

APPLICATION OF NUMERICAL SOLUTION OF THE DIFFUSION EQUATION TO MODELLING PHASE TRANSFORMATION DURING HEATING OF DP STEELS IN THE CONTINUOUS ANNEALING PROCESS*

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Abstract

Physical basis for modelling of phase transformation during heating of DP steels is given in the paper. Basic models are discussed briefly. The model based on the solution of the diffusion equation with moving boundary was selected as an alternative with extensive predictive capabilities, which include determination of the carbon segregation in the austenite. The diffusion equation was solved using finite difference method for 1D domain and finite element method for 2D domain. Model was validated qualitatively by comparison the results with the dilatometric tests data and good agreement was obtained.

Key words: DP steels, continuous annealing, phase transformation during heating, diffusion

1. INTRODUCTION

The dynamics of the development of the automotive industry depends on the availability of new materials with exceptional properties. Scientists are constantly looking for new materials by changing chemical composition or are trying to improve properties of existing ones without changing their chemistry. Aluminium and magnesium alloys, polymer composites, nanomaterials and smart materials have been developed over recent years, but still more than 60% of the car is built of steels.

The current requirements of the automotive industry for materials is high strength and good plastic properties matched with the low density. Thus, it is possible to reduce the vehicle weight and conse-

quently to reduce adverse effects on the environment by decreasing the amount of exhaust emissions. Another important factor is cost reduction.

Properties of materials depend on their structural composition. The strength properties increase with increasing volume of phases of high hardness as pearlite, bainite, and martensite. The presence of soft ferritic phase improves the workability. Studies on the development of multi-phase steel structure have been conducted for many years. This led to the development of Advanced High Strength Steels (AHSS) of the first generation (Matlock & Speer, 2009; Hofmann et al., 2009; Pichler et al., 2007). Soft ferrite is the main component of these steels. DP steels with ferritic-martensitic structure, transformation induced plasticity TRIP steels with ferrite, bainite and retained austenite, CP steels with ferrite, martensite, bainite and MART steels with martensitic structure, belong to the AHSS. All these steels are

* This paper will be presented at the KomPlasTech 2013 Conference, which will be held in Zakopane, Poland on January 13-16, 2013.

still widely investigated, beyond listed papers on manufacturing of multiphase steels, wide research on in-use properties are carried out, see for example works of Hodgson and co-workers (Asgari et al., 2004; 2012; Pereira et al., 2005; Nihare et al., 2010) or (Thomser et al., 2009).

The second generation of AHSS are austenitic steels with high manganese content, including twinning induced plasticity TWIP steels (Bouaziza et al., 2011). Preferably the mechanical properties of these steels are strongly dependent on the chemical composition, including the concentration of manganese, which determines the main mechanism of deformation during forming process. Unfortunately, this high content of alloying elements increases the cost of production and creates problems in casting and heat treatment. In consequence, these steels are used only for the most important elements of the crumple zone.

High costs of manufacturing of the second generation of AHSS caused that intensive research is still focused on improvement of conventional steels without changing their chemical composition. This research led to development of the third generation AHSS, which are currently intensively developed (Matlock & Speer, 2009). These steels are designed to achieve better properties than the first generation steels, while low manufacturing cost are maintained. DP and TRIP steels are modified primarily due to the possibility of manufacturing them in a wide range of parameters, for example by strain hardening, precipitation strengthening, or the grain refinement. Control of morphology of the second phase is the next possible method of improvement of steel properties.

One of the methods of obtaining of multi-phase microstructure in steels is proper thermal cycle during the annealing-galvanizing process. Due to several complex microstructural phenomena occurring during this process its control and optimization is difficult. It is expected that numerical modelling can be a support for investigation of various thermal cycles and design of new materials. There are three main processes in the continuous annealing, which are mutually dependent and which have to be considered by the model: i) ferrite recrystallization during heating, ii) transformation of the ferritic-pearlitic microstructure into austenite, iii) austenite decomposition during cooling. Recrystallization of ferrite is usually modelled by the Avrami equation but more advanced models based on the Cellular Automata (CA) are also used. A lot of work was done on mod-

elling phase transformations during cooling, see for example authors papers (Kuziak & Pietrzyk, 2011; 2012; Pietrzyk et al., 2010). In all these papers an assumption of purely austenitic microstructure at the beginning of transformation was made. It is known, however, that continuous annealing processes are performed in the intercritical temperature range and at the beginning of the cooling stage a complex ferritic/austenitic microstructure is encountered. Moreover, segregation of elements in the austenite is observed. Therefore, there is a need for prediction of microstructure after heating stage in the annealing process and to use these data as starting for simulation of the cooling stage.

The objective of the present paper is investigation of phenomena occurring in multi phase steels during heating in the continuous annealing process and evaluation of possibility of application of advanced numerical model to simulations of these phenomena. The numerical model based on the solution of the diffusion equation with moving boundary was applied. Basic idea of this model was presented by Pernach and Pietrzyk (2008) for the austenite-ferrite transformation during laminar cooling. This model gave good insight into phase transformations occurring in steels during its manufacturing and allowed to determine the correlation between process parameters and changes in the microstructure and the properties of products. The model (Pernach & Pietrzyk, 2008) assumed purely austenitic microstructure at the beginning of cooling and it cannot be used for simulation of cooling from the intercritical temperature in the continuous annealing. Therefore, application of the solution of diffusion equation to the phase transformation during heating was the particular objective of the present work. This model gives the carbon distribution in austenite at the intercritical temperature and can be further used as starting point for simulation of cooling in the continuous annealing process.

2. PROCESSES OF DP STEEL PRODUCTION

DP steel plates are produced by hot rolling and laminar cooling, or by cold rolling and intercritical annealing. In the former case steel strips of a thickness exceeding 3 mm are obtained, in the latter thin strips with a thickness of 0.16-3 mm are produced. Very brief description of manufacturing of these steels is given below.



2.1. Hot rolling and laminar cooling

Selection of the hot rolling parameters such as rolling velocity, temperatures and reductions is typical for hot rolling of strips. The multiphase microstructure is obtained during special thermal cycle in the laminar cooling. In practice, the following stages can be distinguished in the hot rolling of strips with thickness exceeding 3 mm:

- Roughing and finishing rolling, during which a grain refinement is obtained by static recrystallization,
- Fast cooling to the temperature of fast ferritic transformation,
- Isothermal holding to obtain required volume fraction of ferrite,
- Fast cooling to transform remaining austenite into martensite and to avoid bainitic transformation.

For practical reasons, in industrial processes often the isothermal holding is avoided and the microstructure composed of ferrite, bainite and martensite is obtained.

2.2. Cold rolling and continuous annealing

Similarly to the hot rolling, conditions of the cold rolling process of the DP steels are also similar as typical conditions used for carbon-manganese steels and the multiphase microstructure is obtained during continuous annealing after rolling. Annealing is usually combined with galvanization, what puts additional constraints on designing the thermal cycle. The input microstructure is a mixture of ferrite and pearlite, which is deformed in rolling. During the heating before annealing recrystallization of ferrite takes place first. Dual phase structure is obtained by isothermal holding in the intercritical temperature followed by a special cooling cycle. The part of the austenite transforms into ferrite during slow cooling. Structure of martensite and retained austenite is the result of subsequent fast cooling. Processes occurring during annealing: recrystallization of ferrite, pearlite and ferrite transformation into austenite, austenite transformation into ferrite and subsequently austenite transformation into martensite have joint influence on the final structure (Rocha et al., 2005).

A number of papers dealing with the continuous annealing process can be found in the scientific literature. Modelling of the ferrite recrystallization kinetics was described by Ferry et al. (2001). Thor-

ough discussion of the annealing process can be found in the works of Pichler et al. (1999; 2000; 2007). Authors of these papers discuss correlation between thermal cycle parameters and properties of the DP steel (Pichler et al., 1999) and transformations during cooling (Pichler et al., 2000). Recapitulation of these works can be found in Pichler et al. (2007). Less attention was paid to the simulation of transformation of heating to the intercritical temperatures and this problem is discussed in further chapter of the present work.

3. PHASE TRANSFORMATION DURING HEATING

Heating is an important part of the continuous annealing. The low carbon steel that is in the equilibrium state has a ferrite plus pearlite microstructure. The process of austenitization is carried out in two stages. The first stage is the pearlite dissolution and the second one is transformation of ferrite into austenite. Both processes are controlled by diffusion. Thus, the mechanism is based on the lattice reconstruction $Fe\alpha$ into $Fe\gamma$ and the carbon diffusion. The kinetics of nucleation and grain growth is conditioned by the energy of the system. Simulation of the phase transformation during heating of the DP steel accounting for the diffusion of carbon is the objective of this paper. The physical basis for the developed model is described in this chapter.

3.1. Pearlite dissolution

Pearlite is a mixture of cementite containing 6.67%C and ferrite, in which the carbon concentration reaches a maximum value of 0.025%. The transformation of pearlite to austenite begins when the temperature exceeds A_{e1} . Austenite nucleates mainly at the pearlitic colony boundaries (high angle boundaries and lattice mismatch), but nucleous can also occur between the plates of ferrite and cementite and between pearlite and ferrite (figure 1a).

Austenite grains grow along the ferrite plates, increasing its volume and finally replacing the ferrite in pearlite colonies. The cementite plates dissolve in this austenite, but austenite grains grow at a faster rate than that at which the cementite plates dissolve. As a result, there are areas in which the pearlite colonies have been transformed, and those in which the process of dissolution of cementite is still ongoing (figure 1b).

Pearlite dissolution process is inversely proportional to the inter-lamellar spacing of the pearlite



and it can take from few seconds to tens of seconds, depending on the heating rate. It is assumed that the rate of transformation is inversely proportional to the interlammellar spacing in the pearlite. Austenite rich in carbon (at the beginning it is concentration of the eutectoid point S) is formed in the original volume of pearlite colonies.

The numerical model developed in the present work does not take into account the phenomena occurring in the pearlite and it assumes pearlite as a single uniform phase with the average carbon concentration of 0.64% for the investigated DP steel. Austenite grain growth is determined by the diffusion of carbon from pearlite into growing austenite grain. Assuming the controlling effect of carbon diffusion one can determine the conditions of local equilibrium at the γ - α interface on the basis of the Fe-Fe₃C diagram (figure 2a).

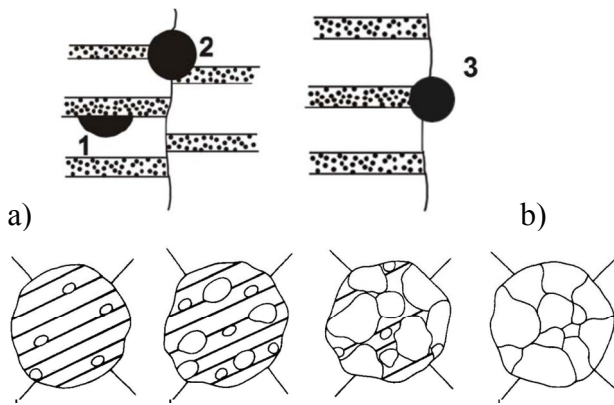


Fig. 1. a) Locations of austenite nuclei, 1) boundary between cementite and ferrite lamellas, 2) pearlite-pearlite boundary, 3) perlite-ferrite boundary; b) scheme of pearlite transformation into austenite (Savran, 2009).

3.2. Ferrite-austenite transformation

When pearlite decomposition is completed, original ferrite and newly created austenite coexist in the steel. The volume fraction of austenite is close to the initial volume fraction of the pearlite in steel. It is assumed that an average carbon content in austenite is around $c_p = 0.64\%$, which is the eutectoid point S (figure 2a). During further heating or isothermal annealing in the intercritical range of temperatures $A_{c1} - A_{c3}$, transformation of ferrite into austenite is launched. This transformation involves the lattice reconstruction and diffusion of carbon. The latter leads to austenite with equilibrium carbon concentration determined by the line GS in figure 2a. Progress of the ferrite-austenite transformation is presented schematically in figure 2b for two locations of the interface ξ . It is shown (Savran, 2009) that at

higher temperatures the transformation is controlled by carbon diffusion, at lower temperatures it is controlled by manganese diffusion.

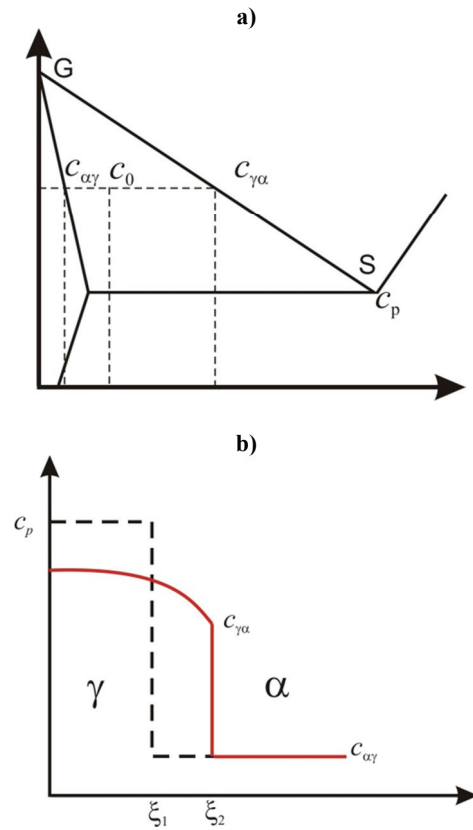


Fig. 2. a) Part of the Fe-Fe₃C diagram, b) Changes of the distribution of the carbon concentration during ferrite-austenite transformation.

4. EXPERIMENT

DP steel with the chemical composition in table 1 was investigated. The tests were performed on the dilatometer DIL805. The dilatometer is equipped with the LVDT measurement head with a theoretical resolution $\pm 0.057 \mu\text{m}$ and with electronic stabilization of cold ends. Tubular samples measuring $\phi 4/2 \times 10 \text{ mm}$ were used. The samples were heated with the rate of 3°C/s , which is a typical heating rate for industrial continuous annealing lines. Measured kinetics of transformation is compared with the equilibrium volume fraction of austenite in figure 3. Very good agreement between measured and calculated kinetics of transformation was obtained.

Table 1. Chemical composition of the investigated DP steel, wght%.

C	Mn	Si	P	S	Cr	Mo	V
0.11	1.45	0.16	0.014	0.009	0.27	0.005	0.005



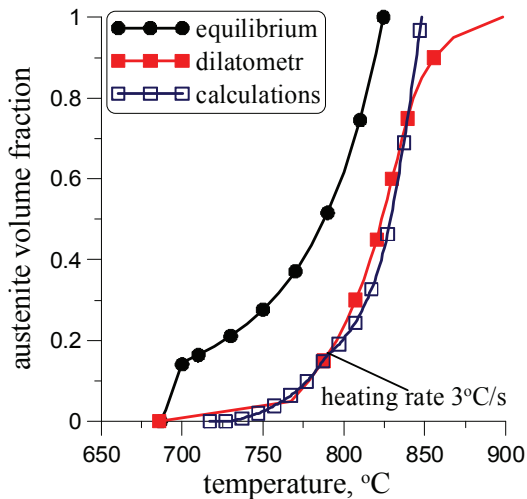


Fig. 3. Equilibrium content of austenite (solid line) and kinetics of transformation obtained from the dilatometric test and from the model for heating rate 3°C/s.

5. NUMERICAL MODELS OF PHASE TRANSFORMATIONS DURING HEATING OF DP STEELS

5.1. Introduction

As it has been mentioned, AHSS steel sheets can be produced either in the hot rolling process followed by laminar cooling or in the processes of cold rolling and continuous annealing. Proper selection of the thermal cycle during laminar cooling or continuous annealing affects the ratio of ferrite, martensite and bainite phases in the final microstructure (Pietrzyk & Kuziak, 2012). Determination of the optimum process parameters, such as temperature and time of annealing and the cooling rate, is possible by application of numerical models of phase transformations. These models take into account real physical phenomena to various extent, what affects the efficiency and accuracy of these models. Among currently used models Avrami (1939) equation, phase field method (Militzer, 2011), and cellular automata (CA) (Lan et al., 2004) should be mentioned, see Szeliga (2012) for more details. Particular attention should be paid to the Bos et al. (2010) paper, where application of the CA method to modelling continuous annealing is presented.

Recapitulating, the Avrami equation is limited to prediction of average volume fractions of phases and it does not allow a complete description of the development of the microstructure during transformations. The more complex models (CA, phase field) are capable of simulating of carbon segregation as well as morphology of growing phases but they are characterized by high computing costs, what makes 3D solution for the whole annealing

cycle practically impossible. In general, all these models can be used for both ferrite-austenite transformation during heating and austenite decomposition during cooling. Brief description of basic principles of these models is given in sections 5.2, 5.3, 5.4 and 5.5.

The results presented by Pernach and Pietrzyk (2008) show exceptional predictive capabilities of the model based on the numerical solution of the diffusion equation with moving boundary. More accurate modelling of the carbon segregation is the most important advantage of this model, which inspired Authors of the present paper to apply this model to simulations of the phase transformation during heating stage. The main aspects of this model are discussed in Chapter 5.

5.2. Models based on the thermodynamic relations

The most popular models of phase transformation are directly based on thermodynamic relationships. Commercial program ThermoCalc and the associated Dictra package, based on the CALPHAD method, are examples of such a solution. This method allows to determine the phase diagram based on the thermodynamic database, assuming the equilibrium condition at the interface. Thermodynamic equilibrium state means that minimum of the free Gibbs energy is achieved and the chemical potentials of each component are the same in all phases. In the case of DP steels and transformation during heating ternary system Fe-C-Mn should be considered and the condition of local equilibrium of potentials for all components is:

$$\mu_i(\gamma) = \mu_i(\alpha) \quad (1)$$

Global equilibrium state is practically not possible and limited equilibrium (paraequilibrium) is introduced in modelling. This idea was proposed by Singer-Loginova and Singer (2008), Steinbach et al. (1996) and Apel (2006). In the paraequilibrium state the ration between alloying element and iron is constant for all phases. This state for the Fe-Mn-C system is defined as:

$$\begin{aligned} \mu_C(\gamma) &= \mu_C(\alpha) \\ \frac{x_{Mn}(\gamma)}{x_{Fe}(\gamma)} &= \frac{x_{Mn}(\alpha)}{x_{Fe}(\alpha)} = \frac{x_{Mn}^0}{x_{Fe}^0} \end{aligned} \quad (2)$$

where: $\mu_i(\gamma)$, $\mu_i(\alpha)$ – chemical potentials of the i component in phases γ and α , $x_i(\gamma)$, $x_i(\alpha)$ –



concentrations of the i component in phases γ and α , x_{Mn}^0 , x_{Fe}^0 - initial concentrations of the i component of the system Fe-Mn-C.

The general paraequilibrium condition is (Provatas, 1999):

$$\left[\mu_{Fe}(\gamma) - \mu_{Fe}(\alpha) \right] + \frac{x_{Mn}^0}{x_{Fe}^0} \left[\mu_{Mn}(\gamma) - \mu_{Mn}(\alpha) \right] = 0 \quad (3)$$

The paraequilibrium condition for the Fe-Mn-C system are shown schematically in figure 2. The plane tangent to surfaces of free energy of austenite and ferrite demonstrate the equilibrium conditions at the interface. According to these conditions the chemical potentials of the carbon is the same in both phases and difference in potentials of iron is compensated by difference in potentials of alloying elements. The planes cross each other along the line, which when projected on the Fe-Mn-C plane gives lines connecting paraequilibrium states. Iron/manganese ratio for this line is constant. γ - α interfaces, which are in a paraequilibrium state, are inside of the area of coexistence of these phases in the global equilibrium (figure 2a)

An example of application of thermodynamic calculations for the numerical modelling of phase transformation in the continuous annealing of the DP steel sheets can be found in (Kuziak et al., 2010). This approach determines the stationary equilibrium state and it gives a constrain for all remaining models, which are used to simulate transient states during overheating of ferritic-pearlitic microstructure. Thus, the ThermoCalc software was used in the present work to determine the equilibrium parameters in the Avrami model described in the next section. The following equations were obtained for the steel chemical composition given in table 1:

$$\begin{aligned} c_{\gamma\beta} &= -1.46583 + 0.002887T \\ c_{\gamma\alpha} &= 4.8513 - 0.005776T \end{aligned} \quad (4)$$

$$\begin{aligned} c_{\alpha} &= -0.05869 + 0.0003827T - 8.288688 \times 10^{-7} T^2 + 5.997 \times 10^{-10} T^3 & \text{for } T \leq 637^\circ \text{C} \\ c_{\alpha} &= -0.0208533 + 0.000102818T - 9.36396 \times 10^{-8} T^2 & \text{for } T > 637^\circ \text{C} \end{aligned} \quad (5)$$

where: $c_{\gamma\alpha}$ - carbon concentration in austenite at the γ - α phase boundary, $c_{\gamma\beta}$ - carbon concentration in austenite at the γ -cementite phase boundary, c_{α} - carbon content in ferrite.

Equilibrium temperatures A_{e1} and A_{e3} calculated by the ThermoCalc software were 729.2°C and

827.6°C , respectively. The equilibrium parameters are the boundary conditions for the transient models for preheated ferrite or under cooled austenite.

5.3. Model based on Avrami equation

Models based on the solution of Avrami (1939) equation are still commonly used for simulations of phase transformations. The basic form of the Avrami equation is:

$$X = 1 - \exp(-kt^n) \quad (6)$$

Theoretical considerations show that a constant value of n in equation (6) can be used for modelling transformations in steels. On contrary, value of the coefficient k must vary with temperature. The formalism of the function $k = f(T)$ must be carefully chosen to describe properly the temperature dependence of transformation kinetics. The following function was selected:

$$k = k_1 \exp\left[\frac{k_2}{R(T+273)}\right] \quad (7)$$

Incubation time τ_a for the ferrite-austenite transformation is calculated from the equation:

$$\tau_a = \frac{a_1}{(T - Ae_1)^{a_3}} \exp\left[\frac{a_2}{R(T+273)}\right] \quad (8)$$

Coefficients $n = 0.229$ in equation (6), $k_1 = 9636.1$ and $k_2 = 79.4$ in equation (7) and $a_1 = 9636.1$, $a_2 = 79.4$ and $a_3 = 79.4$ in equation (8) were determined on the basis of the inverse analysis of dilatometric tests.

This simple model in connection with Scheil (1935) additivity rule has been widely used in the description of phase transformations, and it is efficient in supplying information regarding phase volume fractions, see for example papers for lamellar cooling (Kuziak & Pietrzyk, 2011) and continuous

annealing (Pietrzyk & Kuziak, 2012). The results of numerical simulations allowed to determine thermal cycle parameters, for which required volume fractions of the phases were obtained. Models based on the Avrami equation correctly describe the kinetics of transformation, but they do not allow for determi-



nation of carbon concentration profile in the final structure and morphological features of the two-phase microstructure. This model is used in the present work to supply data for evaluation of the solution of the diffusion equation described in chapter 6.

5.4. Phase field model

Phase field method (PFM) is more advanced and it is used to simulate the development of the microstructure (Singer-Loginova & Singer, 2008; Steinbach et al., 1996; Apel, 2006; Militzer, 2011). This method is based on the assumption of diffusive shape of the interface. According to this assumption, the boundary between the two phases is defined as narrow area in which the parameter field Φ is changing gradually between the two characteristic values for the two phases. Outside this area parameter Φ takes a constant value. Phase field parameters represent the shape of grains and their distribution and they are continuous functions in time and space. The value of the parameter Φ is determined by a solution of a system of partial differential equations taking into account the thermodynamics and kinetics of the processes occurring during the development of microstructure. In consequence, numerical models based on the MPF correctly describe the kinetics of phase transformations. The main disadvantage of this method is a necessity of using very fine mesh, which increases the computation time. On the other hand, it is possible to eliminate this problem by the introduction of adaptive networks (Provas, 1999).

The phase field method was applied by Savran (2009) to simulation of transformation of the ferritic-pearlitic microstructure into austenite. As it has been mentioned above, the kinetics of the phase transformation is described by the phase field parameter Φ_i ($i = 1 \dots, N$), which is equal 1 inside the grain and 0 outside. In the interface between the grains parameter $\phi_i + \phi_j = 1$ (i, j – numbers of neighbouring grains). Rate of changes of Φ is determined by mutual interaction between neighbouring grains:

$$\frac{d\phi_i}{dt} = \sum_j \mu_{ij} \left[\sigma_{ij} \left(\phi_i \nabla^2 \phi_j - \phi_j \nabla^2 \phi_i + \frac{\pi^2}{2\eta_{ij}^2} (\phi_i - \phi_j) \right) \right] + \frac{\pi}{\eta_{ij}} \sqrt{\phi_i \phi_j} \Delta G_{ij} \quad (9)$$

where: μ_{ij} – mobility of the interface, σ_{ij} – energy of the interface, η_{ij} – thickness of the interface, ΔG_{ij} – driving force.

In the case when two adjacent grains belong to the same phase, $\Delta G_{ij} = 0$ and growth of grains is controlled by the energy and the curvature of the interface. Mobility of the interface depends on the temperature:

$$\mu_{ij} = \mu_{ij}^0 \exp\left(-\frac{Q_{ij}}{kT}\right)$$

$$\mu_{ij}^0 = \frac{d_{ij}^4 v_D}{kT} \quad (10)$$

$$d_{ij} = \frac{1}{2} (V_i^{1/3} + V_j^{1/3})$$

where: μ_{ij}^0 – coefficient of the mobility of the interface, Q_{ij} – activation energy, k – Boltzman constant, v_D – Debye frequency, V_i, V_j – atomic volume of two grains in contact.

Range of appearance of ferrite, pearlite and austenite is determined from the equilibrium diagram using ThermoCalc software. Diffusion of carbon, which controls the transformation of ferrite+pearlite into austenite, is modelled by introduction of the function, which determines changes of carbon concentration in time:

$$\frac{\partial x_i}{\partial t} = \nabla \left[\phi_i D_i^C \nabla x_i^C + \phi_j D_j^C \nabla x_j^C \right] \quad (11)$$

where: D_i^C, D_j^C – diffusion coefficient in two adjacent grains, x_i^C, x_j^C local carbon concentration in grains i, j .

5.5. CA model

In the cellular automata model of phase transformation the lattice of cells represents the image of microstructure and reproduces topological relations between grains. The state of each cell is represented by such state variables as carbon concentration, orientation and assignment to a grain. The image of initial microstructure is a starting point for calculations. This initial microstructure is usually generated using CA algorithm of a normal grain growth (eg. Gawład, 2007). Example of generated microstructures is presented in figure 4. It is a schematic CA



space, in practical applications the space between 300×300 cells and 800×800 cells is used.

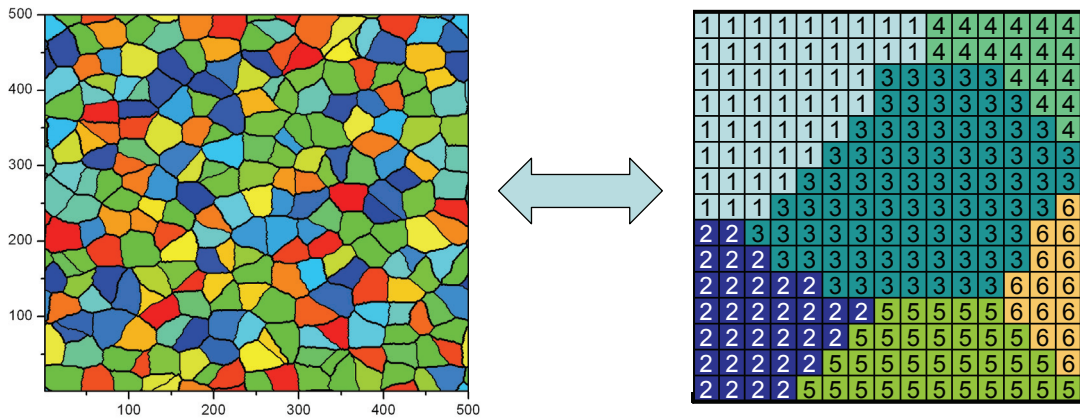


Fig. 4. Representation of the microstructure in the CA space.

Changes of states of cells are controlled by transition rules. Definition of the transition rules is crucial for the reliability of the CA method. These rules define the new state of the cell in the next time step on the basis of the state of the neighbours of this cell and the state of this cell itself in the previous time step:

$$Y_{k,l}^{t+1} = \begin{cases} \text{if } (\Lambda) \Rightarrow \text{new state} \\ \text{else } \Rightarrow Y_{k,l}^t \end{cases} \quad (12)$$

where: $Y_{k,l}^t, Y_{k,l}^{t+1}$ – state of the cell (k,l) in the previous and current time step, respectively, Λ – logical function, which controls changes of the state of the cell.

For a particular case of phase transformations separate functions Λ are introduced for nucleation and growth mechanisms (Opara et al, 2012). There are several examples of application of the CA model to simulation phase transformations during cooling (Lan et al., 2004; Opara et al, 2012). Applications to phase transformation during heating are scarce. Boss (2010) presented such a solution for a cubic CA space and periodic boundary conditions. In each time step Δt each of the cells belonged to one grain. Velocity of motion of the interface was calculated as:

$$v = \mu_{ij} \sum_{i=1}^3 x_i^n (\mu_i^p - \mu_i^n) \quad (13)$$

where: μ_{ij} - mobility of the interface, x_i^n - concentrations of the i component in the new phase, μ_i^p, μ_i^n – concentration of the i component in the old and new phase, respectively.

Model proposed by Bos et al. (2010) provides information about grain size, phase volume fraction

and grain distribution. Good correlation with Avrami equation was observed. Material structure was generated randomly using Voronoi algorithm, what can influence the correctness of the results. The long computation time is a disadvantage of the CA model.

6. MODEL BASED ON THE SOLUTION OF THE DIFFUSION EQUATION

Ferritic transformation is controlled by diffusion, therefore, solution of the diffusion equation is often used for modeling this transformation, see for example (van Leeuwen et al., 2003). The model developed by the Authors of the present paper and based on (Pernach & Pietrzyk, 2008) is described in the next section.

6.1. Mathematical formulation

The solution of the diffusion equation with the moving boundary allows for a full description of the transformation of ferrite+pearlite into austenite, as well as a clear definition of the structure, by determining the volume fraction of phases, grain size and carbon concentration. Mathematical formulation is based on the solution of the second Fick law:

$$\nabla \cdot (D \nabla T) = \frac{\partial c}{\partial t} \quad (14)$$

where: D – diffusion coefficient, t – time.

The initial and boundary conditions at the interface are:

$$\begin{aligned} c(\mathbf{x}, 0) &= c_p & \mathbf{x} \in d_\gamma, \\ c(\xi, t) &= c_{\gamma\alpha} \end{aligned} \quad (15)$$



$$\frac{\partial c}{\partial \mathbf{n}}(\xi, t) = 0$$

where: ξ – location of the interface, d_γ – austenite grain, which was formed from the pearlite at $t = 0$, \mathbf{n} – unit vector normal to the surface, c_p – average carbon concentration in pearlite, which for the investigated steel chemical composition was 0.64%.

The finite difference solution of equation (14) was performed first to obtain qualitative information about carbon segregation. The explicit integration scheme was applied and front tracking method was used to move the interface controlled by the mass balance. This is well known solution and it is not described in the paper.

The finite element method was used to solve Fick equation in two dimensions. The finite element discretization in the V domain was performed. The concentration inside an element is presented as a function of nodal values:

$$\mathbf{c} = \mathbf{n}^T \mathbf{c} \quad (16)$$

where: $\mathbf{n} = \{n_1, n_2, \dots, n_n\}^T$ is a vector of shape functions, $\mathbf{c} = \{c_1, c_2, \dots, c_n\}^T$ is a vector of concentrations in nodes of the finite element mesh.

The solution of Fick equation is based on the variational principle, which states that the function of concentrations c , which solves equation (14), gives the minimum of the general functional, for which equation (14) is the Euler equation. The following functional meets this condition:

$$J = \int_V \left[\frac{D}{2} \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{c} \right)^2 + \frac{D}{2} \left(\frac{\partial \mathbf{n}^T}{\partial y} \mathbf{c} \right)^2 \right] dV - \int_S q \sum \mathbf{n}^T \mathbf{c} dS \quad (17)$$

Equation (17) describes stationary problem, when $\partial c / \partial t = 0$. Substitution of relationship (16) into equation (17) leads to:

$$\frac{\partial J}{\partial \mathbf{c}^T} = \int_V \left(D \frac{\partial \mathbf{n}^T}{\partial x} \frac{\partial \mathbf{n}}{\partial x} \mathbf{c} + D \frac{\partial \mathbf{n}^T}{\partial y} \frac{\partial \mathbf{n}}{\partial y} \mathbf{c} \right) dV - \int_S q \mathbf{n} dS = 0 \quad (18)$$

Minimization of the discretized steady state functional (18) requires calculation of the partial derivatives with respect to nodal concentrations and it results in the following set of linear equations:

$$\mathbf{H} \mathbf{c} = \mathbf{p} \quad (19)$$

where:

$$H_{ij} = \int_V (\nabla n_i)^T D (\nabla n_j) dV$$

$$p_i = \int_S q n_i dS$$

In equation (19) q represents mass flux through the grain boundary, which in the case of phase transformation is equal zero, see equation (15). Accounting for the fact that the concentration is a function of time leads to:

$$\mathbf{H} \mathbf{c} + \mathbf{C} \frac{\partial}{\partial t} \mathbf{c} = \mathbf{p} \quad (20)$$

where:

$$C_{ij} = \int_V n_i n_j dV$$

Assumption of the quasi-stationary state during time step Δt and application of the Galerkin time integration scheme yields the final set of equations:

$$\hat{\mathbf{H}} \mathbf{c} = \hat{\mathbf{p}} \quad (21)$$

where \mathbf{c} is the vector of carbon concentrations in nodes at the end of the time interval, and:

$$\hat{\mathbf{H}} = \left[2\mathbf{H} + \frac{3}{\Delta t} \mathbf{C} \right]$$

$$\hat{\mathbf{p}} = \left[-\mathbf{H} + \frac{3}{\Delta t} \mathbf{C} \right] \mathbf{c}_i - 3\mathbf{p} \quad (22)$$

6.2. Physical aspects of the model

The initial microstructure was composed of ferrite and pearlite. It was assumed that pearlite transforms into austenite first and that austenite containing c_p of carbon is created. Right after that process is completed the transformation of ferrite into austenite begins. This process is controlled by the diffusion in austenite and diffusion in ferrite is neglected. Carbon diffuses in austenite towards the interface with ferrite until the equilibrium concentration for the current temperature is reached. Motion of the boundary is made then and the simulation of the diffusion is continued until the equilibrium is reached (for isothermal transformation) or the whole ferrite is transformed into austenite (transformation during heating). At this stage the model does not account for the diffusion of the manganese and other elements, what may cause some errors.

7. RESULTS

Modelling of phase transformation by the solution of the diffusion equation (14) was the objective



of the paper, however, for comparison, some results of earlier works based on the Avrami equation are presented, as well.

7.1. Results for Avrami equation

Kinetic of transformation calculated using Avrami equation was compared with the dilatometric data in figure 3 and good agreement was obtained. It means that this equation can be effectively used for simulation and optimization of the heating part in the continuous annealing process when volume fractions of phases are of interest. This model allows also to calculate changes of the average carbon concentration in austenite. Selected example of simulations of the kinetics of transformation and the segregation of carbon in austenite during the whole annealing cycle is presented below. Figure 5a shows changes of the temperature, recrystallized volume fraction and volume fractions of phases and figure 5b shows changes of the carbon concentration during the annealing cycle, which gives 27% of martensite in the final microstructure. C_0 in this figure represents average carbon content in steel. Model of ferrite recrystallization is described elsewhere (Kuziak & Pietrzyk, 2011) and is not repeated here. It is seen in figure 5 that simple Avrami equation predicts properly changes of volume fractions of phase and it can be efficiently used for the design of annealing cycles. Changes of the average carbon concentration in austenite are calculated from the current volume fraction of ferrite, therefore, the equilibrium concentration is obtained during the heating stage. During cooling the model shows how carbon concentration in austenite increases with the progress of transformation.

7.2. Finite difference simulation results

Carbon distributions calculated for isothermal transformations at 800°C and 820°C are presented in figure 6. Diffusion diminishes when austenite volume fraction reaches values 0.41 and 0.8, which are close to the equilibrium respectively at 800°C and 820°C.

Carbon distributions calculated for transformations at constant heating rates of 2°C/s and 3°C/s are presented in figure 7. Diffusion ceases when austenite volume fraction reaches values 0.41 and 0.8, which are close to the equilibrium respectively at 800°C and 820°C. The transformation is completed at 840°C and 855°C respectively for heating rates

of 2°C/s and 3°C/s. After completion of the transformation carbon concentration is not uniform and some time is needed to homogenize this concentration.

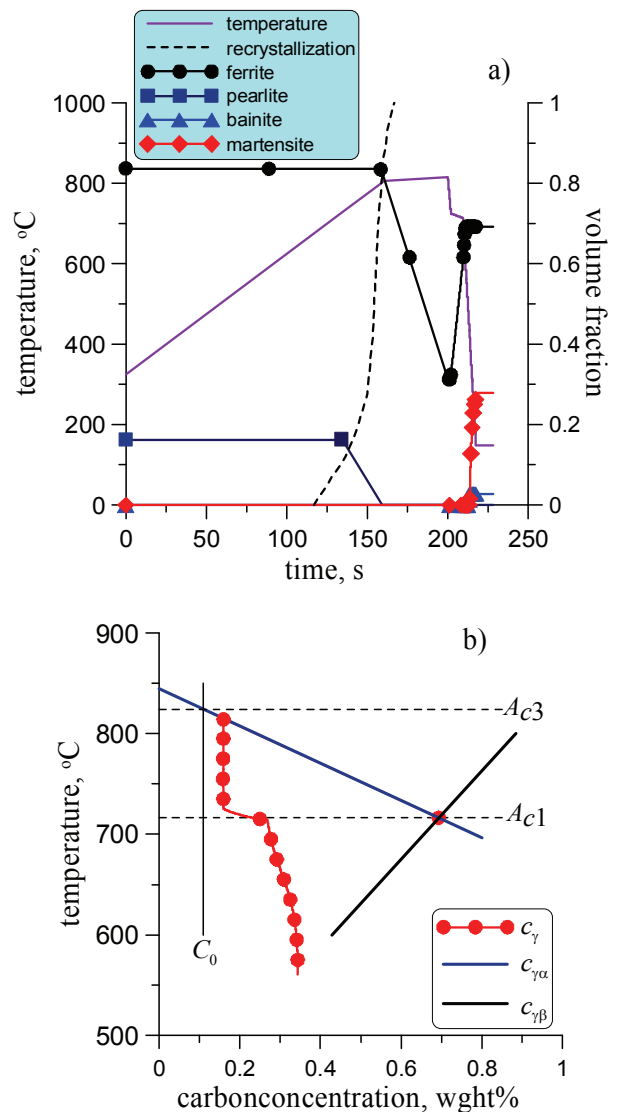


Fig. 5. Changes of the temperatures and volume fractions of phases (a) and equilibrium content of austenite c_γ compared to equilibrium content.

Although one dimensional solution cannot give quantitatively good result as far as kinetics of transformation is considered, the presented results show interesting predictive capabilities of the model. When this model is applied to the continuous annealing process an information regarding carbon distribution in austenite at the end of the intercritical heating will be available. This information will be a starting point for simulation of transformations during cooling.



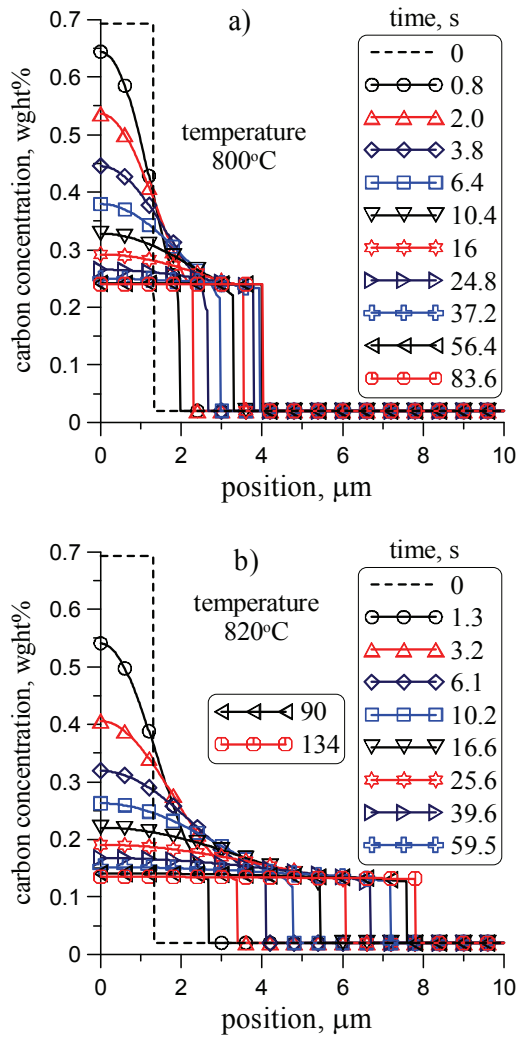


Fig. 6. Changes of the carbon distribution for isothermal transformation at 800°C (a) and 820°C (b).

7.3. Finite element simulation results

FE model described in section 6.1 was used for simulation of carbon diffusion in austenite during heating. An arbitrary ferrite grain with two pearlite islands located in the corners was assumed as the domain of the solution, see figure 8. Maps of the carbon distribution in austenite for the phase transformation during heating with 2°C/s are shown in figure 9. Carbon distribution along the line connecting two corners of the grain (dotted line in figure 8) at subsequent stages of the transformation are shown in figure 10.

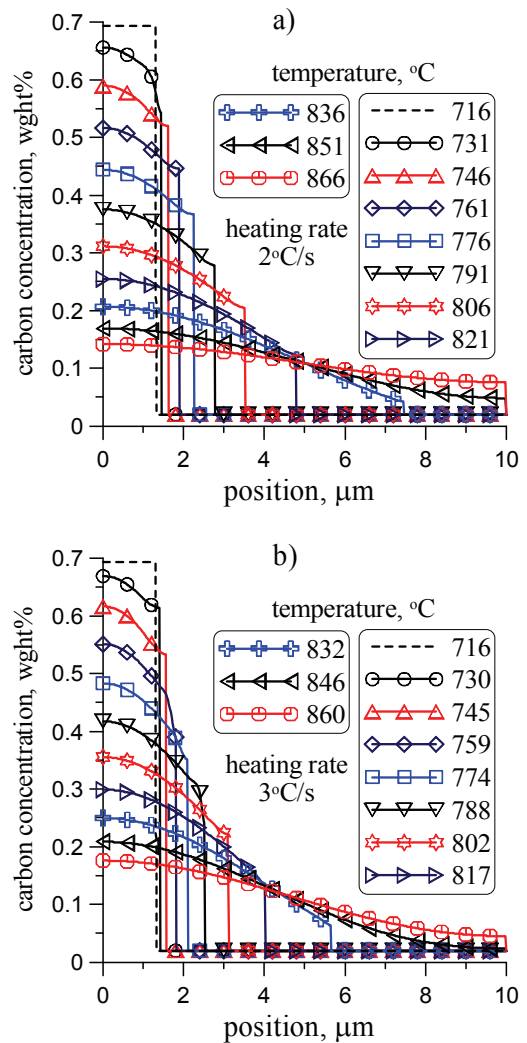


Fig. 7. Changes of the carbon distribution for constant heating rate transformation at 2°C/s (a) and 3°C/s (b).

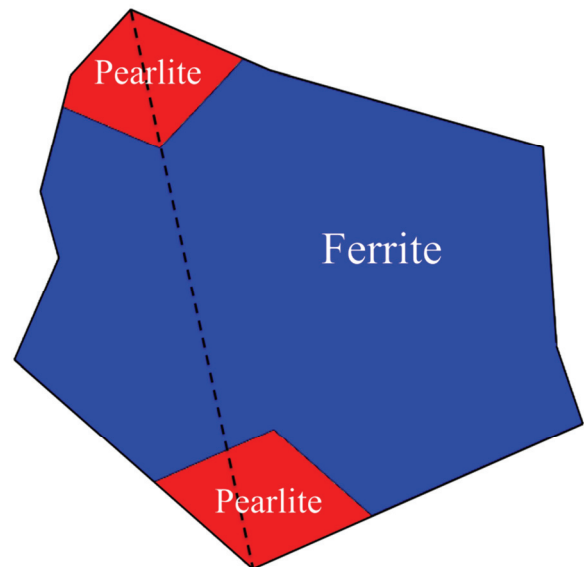


Fig. 8. Computational domain, which is ferrite grain with two pearlite islands located in the corners.



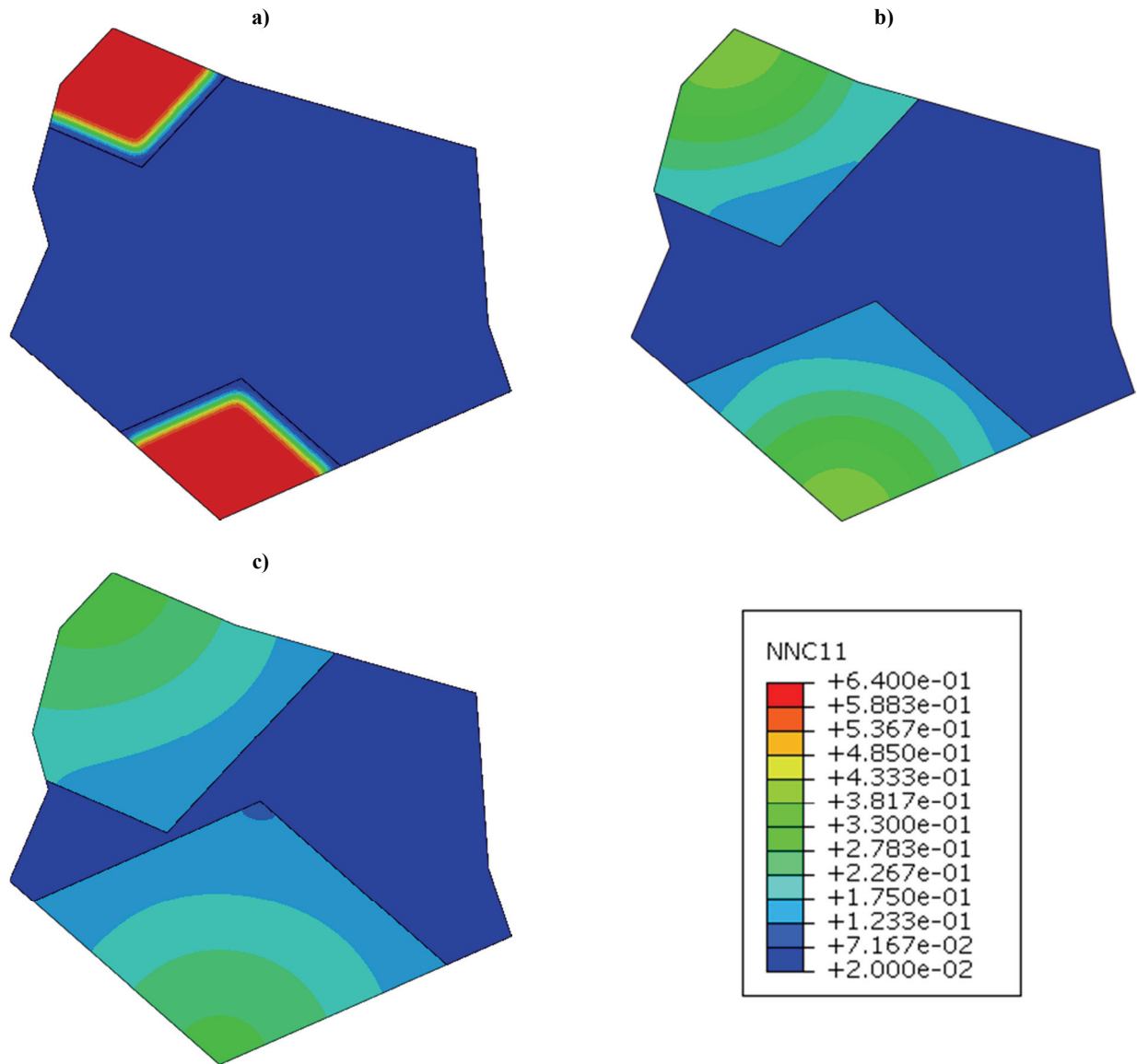


Fig. 9. Carbon distribution in austenite at subsequent stages (a, b, c) during transformation at the heating rate of 2°C/s.

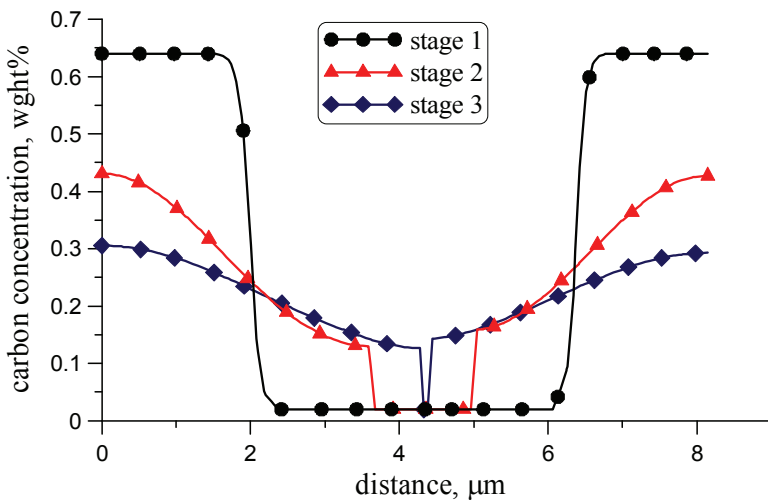


Fig. 10. Changes of the carbon distribution along the dotted line in figure 8 at various staged of the process for heating rate 2°C/s.

2D simulations confirmed good predictive capabilities of the model, which were expected from the 1D results. 2D solution is much more reliable and it will be very useful when this model is applied to the continuous annealing process. An information regarding carbon distribution in austenite will allow to control locally kinetics of transformation during cooling. This information will also allow to predict better the carbon distribution in the martensite.

8. CONCLUSIONS

The model, which predicts carbon distribution in austenite during heating, was presented. The model has extensive predictive capabilities. It supplies information regarding carbon distribution during heat-



ing stage of the intercritical annealing. This information is important for simulation of transformations during cooling. It is expected that the model and will be very useful in simulation the whole continuous annealing cycle and will improve the reliability of simulations.

Numerical tests of the model were performed and its qualitatively good predictive capabilities were confirmed. The parameters in the model have to be identified by the inverse analysis of experimental data what will be the goal of further research.

Acknowledgements. Financial assistance of the NCN, project no. 2011/03/B/ST8/06100 is acknowledged.

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**ZASTOSOWANIE NUMERYCZNEGO ROZWIĄZANIA
RÓWNAŃ DYFUZJI Z RUCHOMĄ GRANICĄ DO
MODELOWANIA PRZEMIANY FAZOWEJ PRZY
NAGRZEWANIU W PROCESIE CIĄGŁEGO
WYŻARZANIA**

Streszczenie

W artykule przedstawiono fizyczne podstawy modelowania przemiany fazowej przy nagrzewaniu stali DP w procesie ciągłego wyżarzania. Omówiono najważniejsze modele stosowane dla tej przemiany. Model wykorzystujący rozwiązanie równania dyfuzji z ruchomym brzegiem wybrano jako alternatywę dającą szerokie możliwości przewidywania parametrów przemiany fazowej, obejmujące wyznaczenie segregacji węgla w austenicie. Rozwiązanie równania dyfuzji przeprowadzono metodą różnic skończonych w obszarze 1D i elementów skończonych w obszarze 2D. Model został zweryfikowany przez jakościowe porównanie wyników obliczeń kinetyki przemiany z danymi dylatometrycznymi i uzyskano dobrą zgodność.

Received: December 18, 2012

Received in a revised form: January 01, 2013

Accepted: January 11, 2013

