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MODELING OF THE KINETICS OF CARBONITRIDES PRECIPITATION PROCESS AND SIMULATE THE IMAGE OF MICROSTRUCTURE USING CELLULAR AUTOMATA METHOD IN MICROALLOYED STEELS

Microalloying elements such as Ti, Nb, V, entered into steel they influence their microstructure and mechanical properties, because formation of carbonitrides, M(C,N). Influence of carbonitrides to the microstructure and mechanical properties depends on their basic stereological parameters: volume fraction, V_v , and their size, r . In this work the Cellular Automata model of the kinetics of the carbonitrides precipitation which enable to predict the image of the microstructure and calculate the size of carbonitrides formed during isothermal annealing of supersaturated steel is presented. In the high temperature the microalloying elements inhibit the austenite grains growth. Chemical composition of steel has influence to volume fraction and size of precipitations. The work is supplemented with examples of experimental comparison.

Keywords: cellular automata; precipitation; carbonitrides; microalloying elements; microalloyed steel

1. Introduction

Carbonitrides precipitations of microalloying elements such as V, Nb and Ti, strongly influence the microstructure and mechanical properties of high strength low alloy steels. To predict the mechanical properties of these steels parameters of precipitates such as size (mean radius) and content (volume fraction) are required. The development of computer science enables simulations of precipitation process. The models are based on the algebraic equations describing the nucleation and growth kinetics of precipitates. Important group of structural steels are microalloyed steels with ferrite-pearlite microstructure, where high mechanical properties are achieved through small additions of elements such as Ti, Nb, V, introduced separately or comprehensively. These elements have high chemical affinity for interstitial elements C, N and form sparingly soluble compounds, carbides and nitrides. Due to the similarity of the crystal lattice these compounds exhibit mutual solubility which results in forming complex compounds carbonitrides, M(C,N). The carbonitrides undissolved at austenitisation temperature inhibit the growth of austenite grains, providing a fine grain of supercooled austenite transformation products. Effect of the carbonitride parameters, volume fraction, V_v , and the average radius

of the precipitations, r , on the average radius of the austenite grains, R_a , describes the Smith-Zener equation [1]:

$$R_a = \frac{4r}{3V_v} \quad (1)$$

Knowledge of parameters carbonitrides precipitations, both undissolved in austenite at high temperatures and formed in ferrite during phase transformations of undercooled austenite allows to predict the mechanical properties after manufacturing process using the knowledge of the steel chemical composition and process parameters [6]. Carbonitride precipitations parameters, their contents, V_v , and size distribution of precipitates can be calculated using mathematical models [2-4].

It is very hard to find any information in publications about modelling of precipitation using the Cellular Automata. In 1995 Karapiperis proposed modelling of precipitation/dissolution reactions coupled with solute transport [28]. In this model solute molecules perform a random walk on a regular lattice and react according to a local probabilistic rule. One of the first work on modelling of the kinetics of carbonitrides precipitation process using Cellular Automata method is presented in [8]. Objective of the present paper is to show how to apply Cellular Automata technique to simulate the image of microstructure of steel during

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the carbonitrides precipitation process and calculate the parameters of precipitates such as size (mean radius) and content (volume fraction).

2. Physical base of precipitation in microalloyed steels

The one of microalloying element such as Nb, Ti or V is added into low alloyed steels to control their microstructure and mechanical properties. High chemical affinity of this element for interstitials (N, C) results in precipitation of binary compound, nitrides and carbides and products of their mutual solubility – carbonitrides [5]. The composition of carbonitrides depends on the composition of steel as well as on the temperature. For calculation of the chemical composition of austenite, the composition and volume fraction of carbonitrides the thermodynamic models were developed [6-11]. They are based on the regular solution model for stoichiometric phases developed by [12]. The effect of addition of Ti, Nb and V in low alloyed steels on the thermodynamic equilibrium state is described by Adrian model [1]. The final form of equations describing the state of thermodynamic equilibrium in the $Fe - M' - M'' - M''' - C - N$ system is as follows [1]:

$$\left\{ \begin{array}{l} y \ln \frac{xyk_{MC}}{[M'_a][C_a]} + (1-y) \ln \frac{x(1-y)k_{MN}}{[M'_a][N_a]} + \\ + y(1-y) \frac{L_{CN}}{RT} = 0 \\ y \ln \frac{vyk_{M''C}}{[M''_a][C_a]} + (1-y) \ln \frac{v(1-y)k_{M''N}}{[M''_a][N_a]} + \\ + y(1-y) \frac{L_{CN}}{RT} = 0 \\ y \ln \frac{zyk_{M'''C}}{[M'''_a][C_a]} + (1-y) \ln \frac{z(1-y)k_{M'''N}}{[M'''_a][N_a]} + \\ + y(1-y) \frac{L_{CN}}{RT} = 0 \\ vy \ln \frac{x[M'_a]k_{MC}}{v[M'_a]k_{M''C}} + z(1-y) \ln \frac{z[M'_a]k_{M''N}}{x[M'_a]k_{MN}} + \\ + (1-y) \ln \frac{x(1-y)k_{MN}}{[M'_a][N_a]} + y(1-y) \frac{L_{CN}}{RT} = 0 \end{array} \right. \quad (2)$$

where: $[M'_a], [C_a], [N_a]$ – atomic fraction of element dissolved in austenite, y – atomic fraction of carbon in carbonitride, 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 (C or N) elements, L_{CN}^M – parameter of mixing, (-4260 J/mol [13]), $z = (1 - x - v)$.

The system of equations Eq. (2) contains 8 unknown atomic fractions: $[M'_a], [M''_a], [M'''_a], [C_a], [N_a]$ and x, v, y . Additional equa-

tions resulting from the mass balance of the elements that make up the reaction and produce carbonitride, are required [1]:

$$\left\{ \begin{array}{l} M'_a = \frac{x}{2} f + (1-f) [M'_a] \\ M''_a = \frac{v}{2} f + (1-f) [M''_a] \\ M'''_a = \frac{z}{2} f + (1-f) [M'''_a] \\ C_a = \frac{y}{2} f + (1-f) [C_a] \\ N_a = \frac{1-y}{2} f + (1-f) [N_a] \end{array} \right. \quad (3)$$

where: f – is the atomic fraction of the $M'_x M''_y M'''_{1-x-y} C_y N_{1-y}$, M'_a, C_a, N_a – the content of the elements in steel, expressed in atomic %.

Presented thermodynamic model allows to calculate the chemical composition of austenite, the composition and volume fraction of carbonitrides at given temperature under thermodynamic equilibrium conditions based on the knowledge of the chemical composition of the steel. The thermodynamic model does not allow for the calculation of the size of precipitations. Information about the size of precipitations produced under non-equilibrium thermodynamic conditions enables the models of kinetics of carbonitride precipitation [6-11]. The equations describing the state of thermodynamic equilibrium in the $Fe - M' - M'' - M''' - C - N$ system can be transformed to systems containing two or one microalloying element.

- $Fe - M' - M'' - C - N$ system [1]:

$$\left\{ \begin{array}{l} y \ln \frac{xyk_{MC}}{[M'_a][C_a]} + (1-y) \ln \frac{x(1-y)k_{MN}}{[M'_a][N_a]} + \\ + y(1-y) \frac{L_{CN}}{RT} = 0 \\ y \ln \frac{(1-x)k_{M'''C}}{[M'''_a][C_a]} + (1-y) \ln \frac{(1-x)(1-y)k_{M'''N}}{[M'''_a][N_a]} + \\ + y(1-y) \frac{L_{CN}}{RT} = 0 \\ x \ln \frac{x(1-y)k_{MN}}{[M'_a][N_a]} + (1-x) \ln \frac{(1-x)(1-y)k_{M'''N}}{[M'''_a][N_a]} + \\ + y^2 \frac{L_{CN}}{RT} = 0 \end{array} \right. \quad (4)$$

- $Fe - M - C - N$ system [1]:

$$\left\{ \begin{array}{l} \ln \frac{yk_{MC}}{[M_a][C_a]} + (1-y)^2 \frac{L_{CN}}{RT} = 0 \\ \ln \frac{(1-y)k_{MN}}{[M_a][N_a]} + y^2 \frac{L_{CN}}{RT} = 0 \end{array} \right. \quad (5)$$

Additional equations resulting from the mass balance of the elements that make up the reaction and produce carbonitride, are required (Eq. (3)) [1].

3. Model of the kinetics of carbonitrides precipitation process

To calculate the kinetics of the carbonitrides precipitation process in the low alloy steel a model based on the classical theory of nucleation and growth (CNGT) was developed. CNGT is based on the change in free energy, ΔG , associated with the formation of an embryo in a supersaturated solid solution. In the process of carbonitrides precipitation there are three stages: nucleation, growth and coalescence, which can occur simultaneously. The nucleation rate V_n , is described by the equation [14]:

$$V_n = \frac{dN}{dt} = N_0 Z \beta^* \exp\left(-\frac{\Delta G^*}{kT}\right) \exp\left(-\frac{\tau}{t}\right) \quad (6)$$

where: β^* – the condensation rate of solute atoms in cluster of critical size, Z – Zeldovich parameter, N_0 – number of nucleation site per unit volume, ΔG^* – critical Gibbs free energy for nucleus formation, k – Boltzmann constant, T – temperature, τ – incubation time, t – time.

Embryo critical radius r^* , parameters β^* and Z represent the following equations [14]:

$$r^* = -\frac{2\gamma}{\Delta G_v} \quad (7)$$

$$\beta^* = \frac{4\pi r^{*2} D X}{a^4} \quad (8)$$

$$Z = \frac{v_{at}^p}{2\pi r^{*2}} \sqrt{\frac{\gamma}{kt}} \quad (9)$$

The incubation time, τ is given by equation [14]:

$$\tau = \frac{4}{2\pi\beta^* Z^2} \quad (10)$$

where: γ – interphase boundaries energy, ΔG_v – the driving force for precipitation per unit volume, D – diffusion coefficient of the metallic element, X – a fraction of the atomic metallic element dissolved in matrix, a – lattice parameter, v_{at}^p – the average volume of an atom in precipitation.

In the case of the formation of precipitates of carbonitrides, described by formula MC_yN_{1-y} driving force of nucleation is equal to [14]:

$$\Delta G_v = -\frac{RT}{V_{MCN}} \left[\ln\left(\frac{X_M^S}{X_M^e}\right) + y \ln\left(\frac{X_C^S}{X_C^e}\right) + (1-y) \ln\left(\frac{X_N^S}{X_N^e}\right) \right] \quad (11)$$

where: X_i^S – the atomic fraction of the component X in the solution i , X_i^e – equilibrium atomic fraction of component X in solution. V_{MCN} – molar volume of carbonitride MC_yN_{1-y} .

Growth rate, V_{gr} , is described by equation [14]:

$$V_{gr} = \frac{dr}{dt} = \frac{D}{r} \left(\frac{X - X^i(r)}{\alpha X^p - X^i(r)} \right) \quad (12)$$

where: D – diffusion coefficient of metal M , X , X^p , atomic fractions of X in matrix and in precipitate, $X^i(r)$ – equilibrium solute fraction of X at precipitate/matrix interface taking into account the Gibbs-Thomson effect, $\alpha = \frac{v_{at}^M}{v_{at}^p}$ – ratio of matrix to precipitate volumes.

In the last stage the precipitations undergo the coagulation process involving of dissolution of small precipitates and growing of large precipitation at constant V_V and $\bar{r} = r^*$. The coarsening process of precipitates is described by equation [1]:

$$V_{coarse} = \frac{d\bar{r}}{dt} = \frac{4}{27} \left(\frac{X^i}{\alpha X^p - X^i} \right) \frac{2\gamma v_{at}^p D}{kT \bar{r}^2} \quad (13)$$

Consequently, mean radius, \bar{r} , of precipitates is an increasing function of time. As a result, the particle density, N_V , decreases and size distribution as a probability density function, $g(r)$, with a negative asymmetry moves toward larger particle size.

4. Cellular Automata model

Cellular Automata (CA) model is very efficient in modeling various phenomena in materials science. The main principles of the applications of the CA method in materials science were discussed by Raabe [15]. Modelling microstructure evolution is the most frequent application of the CA. 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.

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:

$$Y_{i,j}^{t+1} = \begin{cases} \text{if } (\Lambda) \Rightarrow \text{new state} \\ \text{else } \Rightarrow Y_{i,j}^t \end{cases} \quad (14)$$

where: $Y_{i,j}^{t+1}$, $Y_{i,j}^t$ – 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:

$$\Lambda = \Lambda(Y_{i,j}^t, Y_{k,l}^t, \mathbf{p}, \mathbf{q}) \quad (15)$$

where: $Y_{k,l}^t$ – 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, e.g. temperature, \mathbf{q} – vector containing internal variables, e.g. carbon concentration.

Since the transition rules control the cells behaviour during calculations, the proper definition of these rules in designing a CA model critically affects the accuracy of this approach.

4.1. Cellular Automata model – MCN_CA computer program

MCN_CA computer program was written in Delphi 4.0. In MCN_CA program two dimensional CA space was created with square shape. Each cell in space has square shape. In CA model constructing the anisotropy of grid was not considered. 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 ($-P$). Growing of cells in every direction (up, down, left, right, and corners) is determined by Moore's neighborhood. Shape of precipitations on the image is determined by shape of cells. CA method needs some simplifications to be done. At the boundary of CA was considered absorbing conditions, means that every cell in boundary has the same value which cannot be changed. At the interfacial boundaries was considered the reflective condition. Before changing state of the cell the states of neighbors cells are checked. If there is minimum one of a cell with state of precipitation, the state of initial cell cannot be change. Each cell in CA has the same dimension and was divided to 10 layers, every layer has the same size. Every time step during simulation the change of radius is calculated (Δr). When calculated Δr is lower than value in cell, the information about it is updated. If Δr has size of one or more layer, information about occupied layers is updated. When all layers become to be occupied the whole cell becomes to be new cell of precipitate. One simple layer is represented the boundary region between precipitation and austenite. When Δr is higher than value in cell, the information about occupied layers is updated, layers are removed. Those processes are described as growing and coagulation. The CA model takes into account a simulation of solute diffusion. Growth rate and the coarsening process (Eq. 12 and 13) includes diffusion coefficient. The diffusion is considered only like the same in whole simulated space. Each cell in CA has the same value of diffusion but changing with temperature and content of solute. In whole space of CA the diffusion as a process is not consider. In MCN_CA program there are two parameters:

time start and time stop of simulation. Start time is set up to 0,00000001 sec. End time can be set up. Each time step in simulation is not the same. Time step is calculated on a logarithmic scale. In the beginning of the process time steps are very small and growing logarithmically until reaching time stop. It is very hard to find in literature any information about Cellular Automata method to simulate image of microstructure during carbonitrides precipitation process. More information can be found in [27].

5. Example of modelling of carbonitride precipitation

Developed computer program, MCN_CA, was used to simulate the image of carbonitride precipitates, Nb(C,N) and V(C,N), in microalloyed steel. Simulation of Nb(C,N) precipitation process was carried out for two steels A and B subjected to heat treatment austenitization at 1250°C with following holding at $T = 850, 900$ and 950°C for time, t , from $t = 0.00001$ to 100000 s. Results of the simulations were compared with the experimental data of the average radius of precipitates, measured after similar temperature of austenitization with holding at 850, 900 and 950°C for 100, 1000 and 10000 s [16].

TABLE 1

Chemical composition of steels [16], % mass

Steel	C	N	Nb	Mn
A	0.11	0.01	0.030	1.35
B	0.1	0.01	0.095	1.24

Simulation of V(C,N) precipitation process was carried out for two steels C and D subjected to austenitization at 1200°C with following holding at $T = 790^\circ\text{C}$ for 25 h (90 000 s) and quenching in water [17].

TABLE 2

Chemical composition of steels [17], % mass

Steel	C	N	V
C	0.02	0.022	0.26
D	0.05	0.0002	0.27

For the simulations in MCN_CA program the input data used during calculations are presented in the TABLE 3:

TABLE 3

Main parameters used in simulations

Parameter	Symbol	Value	Lit.
1	2	3	4
bulk diffusion of Nb	D_0 (m ² /s)	$1.4 \cdot 10^{-4}$	[18]
bulk diffusion of V	D_0 (m ² /s)	$0.25 \cdot 10^{-4}$	[19]
activation energy of Nb	Q (kJ/mole)	270	[18]
activation energy of V	Q (kJ/mole)	264.2	[19]
interfacial energy	γ (J/m ²)	0.5	[20]

TABLE 3. Continued

1	2	3	4
atomic weight, Nb	Nb	92.90	[21]
atomic weight, V	V	50.95	[21]
atomic weight, C	C	12.011	[21]
atomic weight, N	N	14.008	[21]
density, NbC	ρ_{NbC} (g/cm ³)	7.788	[22]
density, NbN	ρ_{NbN} (g/cm ³)	7.300	[22]
density, VC	ρ_{VC} (g/cm ³)	5.820	[22]
density, VN	ρ_{VN} (g/cm ³)	6.170	[22]
solubility product for binary compound, NbN	$\lg([\text{Nb}][\text{N}])$	$3.7 - 10800/T$	[23]
solubility product for binary compound, NbC	$\lg([\text{Nb}][\text{C}])$	$2.26 - 6770/T$	[24]
solubility product for binary compound, VN	$\lg([\text{V}][\text{N}])$	$3.02 - 7840/T$	[25]
solubility product for binary compound, VC	$\lg([\text{V}][\text{C}])$	$6.72 - 9500/T$	[23]
molar volume of carbonitride, $\text{MC}_y\text{N}_{1-y}$	V_{MCN} (m ³ /mol)	$\left(y \frac{(M+C)}{\rho_{MC}} + (1-y) \frac{(M+N)}{\rho_{MN}} \right) \cdot 10^{-6}$	
lattice parameter, NbN	a_{NbN} (nm)	0.4392	[26]
lattice parameter, NbC	a_{NbC} (nm)	0.4471	[26]
lattice parameter, VN	a_{VN} (nm)	0.4139	[26]
lattice parameter, VC	a_{VC} (nm)	0.4166	[26]
lattice parameter, $\text{MC}_y\text{N}_{1-y}$	$a_{\text{MC}_y\text{N}_{1-y}}$ (nm)	$y a_{MC} + (1-y) a_{MN}$	
CA dimensions	x_size, y_size	500×500 cells	
cell dimensions	c_size (nm)	0.5×0.5	
time start	t_S (s)	0.0001	
time finish	t_F (s)	10000 or 100000	

Calculated images of carbonitride Nb(C,N) of A and B steels are presented in Fig. 1 and Fig. 2.

Comparison of calculated mean radius, \bar{r} , of precipitation with experimental data [16] is presented in Fig. 3 and Fig. 4.

At temperature 850°C experimental data lies almost on calculated curve $\bar{r} = f(\text{time})$ for A and B steel. At temperature 900°C experimental data lies slightly above calculated curve $\bar{r} = f(\text{time})$ for A and B steel. At temperature 950°C, \bar{r} precipitates lies below calculated curve. Larger difference between the compared values occurs at 10000 seconds. The comparison of calculated and experimental data shows a satisfactory convergence, which

proves that the developed computer program can be a useful tool supporting the design of heat treatment parameters, providing the desired mechanical properties of steel.

Calculated images of carbonitride V(C,N) are presented in Fig. 5.

Comparison of calculated mean radius, \bar{r} , of precipitation with experimental data [17] is presented in Fig. 6.

For both steels experimental data lies above on calculated curve $\bar{r} = f(\text{time})$. Larger difference between the compared values occurs at 90000 seconds for steel C.

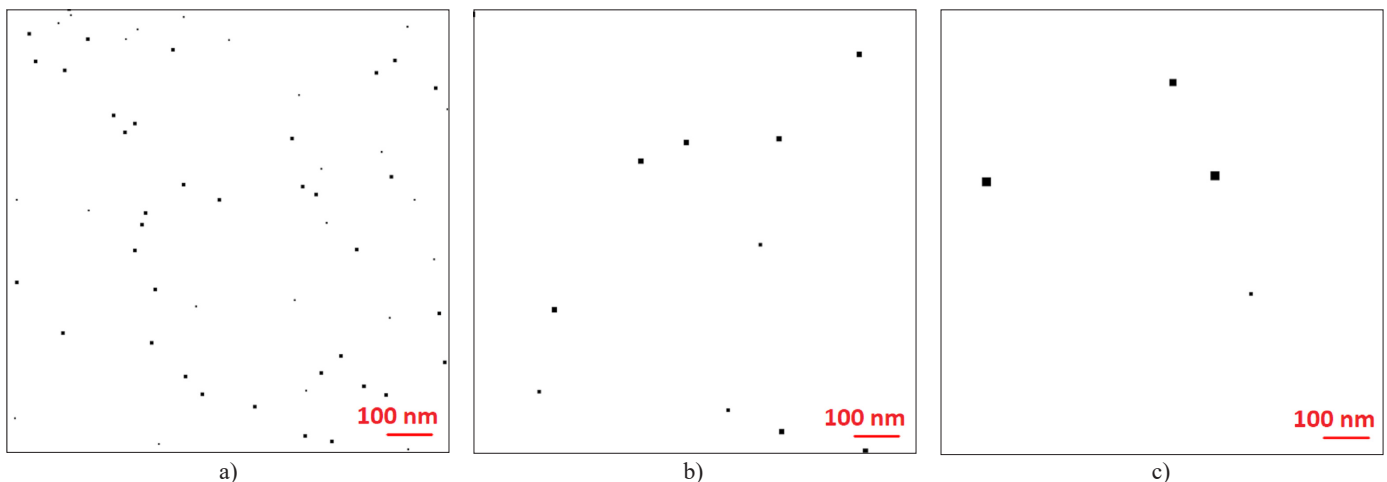


Fig. 1. Simulated microstructures with precipitations of carbonitrides in microalloyed niobium A – 0.11C/0.01N/0.03Nb/1.35Mn steel after heat treatment: austenitization at 1250°C with following isothermal holding at 850°C (a), 900°C (b) and 950°C (c) for 100000 s

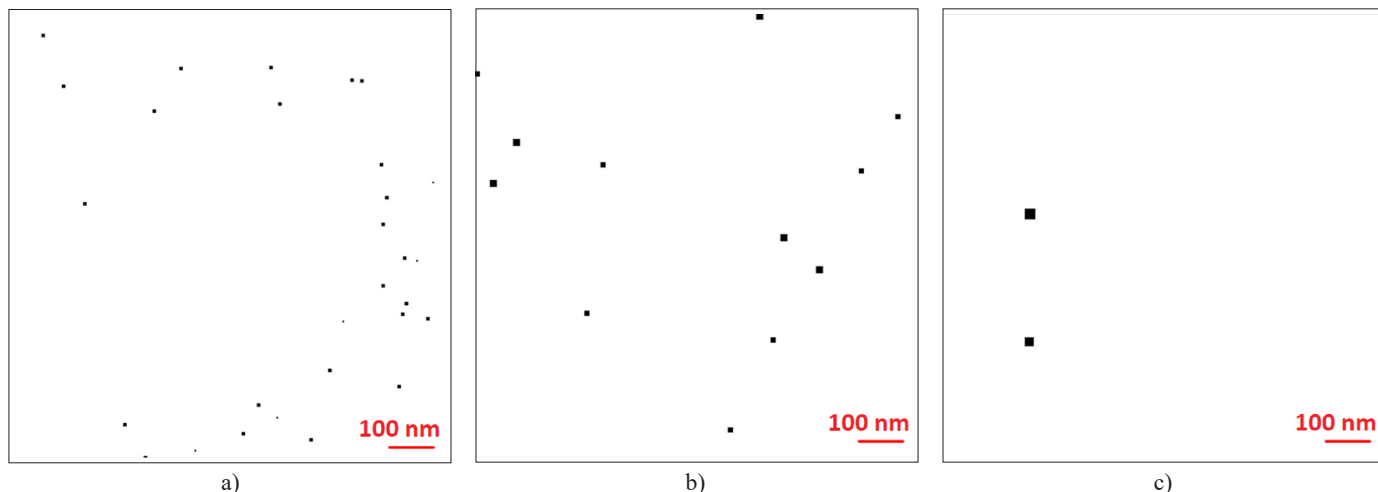


Fig. 2. Simulated microstructures with precipitations of carbonitrides in microalloyed niobium B – 0.1C/0.01N/0.095Nb/1.24Mn steel after heat treatment: austenitization at 1250°C with following isothermal holding at 850°C (a), 900°C (b) and 950°C (c) for 100000 s

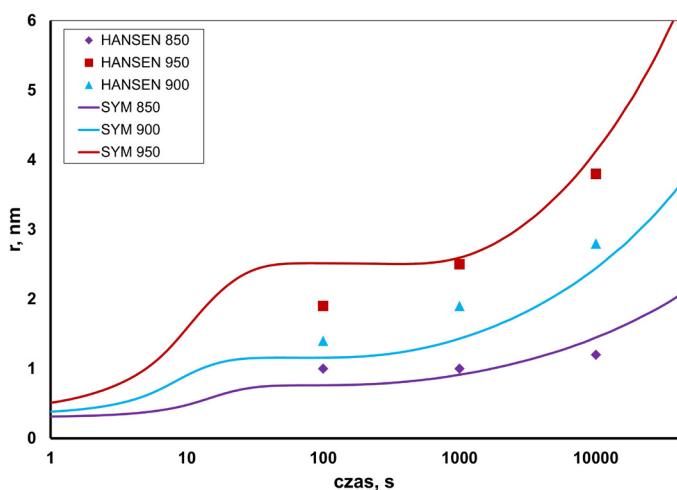


Fig. 3. Comparison of calculated mean radius, \bar{r} (steels A – 0.11C/0.01N/0.03Nb/1.35Mn), of precipitation with experimental data [16], at $T = 850^\circ\text{C}$, 900°C , $T = 950^\circ\text{C}$ for $t = 100000$ s

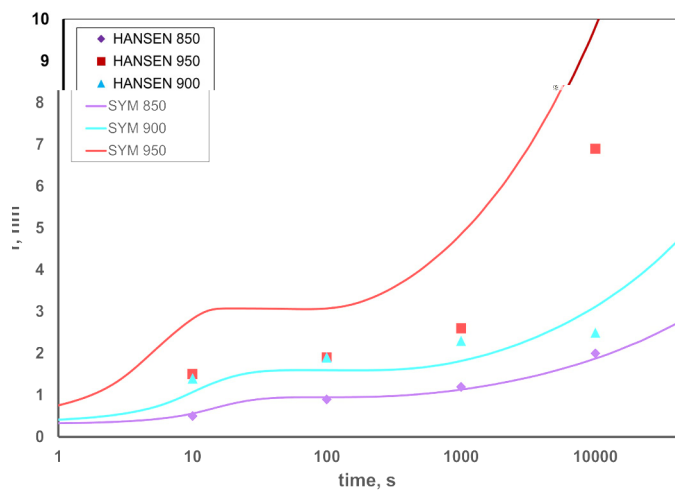


Fig. 4. Comparison of calculated mean radius, \bar{r} (steels B – 0.1C/0.01N/0.095Nb/1.24Mn), of precipitation with experimental data [16], at $T = 850^\circ\text{C}$, 900°C , $T = 950^\circ\text{C}$ for $t = 100000$ s

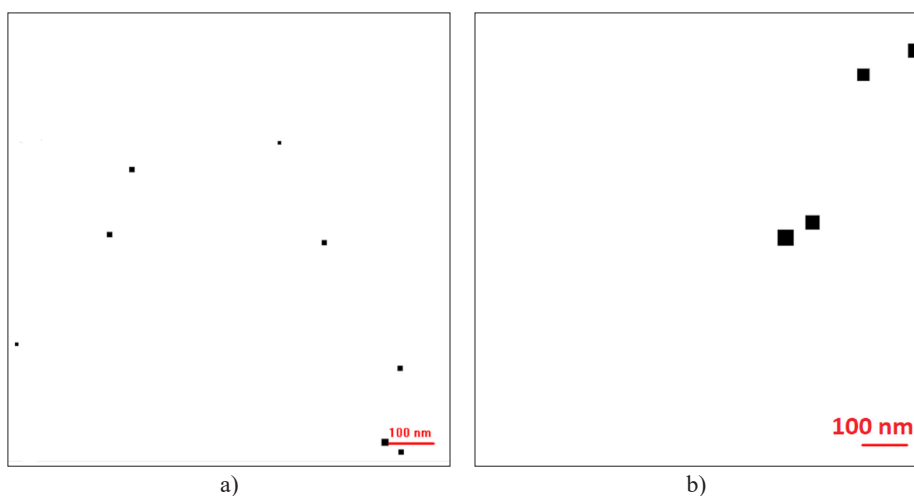


Fig. 5. Simulated microstructures with precipitations of carbonitrides in microalloyed vanadium C – 0.02C/0.022N/0.26V (a) and D – 0.05C/0.0002N/0.27V (b) steel after heat treatment: austenitization at 1200°C with following isothermal holding at 790°C for 90 000 s

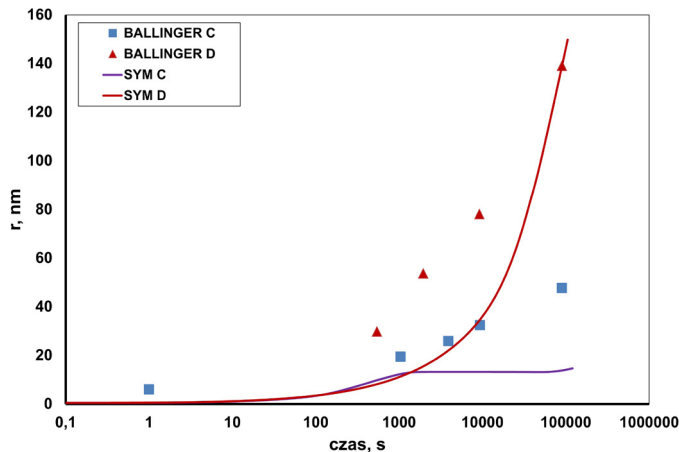


Fig. 6. Comparison of calculated mean radius, \bar{r} , (steel C – 0.02C/0.022N/0.26V and D – 0.05C/0.0002N/0.27V) of precipitation with experimental data [17], at $T = 790^{\circ}\text{C}$ for $t = 90000$ s.

5.1. Results discussion

In Fig. 1 and 2 are presented the simulated images of microstructure of steel A and B with different chemical composition after heat treatment: austenitization at 1250°C with following isothermal holding at 850°C (a), 900°C (b) and 950°C (c) for 100000 s [16]. It can be observed that with increase of the temperature of isothermal holding the size (radius) of precipitations are growing, but the volume fraction of the precipitations is decreasing. Different content of Nb has very small influence to size of the precipitates. In Fig. 3 and 4 is presented the comparison of simulated and experimental mean radius of the precipitations. In lower temperatures (850°C , 900°C) results of simulated and experimental are almost the same, but in the higher temperature (950°C) simulated mean radius lie above the experimental value. The curves show the same conclusion as images of microstructure that with increase of the temperature of isothermal holding the size (radius) of precipitations are growing and different content of Nb has very small influence to size of the precipitate. Fig. 5 shows simulated images of microstructure of steels with different chemical composition after heat treatment: austenitization at 1200°C with following isothermal holding at 790°C (c) for 90000 s [17]. It can be observed that level of N has influence to size of the precipitation. With higher content of N the mean radius of precipitation is lower than with low content of N. In Fig. 6 are presented the comparison of simulated and experimental mean radius of the precipitations. The curves shows the same conclusions as simulated images of microstructure that growing content of N causes lower size of mean radius of precipitation. Results of simulated and experimental data have differences resulting from simplification that have to be used in Cellular Automata model.

6. Conclusion

A particular advantage of the model is the ability to distinguish and track the individual stages of the carbonitride pre-

cipitation process (nucleation, growth, coagulation). It enables to calculate the size distribution of carbonitrides existing in austenite.

In steels with Nb content, different content of Nb has very small influence to size of the precipitates. With increase of the temperature of isothermal holding the size (radius) of precipitations are growing, but the volume fraction of the precipitations is decreasing

It is observed that N has big influence to size of mean radius of precipitation in steels with V content. Growing content of N causes lower size of mean radius of precipitation.

The model needs further development, which should include:

- extending the range of chemical composition of steel for case of simultaneous addition of several microalloying elements in steel, on the carbonitride precipitation process
- calculation of final mechanical properties of steel after heat treatment.

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