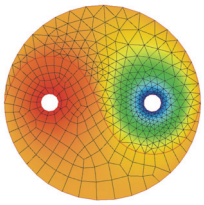

CELLULAR AUTOMATA MODEL OF PRECIPITATION IN MICROALLOYED NIOBIUM STEELS

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Abstract

Proposition of a Cellular Automata model of carbonitride precipitation in microalloyed niobium steels is presented in the paper. Transition rules based on the current knowledge regarding precipitation were formulated. The model accounts for an increase of dislocation density due to plastic deformation and predicts kinetics of precipitation as well as shape of precipitates. Numerical tests confirmed qualitatively good predictive capabilities of the model.

Key words: cellular automata, precipitation, microalloyed steels

1. INTRODUCTION

Precipitation has played crucial role in controlling of properties of alloys for few decades. Numerous research were carried out and development of the High Strength Low Alloyed (HSLA) steels was one of the most spectacular practical effects of these research. Numerical modelling played important role in development of new processing technologies taking advantage of precipitation. By modelling we mean a mathematical description of the relation between the main process variables and the resulting material properties, based on sound physical principles. Variety of models ensuing from the thermodynamics were developed in the second half of the 20th century. Review of these models was presented by Bratland et al. (1997). As far as precipitation of carbonitrides in microalloyed steels is considered works of Dutta and Sellars (1987), Dutta et al. (1991), Dutta et al. (2001), Maugis and Goune (2005) should be mentioned. A model accounting for three alloying elements (Adrian, 1992) was a contribution in this field of one of the Authors of the present paper. All these models are characterized by different complexity of mathematical formulation and different predictive capabilities. In general, the models allow to calculate kinetics of precipitation and changes of the size of precipitates as a function of processing parameters. In the present investigation, the methodology is further developed and Cellular Automata method is applied to precipitation reactions in industrial processing, with particular emphasis on microalloyed steels.

2. CELLULAR AUTOMATA MODEL

Cellular Automata (CA) model proved to be very efficient in modelling various phenomena in materials science. As far as thermomechanical processing of metallic materials is considered, the works dealing with modelling recrystallization and phase transformations should be mentioned.

The main principles of the applications of the CA method in materials science were discussed by Raabe (1998). Following this publication several new applications of this method were published. Modelling microstructure evolution seems to be the most frequent application of the CA in the material science area, see next publication by Raabe (2002).

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During the last 15 years the CA method has been applied to modelling recrystallization by a number of researchers, see for example (Davies & Hong, 1999; Ding & Guo, 2002). Subsequent papers contribute to solution of particular problems in CA modelling of recrystallization, such as influence of the initial microstructure morphology (Kugler & Turk, 2006; Raghavan & Satyam, 2009) or the effect of the neighbourhood on the kinetics of recrystallization (Davies, 1995). First 3D cellular automata models of recrystallization were published at the end of the XXth century (Marx, 1999; Janssens, 2003). Review of published papers with a large list of references was published by (Yang, 2011). Modelling of phase transformations is another large field of applications of the CA in the material science area (Zhang, 2003; Lan et al., 2004). Gołąb et al. (2012) have developed the computer framework for implementation the CA models. Authors of the present paper have applied CA model to simulation of dynamic recrystallization (Gawąd & Pietrzyk, 2007), strain localization (Madej et al., 2009) and phase transformations during cooling (Jabłoński et al., 2012; Opara et al., 2012). Application of the CA model to simulation of ferrite-austenite transformation during heating was presented by Halder et al. (2014).

The main idea of the cellular automata technique is to divide a specific part of the material into one-, two-, or three-dimensional lattices of finite cells. Each cell in this CA space is called a cellular automaton, while the lattice of the cells is known as cellular automata space. Each cell is surrounded by neighbours, which affect one another. Neighbourhoods can be specified in one-, two-, and three-dimensional spaces. The most popular examples are the von Neumann and the Moore neighbourhoods (Wolfram, 1983), where in the 2D case each cell is surrounded by either four or eight neighbouring cells, respectively.

Each cell in the CA space is characterised by its state and by values of internal variables. The cells interactions within the CA space are based on the knowledge defined while studying a particular phenomenon. In every time step, the state of each cell in the lattice is determined by the previous states of its neighbours and the cell itself on a basis of a set of precisely defined transition rules:

$$\mathrm{Y}_{i,j}^{t+1} = \begin{cases} if\,(\Lambda) \Rightarrow newstate \\ else \quad \Rightarrow \mathrm{Y}_{i,j}^{t} \end{cases} \tag{1}$$

where: $\mathrm{Y}_{i,j}^{t+1}, \mathrm{Y}_{i,j}^{t}$ – state of the cell i,j in the current and previous time step, respectively, Λ – logical function, which describes the condition when the state of the cell changes. Function Λ depends on:

$$\Lambda = \Lambda\left(Y_{i,j}^{t}, Y_{k,l}^{t}, \mathbf{p}, \mathbf{q}\right) \tag{2}$$

where: $\mathrm{Y}_{k,l}^{t}$ – state of the cell k,l, which is a neighbour to the cell i,j, in the previous time step, $\mathbf{p}$ – vector containing external variables, eg. temperature, $\mathbf{p}$ – vector containing internal variables, eg. carbon concentration.

Since the transition rules control the cells behaviour during calculations (i.e., during the deformation and precipitation processes), the proper definition of these rules in designing a CA model critically affects the accuracy of this approach. The transition rules of the developed Cellular Automata model of precipitation are based on the knowledge of experts, scientists, experimental observations, and available literature knowledge.

3. PHYSICAL BASE OF PRECIPITATION IN MICROALLOYED STEELS

In high strength low alloyed steels (HSLA) the microalloying elements: Ti, Nb, V are added in order to control their microstructure and mechanical properties. High chemical affinity of these elements for interstitials (N, C) results in precipitation of binary compound, nitrides and carbides and products of their mutual solubility – carbonitrides (Goldschmid, 1967). The composition of carbonitrides depends on the composition of steel as well as on the temperature. For calculation of the chemical composition of austenite as well as the composition and volume fraction of carbonitrides the thermodynamic models were developed (Roberts & Sandberg, 1980; Speer et al., 1987; Liu & Jonas, 1989; Adrian, 1992). They are based on the regular solution model for stoichiometric phases developed by (Hillert & Staffansson, 1970). In steel containing one of the microalloying elements (Ti, Nb, V) the carbonitride described by chemical formula MC_yN_{1-y} is formed, where y means atomic fraction of carbon in carbonitride. The austenite and carbonitride composition, as well as molar fraction of carbonitride, is described by the system of equations:

$$\ln\left(\frac{yK_{MC}}{[M_a][C_a]}\right) + (1-y)^2 \frac{L_{CN}^{M}}{RT} = 0 \tag{3}$$

$$\ln\left(\frac{(1-y)K_{MN}}{[M_a][N_a]}\right)+y^2\frac{L_{CN}^M}{RT}=0 \qquad (4)$$

$$M_a=\frac{f}{2}+(1-f)[M_a] \qquad (5)$$

$$C_a=\frac{yf}{2}+(1-f)[C_a] \qquad (6)$$

$$N_a=\frac{(1-y)f}{2}+(1-f)[N_a] \qquad (7)$$

Where symbol of element X_a, - element content in steel in atomic fraction, symbol of element in bracket, $[X_a]$ - atomic fraction of element dissolved in austenite, L_{CN}^M – parameter of mixing (-4260 J/mol (Adrian, 1992)), R – gas constant (J/(molK)), T –absolute temperature (K), K_{MX} – solubility product for binary compound MX, related to atomic fractions of M and X elements. Solution of the system of equations gives the required data on austenite composition at temperature T, ($[Ma]$, $[Ca]$, $[Na]$ in atomic fractions, molar fraction, f, of the carbonitride and its composition (y).

For the case of simultaneous addition of *Ti*, *Nb* and *V* in HSLA steels the thermodynamic equilibrium state is described by Adrian model (Adrian, 1992). It is necessary to emphasize that in some models describing the kinetics process of compounds precipitation the simplified thermodynamic model is applied, in which the possibility of the mutual dissolution of carbide and nitride forming by microalloying elements is neglected and the effect of nitrogen is considered as equivalent increase of carbon by nitrogen (Dutta & Sellars, 1987).

Existence of the solid solution in the thermodynamically instable condition show a tendency to split into new phases. In consequence, the following products are obtained:

- Matrix, which is the original phase, with different chemical composition but with not changed crystallographic lattice.
- Precipitate, which usually has different crystallographic lattice and different chemical composition.

The state of thermodynamic no equilibrium is usually obtained by decreasing of the temperature or by an increase of the pressure. The way of disintegration of the primary phase depends on a number of parameters and factors and is difficult to predict. Typical micrographs showing precipitates of niobium carbonitrides are shown in figure **1**. General information on the precipitation process of carbonitrides in HSLA steels are described in (Gladman, 1997; Adrian, 2011). Some of these information was used in the present work do develop the transition rules for the Cellular Automata model.

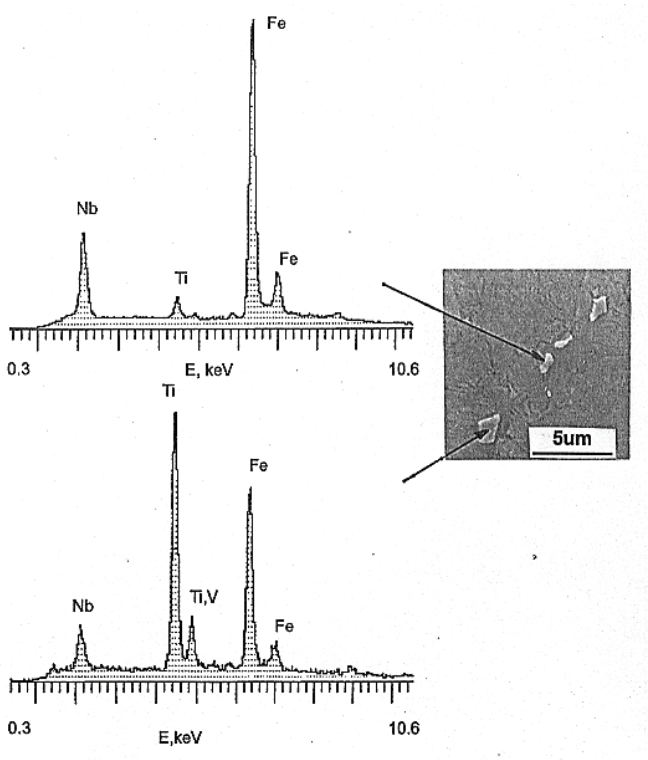

Fig. 1. *Micrographs showing precipitates of niobium carbonitrides.*

4. CELLULAR AUTOMATA PRECIPITATION MODEL

Publications dealing with modelling of precipitation using the Cellular Automata are scarce. Karapiperis (1995) proposed modelling of precipitation/dissolution reactions coupled with solute transport. In this model solute molecules perform a random walk on a regular lattice and react according to a local probabilistic rule. The model is appropriate for the study of the role of intrinsic fluctuations in the presence of reaction thresholds and can be employed to investigate porosity changes associated with the carbonation of cement. Objective of the present work was to apply CA technique to simulate strain induced transport of carbon and niobium in steel and further formation and growth of carbonitride precipitates. Main features of the proposed CA model are given in this Chapter.

4.1. Basic equations describing precipitation of carbonitrides

Conventional equations describing precipitation of carbonitrides, which were used in building the transition rules, are given below. Time between the deformation and beginning of precipitation was calculated as (Dutta & Sellars, 1987):

$$t_{0.05P} = \frac{3\times10^{-6}}{[\mathrm{Nb}]\varepsilon\sqrt{Z}}\exp\left(\frac{270000}{RT}\right)\exp\left\{\frac{2.5\times10^{-10}}{T^3\left[\ln\left(k_s\right)\right]^2}\right\} \quad (8)$$

where: ε – strain, Z – Zener-Hollomon parameter, R – gas constant (J/(molK)), T – absolute temperature (K), k_s – supersaturation ratio, being the ratio of actual amount [Nb] [C + (12/14)N] to the equilibrium amount, defined as:

$$k_s = \frac{[Nb]\left([C]+\frac{12}{14}[N]\right)}{10^{\left(\frac{6770}{T}-2.26\right)}} \quad (9)$$

Critical radius for nucleation, r_{cr}, which is assigned to a new nucleus in the CA model, is determined by the driving force and the equation is:

$$r_{cr} = -\frac{2\gamma_i}{\Delta G_v} \quad (10)$$

where: γ_i – energy of the interface equal to 0.5 J/m^2 (Dutta & Sellars, 2001), ΔG_v – the difference in free energy per unit volume (J/m^3), which is calculated from the formula:

$$\Delta G_v = \frac{-RT\ln\left(k_s\right)}{V_m} \quad (11)$$

where: V_m - molar volume; for Nb(C,N), V_m = 1.28×10^{-5} m^3/mol (Dutta & Sellars, 2001).

At elevated temperatures coagulation of the particles of precipitates occurs, what is modelled by the following equation:

$$r^3 - r_o^3 = \frac{8}{9}\frac{D_{Nb}[Nb]\gamma_i V_m^2}{RT}t \quad (12)$$

where: D_{Nb} – diffusion coefficient for niobium (m^2/s), t – time (s).

Deformation and resulting stresses has strong influence on precipitation. Dislocation density is used in the model as a measure of deformation. Increment of the dislocation density in a time step is calculated from the differential equation proposed by Mecking and Estrin (1984) written in a differential form:

$$\Delta\rho = \left[\frac{\dot{\varepsilon}M}{bl} - B_0\dot{\varepsilon}^n\exp\left(\frac{Q_s}{RT}\right)\rho\right]\Delta t \quad (13)$$

where: t – time, $\dot{\varepsilon}$ – strain rate (1/s), M – Taylor constant, b – length of the Burgers vector (2.59×10^{-10} m (Dutta & Sellars, 2001), l – average free path for dislocations (m), n – coefficient, B_0 – coefficient of recovery, Q_s – activation energy for self diffusion (J/mol).

Presented equations are used in the model to calculate the conditions, which are used in the transition rules.

4.2. General assumptions of the CA model – states of cells and variables

Two dimensional CA space was created. Three alternative neighbours were tested: Moore - as neighbors, assume all cells, the cells lying on the sides and in the corners, Von Neumann - as neighbors, take only the cells lying on the sides of the cell, hexagonal is a modification of Moore neighborhood, reject the cells lying on the diagonal of the cell. Periodic boundary conditions were assumed. Since dimensions of precipitates are few orders magnitude smaller than the grain size, the modelling process was carried out in a domain, which represented very small part of the material. Three possible states of the cell were introduced: *austenite* (γ), *precipitate* (P) and *boundary* (γ-P). Beyond this, each cell was characterised by the internal variables: nucleation rate (N), dislocation density (ρ). The following external variables were assumed: concentration of carbon, nitride and niobium in steel ([C], [N], [Nb]), current radius of the precipitate (r).

4.3. Transition rules and flow of calculations

The transition rules transfer the mathematical model and the knowledge regarding precipitation into the CA space. The cell, which belongs to the austenite grain, will become a nucleus of a precipitate, with certain probability, if:

– It has a dislocation density exceeding critical value ρ_{cr}, which is a function of the temperature (decrease of the temperature results in a decrease of a critical dislocation density).

The cell, which belongs to the austenite grain, will become a precipitate, if:

- It has at least one neighbour, which is a precipitate and the displacement of the γ-P interface is larger than the distance between the cells and the content of niobium in this cell is above equilibrium level.
- The cell, which is a precipitate, will coagulate, if:
- It has at least one neighbour, which is also a precipitate and the increase of the radius r is larger than the distance between the cells.

In each time step calculations begin with determination of the increment of the dislocation density from equation (13). This increment is distributed randomly between all the cell, except the cell which are *Precipitate*. Dislocations are allowed to migrate randomly but they cannot cross austenite grain boundaries. In consequence, random distribution of dislocation density is obtained with higher density close to the grain boundary and lower density inside the grains. The transition rule for the nucleation is checked next. Taking into account mentioned above information, the following transition rule was formulated for nucleation of the precipitate:

$$\mathrm{Y}_{i,j}^{t+1} = \begin{cases} \text{if } (\Lambda) \Rightarrow \mathrm{P} \\ \text{else } \Rightarrow \mathrm{Y}_{i,j}^{t} \end{cases} \tag{14}$$

where:

$$\Lambda = \mathrm{Y}_{i,j}^{t} \equiv \gamma \wedge \rho_{i,j} > \rho_{cr} \wedge l_{(0,1)} < P_{N1} \tag{15}$$

P_{N1} – probability of nucleation (random number between 0.3 and 0.5), $l_{(0,1)}$ – an arbitrary number between 0 and 1, ρ_{cr} – critical dislocation density to create strain induced precipitate (10^{10} 1/m^2 (Estrin & Mecking 1984).

Niobium is removed from the neighbour cells to the precipitate. The transition rule for the nucleation is checked next. The following logical function Λ for a transition rule (14) was proposed for growth of the precipitate:

$$\Lambda = \mathrm{Y}_{i,j}^{t} \equiv \gamma \wedge \rho_{i,j} > \rho_{cr} \wedge \mathrm{Y}_{k,l}^{t} \equiv$$

$$\mathrm{P} \wedge l_{(0,1)} < P_{N2} \wedge \left[\mathrm{Nb}\right]_{i,j} > \left[\mathrm{Nb}\right]_{cr} \wedge \Delta r > d \tag{16}$$

where: P_{N2} – probability of growth (random number between 0.3 and 0.5), $[\mathrm{Nb}]_{cr}$ – critical content of niobium in a cell to form a precipitate, Δr – increase of the precipitate calculated from equation (12), d – cell size (nm).

The transition rules are checked at each time step. When deformation is finished, the dislocation density remains constant, what means that the model at this stage does not account for the recovery. This relation has to be added in each cell separately, because recovery depends on the current level of the dislocation density. It will be added to the model in the future works. Calculations are stopped when the content of niobium in steel is too low to form new precipitate cells.

On the basis of the presented model program in C# was written and implemented in the Visual Studio 2010. Graphical interface was added. The following input data are introduced through the interface:

- Content of niobium, carbon and nitrogen in steel.
- Temperature (constant cooling rate condition is possible)
- Strain rate
- Size of the Cellular Automata space
- Neighbourhood (three neighbourhoods are available).

The following parameters are calculated by the model:

- Distribution of the dislocation density.
- Distribution function for the size of precipitates and an average size of precipitates.

The model contains several parameters, which are not known a'priori. These parameters are critical dislocation density, niobium content necessary to create a precipitate, and probabilities P_{N1} and P_{N2} in equations (15) and ( ) (both random numbers are in the range 0.3 and 0.5). In the present calculations these parameters were assumed. In future works the model will be identified and the coefficients will be determined using inverse analysis for experimental data.

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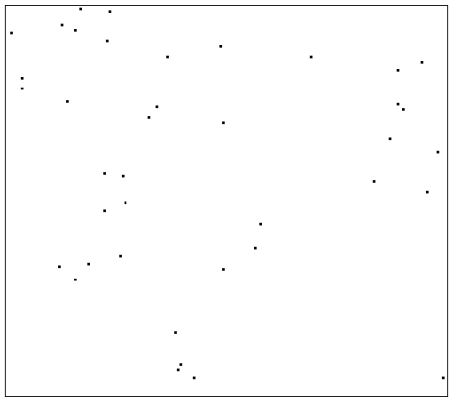
5. RESULTS

Numerical tests were performed to evaluate model's predictive capabilities. Steel containing 0.15%C, 0.43%Mn, 0.038%Nb and 0.007%N was considered. Since precipitates are few orders of magnitude smaller than the austenite grain size, generation of the initial microstructure was limited to initiation of the input parameters. The results presented below were obtained for the 150×150 cells, while the dimension of a single cell was 1 nm. How-

ever, further control of the size of the sample was possible.

5.1. Effect of the neighbourhood

Simulations for various neighbourhoods were performed and negligible effect was observed, see comparison for Moore and hexagonal neighbourhood in figure 2. In these simulations the temperature of 950°C and strain of 0.3 were assumed. Further analysis included the effect of the strain. Figure 3 shows distribution of precipitates for strains of 0.01 and 0.3. Increase of strains leads to rapid decrease of the precipitation time and to larger number of precipitates. It is due to the fact that occurrence of larger number of precipitates leads to a decrease of the niobium content in the austenite and, in consequence, the growth of precipitates is retarded.



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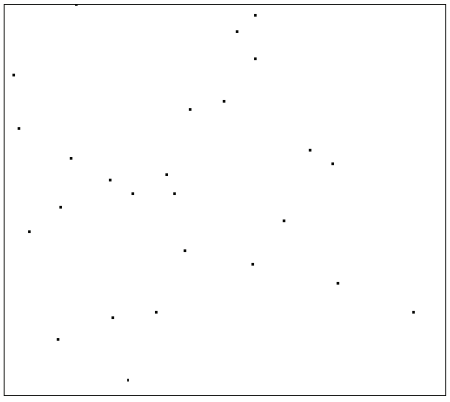
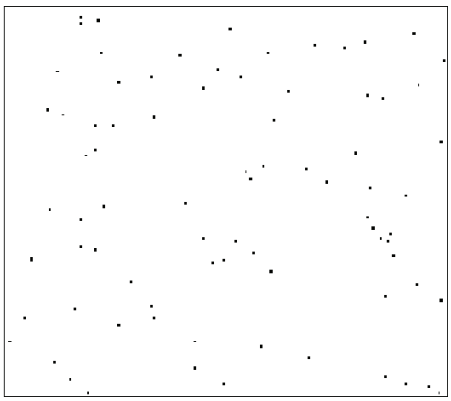


b)

Fig. 2. *Comparison of shape and distribution of precipitates at 950°C for Moore (a) and hexagonal (b) neighbourhoods, strain of 0.3.*

Effect of strain on kinetics of precipitation is presented in figure 4. Changes of an average niobium content in the austenite during precipitation are shown in figure 4a. Changes of an average radius of precipitates are shown in figure 4b. It is seen that the model properly predicts significant acceleration of precipitation caused by plastic deformation.



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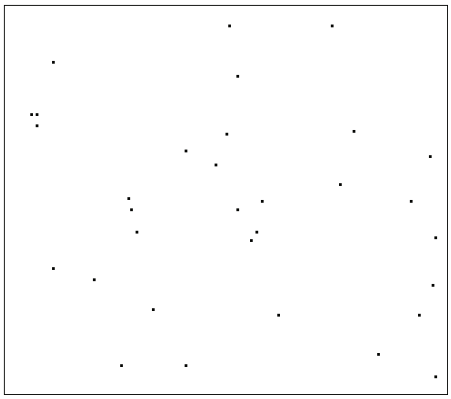
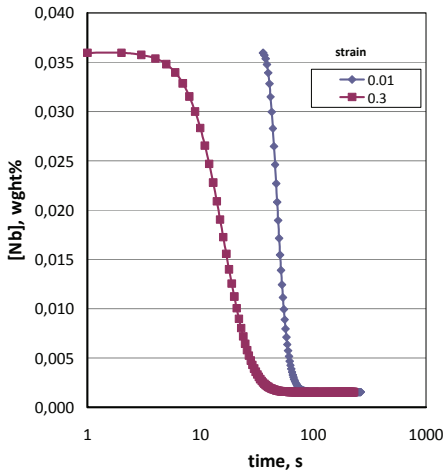


b)

Fig. 3. *Comparison of shape and distribution of precipitates at 850°C for a strain of 0.01 after 110 s (a) and for a strain of 0.3 after 12 s (b) (both are for Moore neighbourhood).*

Precipitation is thermally activated process and strong influence of the temperature is expected. Solubility of niobium in an iron decreases rapidly with a decrease of the temperature. Therefore, sensitivity of the model to temperature was investigated next. Changes of niobium content and radius of precipitates for steel subject to a strain of 0.01 at various temperatures are presented in figure 5.

Decrease of the temperature leads to a decrease of the average radius of precipitates to 7.7×10^{-10} m and to an increase of the number of precipitates. Decrease of the temperature caused also shortening of the time necessary for the first precipitates to occur. On the other hand, the total time until the whole niobium in the austenite precipitates is longer for lower temperature.



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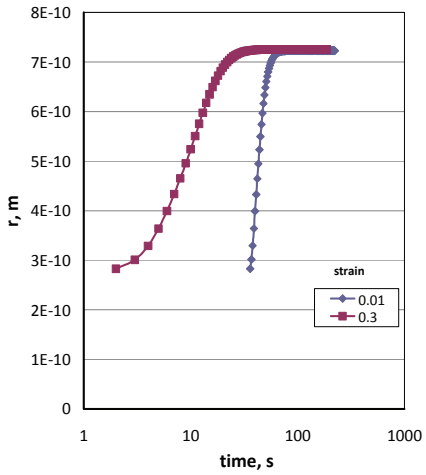
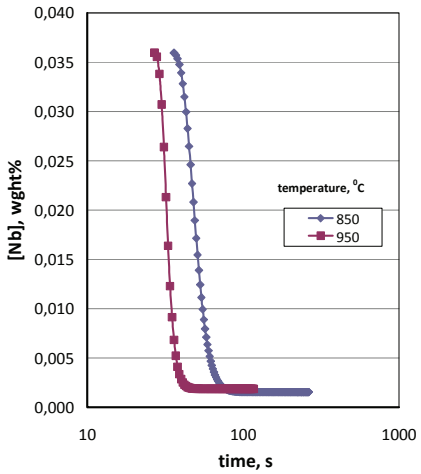


b)

Fig. 4. *Calculated changes of dissolved niobium content, [Nb] (a) and radius, r, of precipitates (b) for various strains. T = 850 °C*



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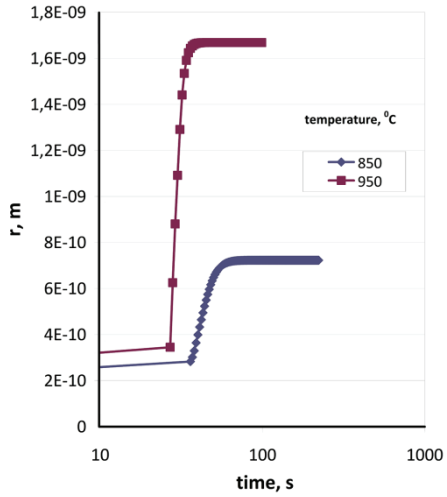

b)

Fig. 5. *Calculated changes of dissolved niobium content, [Nb] (a) and radius, r, of precipitates (b) for various temperatures.*

6. CONCLUSIONS

A proposition of the Cellular Automata model for the precipitation of carbonitrides in niobium steels was presented in the paper. Transition rules for nucleation and growth of precipitates were formulated. Performed numerical tests have shown that model reproduced qualitatively well process of precipitation. Predictions of kinetics of precipitation and changes of the average size of precipitates as well as dependence of these parameters on strains and temperature agreed with tendencies observed in experiments.

The model needs further development, which should include:

– Identification of such parameters as critical dislocation density, niobium content necessary to create a precipitate, and probabilities P_{N1} and P_{N2} in equations (15) and (16).
– Accounting for the effect of recovery after deformation.
– Validation of the model by a comparison of predictions with the experimental data.

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MODEL WYKORZYSTUJĄCY AUTOMATY KOMÓRKOWE DO SYMULACJI PROCESÓW WYDZIELENIOWYCH W STALACH Z MIKRODODATKIEM NIOBU

Streszczenie

W pracy przedstawiono propozycję modelu wykorzystującego metodę automatów komórkowych do opisu kinetyki procesów wydzieleniowych w stalach mikrostopowych z niobem. Wykorzystując wiedzę dotyczącą procesów wydzieleniowych sformułowane zostały reguły przejścia dla modelu. Model uwzględnia zmiany gęstości dyslokacji w wyniku odkształceń plastycznych i przewiduje kinetykę procesu wydzieleniowego oraz kształt wydzieleń węglikoazotków niobu. Wykonane testy numeryczne potwierdziły jakościowo dobrą dokładność modelu.

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