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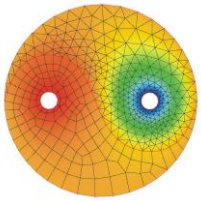

CELLULAR AUTOMATA MODEL OF CARBONITRIDES PRECIPITATION PROCESS IN STEELS

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Abstract

Cellular Automata (CA) model of carbonitride precipitation in microalloyed steels is presented in the paper. The model accounts for an increase of dislocation density due to plastic deformation and predicts kinetics of precipitation as well as stereological parameters of precipitates. Precipitation of compounds plays crucial role in controlling of properties of alloys. In low alloyed steels the microalloying elements: Ti, Nb, V are added in order to control their microstructure and mechanical properties. The most important tool in development of new processing technologies is numerical modelling. Modelling is a mathematical description of the relation between the main process variables and the resulting material properties. Many thermodynamics models were developed in the second half of the 20th century. For example the model of carbonitrides precipitation in microalloyed steels is considered works of Dutta & Sellars (1987), Dutta et al. (1991), Dutta et al. (2001). The models allow calculate kinetics of precipitation and stereological parameters of precipitates as a function of processing parameters. CA model proves to be very efficient in modelling various phenomena in materials science. The transition rules transfer the mathematical model and the knowledge regarding precipitation into the cellular automata space.

Key words: Cellular Automata, Carbonitrides, Microalloyed steels

1. INTRODUCTION

Cellular Automata (CA) model of carbonitride precipitation in microalloyed steels is presented in the paper. The model accounts for an increase of dislocation density due to plastic deformation and predicts kinetics of precipitation as well as stereological parameters of precipitates. Precipitation of compounds plays crucial role in controlling of properties of alloys. In low alloyed steels the microalloying elements: Ti, Nb, V are added in order to control their microstructure and mechanical properties. The most important tool in development of new processing technologies is numerical modelling. Modelling is a mathematical description of the relation between the main process variables and the resulting material properties. Many thermodynamics models were developed in the second half of the 20th century. For example the model of carbonitrides precipitation in microalloyed steels is considered works of Dutta & Sellars (1987), Dutta et al. (1991), Dutta et al. (2001). The models allow calculate kinetics of precipitation and stereological parameters of precipitates as a function of processing parameters. CA model proves to be very efficient in modelling various phenomena in materials science. The transition rules transfer the mathematical model and the knowledge regarding precipitation into the cellular automata space.

2. CARBONITRIDES PRECIPITATION PROCESS IN STEELS

The microalloying elements such as: Ti, Nb, V are added into steels 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 product – carbonitrides (Goldschmidt, 1967). The composition of carbonitrides depends on the composition of steel as

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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 (Adrian, 1992; Liu and Jonas, 1989; Roberts and Sandberg, 1980; Adrian et al., 2014). They are based on the regular solution model for stoichiometric phases developed by Adrian (1992), based on Hillert and Staffansson (1970) model for stoichiometric phases. 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:

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

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

$$M_a=\frac{f}{2}+(1-f)[M_a] \tag{3}$$

$$C_a=\frac{yf}{2}+(1-f)[C_a] \tag{4}$$

$$N_a=\frac{(1-y)f}{2}+(1-f)[N_a] \tag{5}$$

where: symbol of element M_a, C_a, N_a - element content in steel in atomic fraction, symbol of element in bracket, $[X_a]$ - atomic fraction of element X dissolved in austenite, L_{CN}^M – parameter of mixing (-4260 J/mol), 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, $[M_a]$, $[C_a]$, $[N_a]$ in atomic fractions, molar fraction, f, of the carbonitride and its composition (y).

The effect of addition of *Ti*, *Nb* and *V* in HSLA steels on the thermodynamic equilibrium state is described by Adrian model (Adrian, 1992; Adrian, 2011). Some models describing the kinetics process of binary compounds, carbides or nitrides precipitation. In such case simplified thermodynamic model is applied, in which the possibility of the mutual dissolution of carbide and nitride forming by microalloying elements is neglected and in calculation of kinetic of carbide precipitation the effect of nitrogen is considered as equivalent increase of carbon by nitrogen (Dutta and Sellars, 1987). Existence of the solid solution in the thermodynamically unstable condition shows 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 non-equilibrium thermodynamic state 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. General information on the precipitation process of carbonitrides in HSLA steels are described in (Adrian, 2011; Gladman, 1997). Some of these information was used in the present work do develop the transition rules for the Cellular Automata model.

3. BASIC EQUATIONS DESCRIBING PRECIPITATION OF CARBONITRIDES

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 (Dutta and Sellars, 1987):

$$R_a=\frac{4r}{3V_v} \tag{6}$$

The effect of strengthening of ferrite by dispersed carbonitrides precipitations formed during the transformation austenite-ferrite as a result of reactions between elements dissolved in austenite is the second

factor influencing the mechanical properties of microalloyed steel. This effect, which depends on carbonitride precipitation parameters, the mean diameter, d, and volume fraction, V_v, is described by Ashby-Orowan model (Dutta and Sellars, 1987):

$$\Delta\sigma_e = \frac{10.8\sqrt{V_v}}{d}\ln\left(\frac{d}{6.125\cdot 10^{-4}}\right) \tag{7}$$

where: $\Delta\sigma_e$ – increase of the yield point, MPa, d – mean diameter of carbonitride particles, μm.

This equation shows that with increase of carbonitride content and decrease size of precipitation results in improving of yield point of steel.

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. Carbonitride precipitations parameters, their contents, V_v and size distribution of precipitates can be calculated using mathematical models (Dutta and Sellars, 1987; Dutta et al., 1991; Gladmann, 1997; Wagner and Kampmann, 1991; Perez et al., 2008; Maugis and Goune, 2005; Adrian et al., 2014).

4. MODEL OF THE KINETIC 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 (Dutta and Sellars, 1987):

$$V_n = \frac{dN}{dt} = N_0 Z\beta^* \exp\left(-\frac{\Delta G^*}{kT}\right)\exp\left(-\frac{\tau}{t}\right) \tag{8}$$

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* - change of Gibbs free energy of system with the critical radius, r^*, nucleus formation, k - Boltzmann constant, T – temperature, τ - incubation time, t – time.

Embryo critical radius r^*, and parameters β^* and Z represent the following equations (Dutta and Sellars, 1987):

$$r^* = -\frac{2\gamma}{\Delta G_v} \tag{9}$$

$$\beta^* = \frac{4\pi(r^*)^2 DX}{a^4} \tag{10}$$

$$Z = \frac{v_{at}^p}{2\pi(r^*)^2}\sqrt{\frac{\gamma}{kT}} \tag{11}$$

The incubation time, τ, is given by equation (Dutta and Sellars, 1987):

$$\tau = \frac{4}{2\pi\beta^* Z^2} \tag{12}$$

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 MCyN1-y driving force of nucleation is equal to (Dutta and Sellars, 1987):

$$\Delta G_v = -\frac{RT}{V_{MCN}}\left[\ln\left(\frac{X_M^s}{X_M^e}\right) + y\ln\left(\frac{X_C^s}{X_C^e}\right) + (1-y)\ln\left(\frac{X_N^s}{X_N^e}\right)\right] \tag{13}$$

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

Growth rate, V_{gr}, is described by equation (Dutta and Sellars, 1987):

$$V_{gr} = \frac{dr}{dt} = \frac{D}{r}\left[\frac{X - X^i(r)}{\alpha X^p - X^i(r)}\right] \tag{14}$$

where: D – diffusion coefficient of metal the M, X, X_p - atomic fractions of X in matrix and in precipitate, respectively, $X^i(r)$ – equilibrium solute fraction of X at precipitate/matrix interface taking into account the Gibbs-Thomson effect, α – ratio of matrix to precipitate volumes, r – radius of precipitate.

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 $r = r^*$. The coarsening process of precipitates is described by equation (Dutta and Sellars, 1987):

$$V_{coarse} = \frac{dr}{dt} = \frac{4}{27}\left(\frac{X^i}{\alpha X^p - X^i}\right)\frac{2\gamma v_{at}^p}{kT}\frac{D}{r^2} \quad (15)$$

where: V_{coarse} – rate of coarsening.

Consequently, mean radius, 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.

5. CELLULAR AUTOMATA MODEL

The history of cellular automata is only quite recent, coming to life at the hands of two fathers, John von Neumann and Stanislaw Ulam in the early 1950s, although it was re-invented several more Times. In the early 1980s Stephen Wolfram in a seminal paper, "Statistical mechanics of cellular automata", initiated the first serious study of cellular automata. In this work and in a series of subsequent ones Wolfram began producing some of the images that have now become iconic in the field. It is now very much an established scientific discipline with applications found in a great many areas of science. Wolfram has counted more than 10.000 papers referencing his original works on the subject and the field of cellular automata has taken on a life of its own. The cellular automaton paradigm is very appealing and its inherent simplicity belies its potential complexity. Simple local rules govern an array of cells that update the state they are in at each tick of a clock. It has been found that this is an excellent way to analyze a great many natural phenomena, the reason being that most physical processes are themselves local in nature — molecules interact locally with their neighbors, bacteria with their neighbors, ants with theirs and people likewise. Although natural phenomena are also continuous, examining the system at discrete time steps does not really diminish the power of the analysis. So in the artificial cellular automaton world we have an unfolding microcosm of the real world.

Cellular Automata (CA) model is very efficient in modelling various phenomena in materials science. The main principles of the applications of the CA method in materials science were discussed by Raabe (1998). 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. 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.

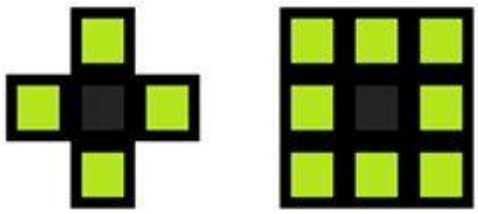

Fig. 1. *Von Neumann and Moore neighborhoods.*

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:

$$Y_{i,j}^{t+1} = \begin{Bmatrix} if\,(\Lambda) \Rightarrow newstate \\ else \Rightarrow Y_{i,j}^{t} \end{Bmatrix} \quad (16)$$

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:.

$$\Lambda = \Lambda\left(Y_{i,j}^{t}, Y_{k,l}^{t}, \mathbf{p}, \mathbf{q}\right) \quad (17)$$

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, **p** – vector containing external variables, e.g. temperature, **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. The transition rules of the developed CA model of precipitation are based on the knowledge of experts, scientists, experimental observations, and available literature knowledge.

5.1 Cellular Automata model of carbonitrides precipitation process

It is very hard to find any information in publications about modelling of precipitation using the Cel-

lular Automata. In 1995 Karapiperis 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. Objective of the present paper is to show how to apply CA technique to simulate strain induced transport of carbon and the niobium in steel and further formation and growth of carbonitride precipitate

5.2 General assumptions of the CA model - states of cells, variables and transition rules

Two dimensional CA space was created. 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, nitrogen and microalloying element, *MA* (titanium, niobium or vanadium) in austenite ([C], [N], [MA]), current radius of the precipitate (r). 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 MA 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. This increment is distributed randomly between all the cells, 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. The following transition rule was formulated for nucleation of the precipitate:

$$Y_{i,j}^{t+1} = \begin{Bmatrix} if\,(\Lambda) \Rightarrow P \\ else \Rightarrow Y_{i,j}^{t} \end{Bmatrix} \tag{18}$$

where:

$$\Lambda = Y_{i,j}^{t} \equiv \gamma \wedge \rho_{i,j} > \rho_{cr} \wedge l_{(0,1)} < P_{N1} \tag{19}$$

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} m^{-2}).

Microalloying element 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 was proposed for growth of the precipitate:

$$\begin{aligned} \Lambda &= Y_{i,j}^{t} \equiv \gamma \wedge \rho_{i,j} > \rho_{cr} \wedge Y_{k,l}^{t} \\ &\equiv P \wedge l_{(0,1)} \left\langle P_{N2} \wedge [MA]_{i,j} \right\rangle [MA]_{cr} \wedge \Delta r > d \end{aligned} \tag{20}$$

PN_2 – probability of growth (random number between 0.3 and 0.5), $[MA]_{cr}$ – critical content of niobium in a cell to form a precipitate, Δr – increase of the precipitate, d – cell size (nm).

Calculations are stopped when the content of MA 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 MA, carbon and nitrogen in steel, temperature, strain rate and size of the Cellular Automata space. 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 and composition of austenite. The model contains several parameters, which are not known a'priori. These parameters are critical dislocation density, MA content necessary to create a precipitate. The schematic diagram of calculation of carbonitrides precipitation process using CA model is shown in figure 2.

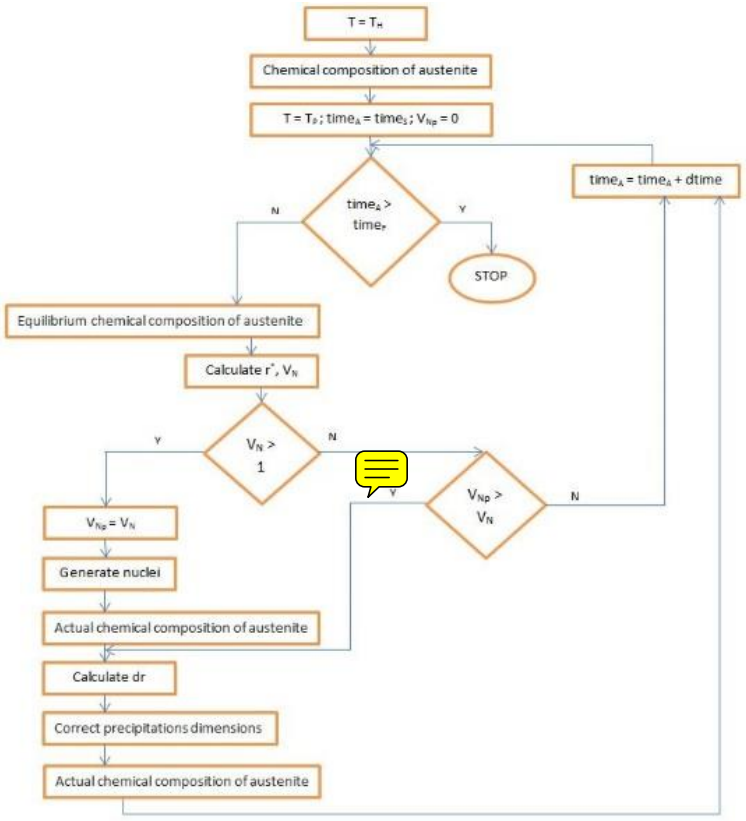

***Fig. 2**. The schematic diagram of calculation of carbonitrides precipitation process using CA model. Main symbols: TH – temperature of heat treatment austenitization, TP – precipitation temperature, timeA – actual time, timeS – start time, timeF – finish time, VN – nucleation rate, VNp – nucleation rate in previous step??*

6. RESULTS OF MODELLING

Steel containing 0.2% C, 0.02% Nb and 0.015% N subjected to heat treatment austenitization at Ta = 1200°C with following holding at T_p for τ (time) enabling of carbonitride Nb(C,N) precipitation from supersaturate austenite 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 of image calculations of microstructure with carbonitride precipitations presented in figure 3 were obtained for the 300×300 cells, while the dimension of a single cell was 1 nm.

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. Decrease of the temperature leads to a decrease of the average radius of precipitates and to an increase of the number of precipitates.

Example of analysis of carbonitride Nb(C,N) precipitation process in the low alloy steel using thermo kinetic model (Adrian et al., 2014) is presented in figures 4 - 7.

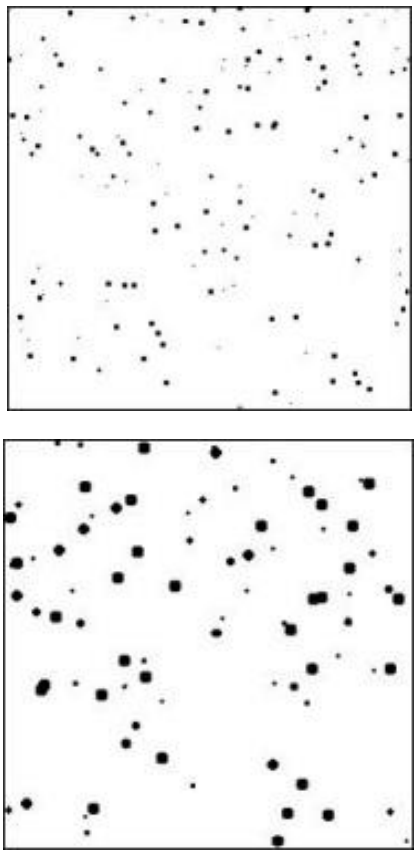

***Fig. 3.** Comparison of simulated microstructures with precipitations of carbonitrides in microalloyed niobium steel after heat treatment: austenitization at 1200°C with following isothermal holding at 880°C (a) and 980°C (b) for 10000 s.*

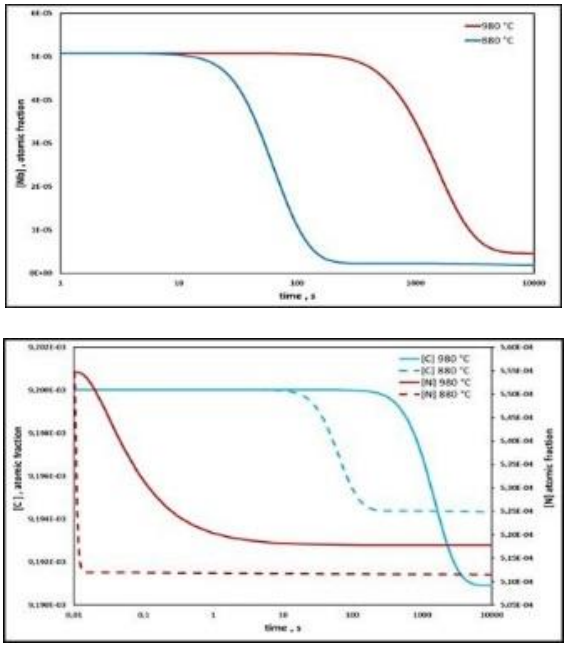

Fig. 4. *Relationships between chemical composition of austenite and time at different temperatures (a) [Nb] = f(time), (b) [C], [N] = f(time).*

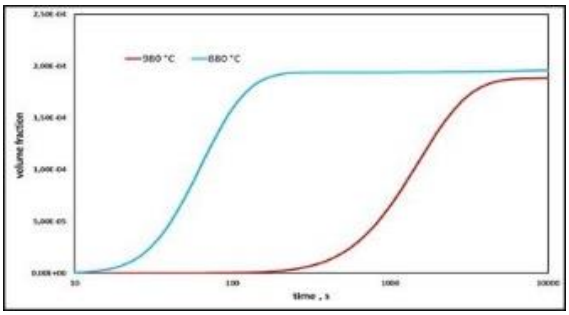

Fig. 5. *Relationships between volume fraction of carbonitride and time at different temperatures.*

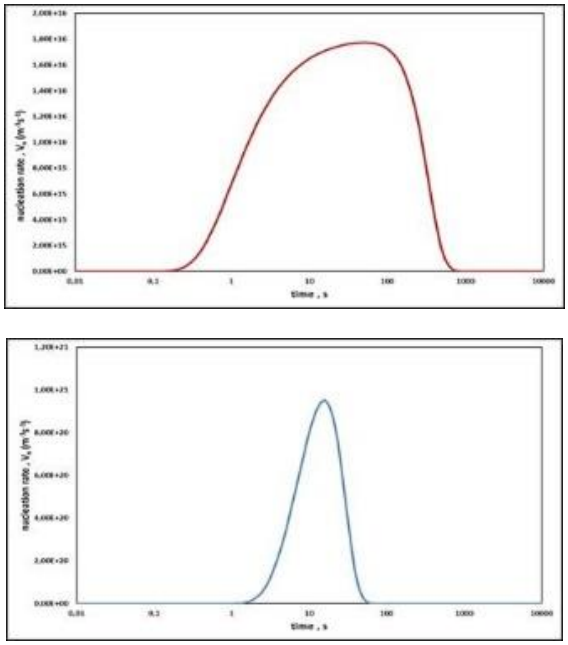

Fig. 6. *Relationships between nucleation rate and time at T = 980°C (a) and at T = 880°C (b).*

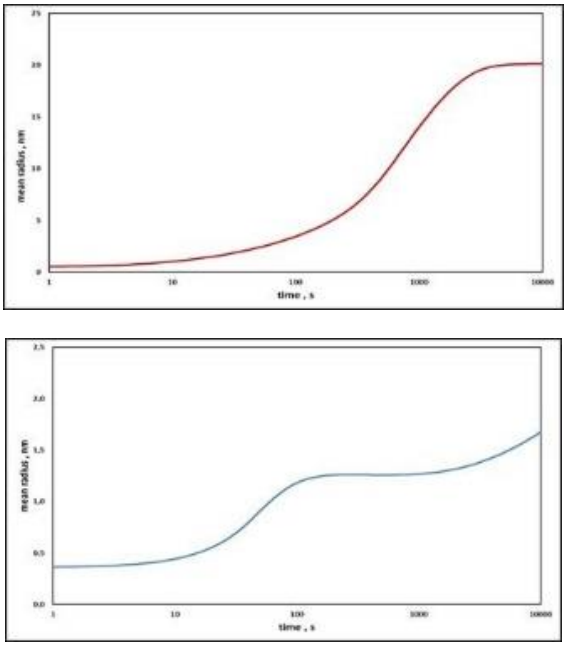

Fig. 7. *Relationships between mean radius, r, of precipitates and time at T = 980°C (a) and at T = 880°C (b).*

With increasing time of holding steel at temperature of carbonitride precipitation, T_p, decreasing of [Nb], [C], [N] contents and increase of volume fraction, V_v, of compound is observed (figures 4 and 5). The relationships between nucleation rate and holding time shows, that nucleation of new carbonitrides take place until 1000 s and 70 s at 980°C and 880°C respectively (figure 6). Temperature of precipitation, T_p and holding time significantly influences on mean size of carbonitride precipitations (figure 7).

7. CONCLUSIONS

Mechanical properties of microalloyed steels are determined by their chemical composition and technological process parameters, which have influence on to the size of carbonitrides precipitations. Precipitations inhabit grain growth. Refining of grains allows to obtain high mechanical properties of steel after cooling after plastic working without additional heat treatment. Based on the chemical composition and size of the precipitations, the effect of microalloying element on mechanical properties of steels can be determined. A proposition of the CA model for the analysis of the precipitation of carbonitrides in microalloyed niobium steels was presented in the paper. The developed "MPCA" computer program allows to calculate the microstructure image from given process parameters (temperature and time) and chemical composition of steel.

ACKNOWLEDGMENTS

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MODEL AUTOMATU KOMÓRKOWEGO DLA PROCESU WYDZIELANIA WĘGLIKOAZOTKÓW W STALACH

Streszczenie

W artykule przedstawiono model Automatu Komórkowego (AK) dla procesu wydzielania węglikoazotków w stalach niskostopowych zawierających dodatki Ti, Nb lub V. Wydzielenia węglikoazotków silnie wpływają na mikrostrukturę i własności mechaniczne tych stali. Parametry wydzieleń takie jak zawartość i rozmiar są wymagane do przewidywania własności mechanicznych stali niskostopowych. Modele matematyczne opisujące proces wydzielania pozwalają określić te parametry. Rozwój nauk informatycznych umożliwia przeprowadzanie symulacji procesów wydzieleniowych. Modele opierają się na równania algebraicznych opisujących zarodkowanie i kinetykę wzrostu wydzieleń, wynikających z termodynamiki stopów. Jednym z możliwych narzędzi informatycznych do przeprowadzenia symulacji procesów wydzieleniowych jest metoda automatów komórkowych, których twórcą jest John von Neumann. Celem pracy było opracowanie programu komputerowego wykorzystującego model automatu komórkowego do obliczania rozmieszczenia i zawartości wydzieleń.

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