



A TWO-DIMENSIONAL CA MODEL TO SIMULATE MICROSTRUCTURE DEVELOPMENT AND CARBON REDISTRIBUTION DURING THE PHASE TRANSFORMATION OF AUSTENITE TO FERRITE USING REALISTIC ANGULAR STARTING MICROSTRUCTURES*

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Abstract

A two-dimensional cellular automaton (CA) model combined with the mixed-mode (MM) approach has been developed to simulate microstructure evolution and segregation of carbon during the phase transformation from austenite to ferrite (γ - α) in DP steels. The model formulated is based on local equilibrium conditions and the assumption that the phase transformation is controlled by both diffusion processes and phenomena occurring at the interface, as formulated in the so-called mixed-mode model. The implementation and integration of the CA and MM models is described in detail. A simple and effective approach is presented to eliminate artificial anisotropy of ferrite growth when using a cubic lattice.

Key words cellular automata, mixed-mode model, diffusion of carbon, phase transformation from austenite to ferrite, digital material representation

1. INTRODUCTION*

Over the last years, dual-phase (DP) steels have been gaining increasing importance for use in the automobile industry. Mechanical properties of DP steels, such as strength and formability can be directly related to volume fractions of ferrite, bainite and martensite and their grain sizes, which are developed as a result of the transformation from austenite. DP steels are produced by two distinct methods, namely, by two-stage cooling from the austenite region after hot rolling, and controlled-cooling of cold rolled strip from the intercritical temperature range, typi-

cally in a Continuous Annealing process (Kim & Thomas, 1981; Nakagawa & Thomas, 1985; Lee et al., 2004). In the second type of heat treatment, a partial transformation of austenite to ferrite, which occurs during the first stage of cooling after intercritical annealing, is very important for further decomposition of austenite into martensite/bainite during the second stage of cooling. As a result of the ferritic transformation, the local chemical composition (elements partitioning) and thermodynamic conditions are established for further austenite transformations during fast-cooling stage. Therefore, the main focus of the paper is put on development of a numerical model capable of predicting not only the ferrite volume fraction changes during the transformation, but also the redistribution of carbon and

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alloying elements between austenite and ferrite and the resulting segregation profiles.

Due to the industrial significance, a lot of papers dealing with the ferritic transformation have been published over several decades (Christian, 1981; Krielaart et al., 1997; Van Leeuwen et al., 2003; Zhang et al., 2003; Loginova et al., 2003; Lan et al., 2004; Mecozzi et al., 2005; Bos & Sietsma, 2009; Zheng et al., 2012). Despite this, not all the features of the γ - α transformation are yet fully understood. Generally, two types of controlling processes are assumed to operate during the ferrite formation, namely, diffusion (diffusion controlled transformation – DC), and phenomena occurring at the interface (interface controlled transformation – IC). However, as the conditions vary during the phase transformation the rate controlling process may be a combination of both or may switch between these mechanisms. Therefore, a mixed-mode approach for austenite to ferrite transformation is adopted in this paper to develop an efficient model capable of tracing the interstitial and substitutional elements (e.g. C and Mn) segregation phenomena in the meso-scale using discrete numerical modeling methods (Krielaart et al., 1997; Van Leeuwen et al., 2003; Bos & Sietsma, 2009).

Modeling of microstructure development in material processing has noticeably progressed over last years. Recently, discrete models, such as Cellular Automata (CA) and Phase Field (PF) methods have been gaining acceptance as valuable tools for microstructure evolution predictions. These models have been successfully applied to the simulation of solidification or phase transformations of austenite (Zhang et al., 2003; Loginova et al., 2003; Lan et al., 2004; Mecozzi et al., 2005; Zheng et al., 2012). They are based on algorithms and computer methods for linking the process conditions to the changes occurring in the microstructure of constructional materials. As a result, they can be used for identification of the principal process controlling phenomena. It is noteworthy that these models are powerful tools in studying the microstructure evolution involving nucleation and growth of grains. An essential advantage of applying CA model is its capability of starting simulations from any realistic initial microstructure. This is a fundamental feature of this model applied to the case of phase transformations.

In the present work, a two-dimensional CA model will be presented to investigate transformation from austenite to ferrite in a DP steel after intercritical annealing followed by cooling. Since

this case does not involve nucleation, a fundamental aspect of modeling of this transformation is the calculation of ferrite growth within the CA lattice. The mixed-mode approach is combined with CA method to set appropriate boundary conditions at the moving interface and to simulate solute diffusion in the CA lattice. An effective and convenient approach in the algorithm implementation of CA model is used, which is called Frontal Cellular Automata (FCA) (Svyetlichnyy, 2010; Svyetlichnyy, 2012). Using these formalisms, a powerful process model is obtained that can simulate the γ - α transformation within a reasonable simulation time, while maintaining an acceptable level of accuracy necessary for exact description of simulated phenomena. Furthermore, the present work describes a new approach to model the transformation for realistic angular starting microstructures without introducing artificial anisotropy as a result of the use of a cubic CA lattice.

2. MODEL DESCRIPTION

2.1. Cellular automata model

The CA model in this work is used to model the behavior of discrete polycrystalline system using a two-dimensional grid of square cells of dimension L_{CA} . Each cell in this CA space is surrounded by neighbors, which influence one another at distances $L_{CA} \cdot \theta$ (where θ is a parameter taking into account the local angularity of the interface, which is to be defined in section 2.9). Periodic boundary conditions are applied on the outer borders. Every cell belongs to one grain and therefore this represents a sharp-interface model. Each CA cell is described by several states and internal variables. Each cell can have one of five different states: *austenite* (γ), *austenite-austenite* (γ/γ), *ferrite* (α), *ferrite-ferrite* (α/α), and *ferrite-austenite* (α/γ). The last state is used to describe CA cells situated at the interface between austenite and ferrite grains. Furthermore, a series of internal variables are defined to describe the initial microstructure including volume fractions of austenite and ferrite in a particular cell, X_A and X_F ; the carbon concentration in each cell c ; the growth length $l_{\gamma \rightarrow \alpha}^i$ of the ferrite phase in the α/γ cell; the physical length of a cell (assumed 0.1 μm) L_{CA} ; the growth velocity $v_{\gamma \rightarrow \alpha}^i$ of an interface cell; the grain number to identify to which grain a cell belongs to; the carbon concentration at interface cells from austenite and ferrite side, respectively c_{γ}^i , c_{α}^i ; and coordinates



x, y, z . These internal variables are used in transition rules to replicate mechanisms controlling phase transformation from austenite to ferrite. In every time step, the state of each cell ($Y_{i,j}^{t+1}$) in the grid is determined by the prior state of its neighbors and the cell itself ($Y_{i,j}^t$), by a set of precisely defined transition rules Λ , as is presented below:

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

The growth of ferrite grain occurs by the following transition rule:

$$\Lambda = T < A_{e3} \wedge (Y_{i,j}^t = \alpha / \gamma \wedge Y_{k,l}^t = \alpha \wedge X_{i,j}^\alpha = 1) \quad (2)$$

where: $X_{i,j}^\alpha$ – ferrite volume fraction in the cell i, j ;
 k, l – coordinates of neighbor cells for the cell i, j .

The kinetics of the moving γ - α interface is determined according to the Christian's (1981) model of the interface-controlled mechanism. The velocity of movement of the interface for the transformation from austenite to ferrite is described by:

$$v_{\gamma \rightarrow \alpha}^i = M_{\gamma \rightarrow \alpha} \Delta G \quad (3)$$

where: $M_{\gamma \rightarrow \alpha}$ – is the effective α/γ interface mobility; ΔG – is the driving force for transformation as a function of the alloying elements.

The ferrite growth length ($l_{\gamma \rightarrow \alpha}^i$) for each interface cell is updated in every time step (Δt) in the following way:

$$l_{\gamma \rightarrow \alpha}^i(t + \Delta t) = l_{\gamma \rightarrow \alpha}^i(t) + \Delta l_{\gamma \rightarrow \alpha} \quad (4)$$

$$\Delta l_{\gamma \rightarrow \alpha} = (v_{\gamma \rightarrow \alpha}^i \Delta t) \Theta \quad (5)$$

where: Θ – is the weight coefficient of the angle of growth, which is based on a normal vector of growth \vec{n} (see Section 2.9). This approach is used to eliminate the problem of artificial anisotropy in 2D CA grid. For interface cells for which the normal vector of growth is parallel to growth direction of ferrite neighbor cells, Θ equals 1 which is its maximum value. The minimum value ($1/\sqrt{2}$) of Θ is obtained for interface cells, for which the symmetry axis is situated on a diagonal at 45° with respect to neighboring ferrite cells. In other cases, the magnitude of Θ is between $1/\sqrt{2} \div 1$.

Subsequently the volume fraction of ferrite is calculated for this interface cell:

$$F_\alpha^i = \frac{l_{\gamma \rightarrow \alpha}^i}{L_{CA}} \quad (6)$$

When the accumulated volume fraction of ferrite reaches the value 1 at the interface cell, the state of this cell is switched to ferrite. Simultaneously, the nearest austenite neighbor cells are transformed into interface cells and the growth of ferrite phase starts to evolve according to equation (6). In case when interface cells of different grains grow simultaneously into the same austenite neighbor cell, the first interface cell that reaches a ferrite volume fraction of 1 defines the grain to which the cell belongs to.

In the CA grid, the solute redistribution is solved using the second Fick's law, which is described in Section 2.6. The diffusion equation in the 2D CA lattice is solved with the Finite Difference Method (FDM). In model developed, the FDM is directly combined with the CA space. As a result of integration of cellular automata method and finite difference solution, detailed information on solute concentration in each CA cell during the phase transformation is obtained.

2.2. Frontal cellular automata

The fundamental idea of the frontal cellular automata (FCA) is that only cells situated near to the front of changes, i.e. near to the moving interface, participate in the calculations (Svyetlichnyy, 2010). This is in contrast to the classical CA method, in which all cells are used at each calculation step. For more details see the publications of Svyetlichnyy (2010; 2012). The frontal cellular automata approach allows a major reduction of the computation time, in modeling phase transformations and microstructure evolution. However, it should be noted that the FCA should be used for calculations of processes, which occur only at interface cells. In simulations involving longer range diffusion the classical CA approach has to be used.

2.3. Mixed-mode approach

Generally, during the diffusional phase transformations two physicochemical processes related to the movement of atoms in the crystal structure occur:

- Migration of the interface, which is responsible for the stepwise change of the crystal lattice of the parent phase into the product phase one.



- Diffusion of atoms in the grains and across the interface, which is responsible for local changes in the chemical composition.

For the simulation of ferrite transformation during cooling after intercritical annealing both these phenomena must be accounted for. Modelling of the growth of newly formed nuclei in the mixed-mode model involves the determination of the interface velocity on the basis of either two models: diffusion-controlled growth model (DC) or the interface-controlled growth model (IC). It is assumed that the interfacial boundary thickness is negligible small (the distance of a few substitutional atoms) in comparison to the austenite grain size, which means that the difference in chemical potential across the phase boundary can be disregarded (Svoboda et al., 2001). In the mixed-mode model for the diffusional phase transformations a solution of the second Fick's law of diffusion for all atoms of alloying elements (see Section 2.6) is required. Due to emergence of a new phase in the crystal lattice, at the interface two admixture fluxes of atoms linked to either the austenite or ferrite are formed, leading to the discharge of the excess or deficiency of admixture in accordance with the reversal of phase transformation, and are described by Fick's first law:

$$J_{\gamma}^e = -D_{\gamma}^e \frac{\partial x_{\gamma}^e}{\partial n} \quad (7)$$

$$J_{\alpha}^e = -D_{\alpha}^e \frac{\partial x_{\alpha}^e}{\partial n} \quad (8)$$

where: $\frac{\partial x_{\gamma}^e}{\partial n}$ and $\frac{\partial x_{\alpha}^e}{\partial n}$ – concentration gradients of solute e , perpendicular to the interface, in austenite and ferrite; $D_{\gamma}^e, D_{\alpha}^e$ – associated diffusion coefficients of element e for austenite and ferrite respectively.

The overall diffusive atom flux ($J_{\gamma \rightarrow \alpha}^{diff}$) for the austenite to ferrite transformation is given by:

$$J_{\gamma \rightarrow \alpha}^{diff} = J_{\gamma}^e - J_{\alpha}^e = -D_{\gamma}^e \frac{\partial x_{\gamma}^e}{\partial n} + D_{\alpha}^e \frac{\partial x_{\alpha}^e}{\partial n} \quad (9)$$

Velocity of the interface movement can then be determined based on the mass balance. When a unit of the interface overcomes the distance ds , from the created volume of a new phase df , the admixture is released or absorbed ($x_{\gamma^*}^e - x_{\alpha^*}^e$). At the same time, t , in which the interfacial boundary overcomes dis-

tance ds , the interface flux J^i must dissipate solute depletion excess to the parent phase or absorb solute depletion from the parent phase, depending on the reversal of the transformation. Therefore, the mass balance requires a fulfillment of the following equation:

$$J^i dt = ds (x_{\gamma^*}^e - x_{\alpha^*}^e) \quad (10)$$

Dividing both sides of equation (10) by dt , the following relation is obtained:

$$J^i = v (x_{\gamma^*}^e - x_{\alpha^*}^e) \quad (11)$$

where: $v = \frac{ds}{dt}$ – velocity of the interface; $x_{\gamma^*}^e$ – content of the element e at the interface from the austenite side; $x_{\alpha^*}^e$ – content of the element e at the interface from the ferrite side.

The velocity of the interface is defined according to the Christian's IC model (Christian, 1981), which is defined by equation (3). The effective interface mobility ($M_{\gamma \rightarrow \alpha}$), in the equation (3), is an integrated parameter which contains multitude of structural effects that influence the mobility, i.e. the degree of coherency of the interface, pinning effect, build up of stresses, solute drag (Krielaart et al., 1997), etc. $M_{\gamma \rightarrow \alpha}$ can be described by the Arrhenius-type equation:

$$M_{\gamma \rightarrow \alpha} = M_{\gamma \rightarrow \alpha}^0 \exp\left(-\frac{Q_g}{RT}\right) \quad (12)$$

where: $M_{\gamma \rightarrow \alpha}^0$ – is a pre-exponential factor; Q_g – is the activation energy of migration; R – is the gas constant; T – is absolute temperature.

The driving force ΔG is assumed to be proportional to the difference of actual and the equilibrium content of e -th element, and can be expressed as:

$$\Delta G = \chi_{\gamma \rightarrow \alpha} (x_{\gamma_{eq}}^e - x_{\gamma}^e) \quad (13)$$

where: $\chi_{\gamma \rightarrow \alpha}$ – is the proportionality factor which can be calculated for example with Thermo-Calc[®] software; $x_{\gamma_{eq}}^e$ – is the equilibrium content of element e in the austenite phase.

Rewriting equation (11) for the austenite to ferrite transformation:

$$J_{\gamma \rightarrow \alpha}^i = v_{\gamma \rightarrow \alpha}^i (x_{\gamma_i}^e - x_{\alpha_{eq}}^e) \quad (14)$$



where: $x_{\gamma_i}^e$ – is the content of the element e at the interface from the austenite phase side; $x_{\alpha_{eq}}^e$ – is the equilibrium content of e -th element in the ferrite phase.

The combination of equations (3, 12-14) gives the final formula for the flux of solute atoms:

$$J_{\gamma \rightarrow \alpha}^i = M_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha} \left[\left(x_{\gamma_{eq}}^e + x_{\alpha_{eq}}^e \right) x_{\gamma_i}^e - \left(x_{\gamma_i}^e \right)^2 - x_{\gamma_{eq}}^e x_{\alpha_{eq}}^e \right] \quad (15)$$

As a result, the net solute flux $\Delta J_{\gamma \rightarrow \alpha}$, for the phase transformation from austenite to ferrite, at the γ - α interface is given by the difference of the two fluxes (Krielaart et al., 1997):

$$\Delta J_{\gamma \rightarrow \alpha} = J_{\gamma \rightarrow \alpha}^i - J_{\gamma \rightarrow \alpha}^{diff} \quad (16)$$

$$\Delta J_{\gamma \rightarrow \alpha} = M_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha}$$

$$\left[\left(x_{\gamma_{eq}}^e + x_{\alpha_{eq}}^e \right) x_{\gamma_i}^e - \left(x_{\gamma_i}^e \right)^2 - x_{\gamma_{eq}}^e x_{\alpha_{eq}}^e \right] - \left(-D_{\gamma}^e \frac{\partial x_{\gamma}^e}{\partial n} + D_{\alpha}^e \frac{\partial x_{\alpha}^e}{\partial n} \right) \quad (17)$$

The equation (17) reflects the interaction between solute diffusion and interface mobility. In the case of constant solute concentration at the interface, the net solute flux $\Delta J_{\gamma \rightarrow \alpha}$ is zero, and it is possible to determine the content of the solute e at the interface from the austenite and ferrite phase side respectively. By solving the partial differential equation for the Fick's first law using the FDM, similarly as in earlier works (Sietsma & van der Zwaag, 2004; Chen & van der Zwaag, 2010), the following final equation is obtained:

$$x_{\gamma_i}^e = \frac{\left(x_{\gamma_{eq}}^e + x_{\alpha_{eq}}^e \right) - \frac{D_{\gamma}^e}{sM_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha} \Delta_{xy}}}{2} + \frac{\left\{ \left[\left(x_{\gamma_{eq}}^e + x_{\alpha_{eq}}^e \right) - \frac{D_{\gamma}^e}{sM_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha} \Delta_{xy}} \right]^2 - 4 \left(D_{\alpha}^e \frac{x_{\alpha_i}^e - x_{\alpha_{i\pm s}}^e}{sM_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha} \Delta_{xy}} + x_{\alpha_{eq}}^e x_{\gamma_{eq}}^e - \frac{D_{\gamma}^e x_{\gamma_{i\pm s}}^e}{sM_{\gamma \rightarrow \alpha} \chi_{\gamma \rightarrow \alpha} \Delta_{xy}} \right) \right\}^{\frac{1}{2}}}{2} \quad (18)$$

where: $x_{\alpha_i}^e$ – is the content of the element e at the interface from the ferrite phase side, and in this case it equals to the equilibrium content; $x_{\alpha_{eq}}^e$; $x_{\alpha_{i\pm s}}^e$, $x_{\gamma_{i\pm s}}^e$ – are contents of the solute e at the defined distance of cells s from interface into interiors of ferrite and austenite grains; Δ_{xy} – is the distance between two nearest nodes on x and y axis and in the model it is the L_{CA} dimension. By integrating the mixed-mode model with the CA method it is possible to simulate the austenite to ferrite phase transformation while also providing direct visualization of microstructure evolution.

2.4. Initialization of the CA grid

An initial microstructure is created in the CA grid using the Digital Material Representation (DMR) scheme (Madej, 2010). The microstructure picture of real physical samples was processed with a program for quantitative analysis and subsequently digitised to represent it using the CA grid. An additional module of microstructure representation was developed for digitizing procedure. The thermal history of the sample was as follows: the sample was heated to the intercritical temperature and then immediately quenched to obtain ferrite-martensite microstructure. In the DMR of the real obtained microstructure, the martensite islands are equivalent to austenite regions prior to the fast quenching, and this is the digital input microstructure for simulations of the phase transformation from austenite to ferrite.

2.5. Ferrite nucleation

It is assumed in the model that no additional ferrite nucleation occurs in the system. It means that during the cooling after annealing at the intercritical temperature a growth of the “fresh” ferrite occurs epitaxially on the remaining ferrite after the intercritical annealing.

2.6. Solute redistribution in austenite and ferrite

Due to the fact that the growth of ferrite is assumed to be both diffusion- and interface-controlled, the solute diffusion is solved with the second Fick's law:

$$\frac{\partial x_{\phi}^e}{\partial t} = D_{\phi} \nabla^2 x_{\phi}^e \quad (19)$$



where: t – is time; x_φ^e – is the solute e concentration in phase φ (γ or α); D_φ – is the associated diffusion coefficient.

The solution of equation (19) using explicit FDM for 2D problem is:

$$x_{k,l}^{t+\Delta\tau} = x_{k,l}^t + D_\varphi \frac{\Delta\tau}{\Delta_{xy}^2} (x_{k+1,l}^t + x_{k-1,l}^t + x_{k,l+1}^t + x_{k,l-1}^t - 4x_{k,l}^t) \quad (20)$$

where: k, l – are the nodes' coordinates; $\Delta\tau$ – is the time step.

Based on the solution of equation (20), the calculated value of solute concentration is assigned to cells' attributes at each time step. The above numerical solution can take into account detailed information of solute concentration in austenite and ferrite grains.

Additionally, at each time step, the average solute concentration at interface cells is determined by:

$$x_{\alpha/\gamma}^e = F_\alpha^i x_{\alpha_i}^e + (1 - F_\alpha^i) x_{\gamma_i}^e \quad (21)$$

Another important aspect of ferrite transformation modeling is to keep calculations with the stability of solution and therefore a proper value of time step should be defined, which will be presented in next section.

2.7. Determination of time step

The time step, $\Delta\tau$, is a key parameter to achieve accurate and realistic results in modeling. Determination of the time step is based on the stability criterion of the solution for the explicit scheme of the FDM. The condition is given by:

$$\Delta\tau \leq \frac{(L_{CA})^2}{4D_\varphi} \quad (22)$$

On the basis of equation (22), considering the diffusion coefficients for austenite and ferrite and the maximum growth velocity (v_{\max}) of newly formed phase, the time step is determined as follows:

$$\Delta\tau = \min \left\{ \frac{L_{CA}}{v_{\max}}, \frac{(L_{CA})^2}{4D_\alpha}, \frac{(L_{CA})^2}{4D_\gamma} \right\} \quad (23)$$

where: “min” – means the minimum value among the three values in the curly bracket.

2.8. Boundary conditions at interface

Defining appropriate boundary condition is one of the most important aspects of modeling. For the CA model integrated with MM model, the Dirichlet boundary conditions are set for the solute concentrations at the interface cells from austenite and ferrite side respectively $x_{\gamma_i}^e, x_{\alpha_i}^e$, as is presented in figure 1 for 1D case.

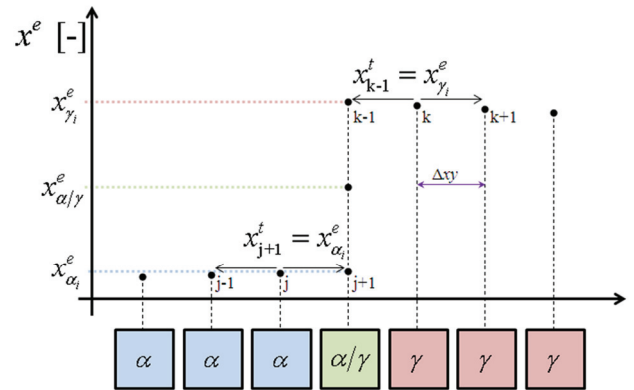


Fig. 1. The Dirichlet boundary conditions for solute diffusion with the second Fick's law in one dimensional CA space, in cells (k,j) which are next to the interface cell.

In the numerical implementation of equation (20) for the austenite cells which are in the neighborhood of interface cells, the solute content from these sides is determined at $x_{\gamma_i}^e$. Similarly the boundary conditions are solved for the ferrite cells with $x_{\alpha_i}^e$.

Neumann boundary conditions are assumed for the gradients of solutes in front of the interface cell in order to calculate the magnitude of the fluxes resulting from equation (9), as presented in figure 2. Figure 3 shows the determination of fluxes of solute for austenite and ferrite (equations 7-8) in the two-dimensional CA grid.

The gradients in equations (7-8) are established using the normal vector of growth \vec{n} (see Section 2.9) and an algorithm to find the neighbor cell with assumed distance (s) of cells according to direction of the \vec{n} .

For each time step and temperature change, the equilibrium conditions are recalculated using linearized Thermo-Calc[®] data for Fe-M-C system. The actual values of $x_{\gamma_{eq}}^e$ and $x_{\alpha_{eq}}^e$ are determined at the interface cells to recalculate values of equations (12-18).



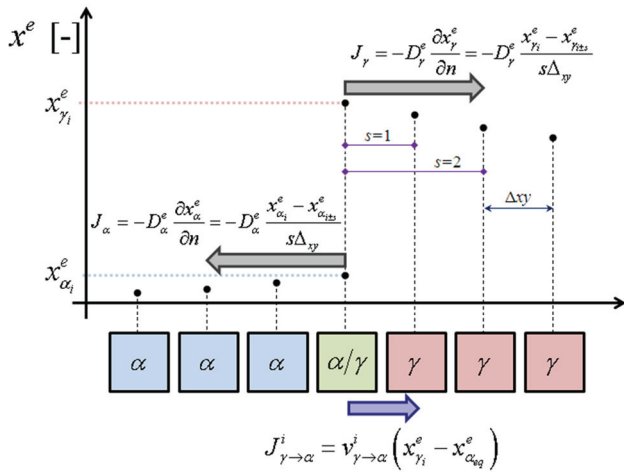


Fig. 2. The Neumann boundary conditions for solute atoms gradient with the first Fick's law for one dimensional CA space, at the interface cell.

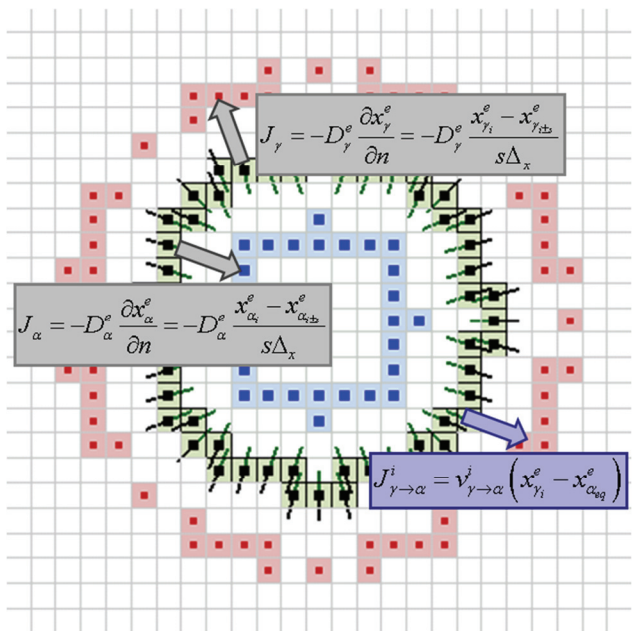


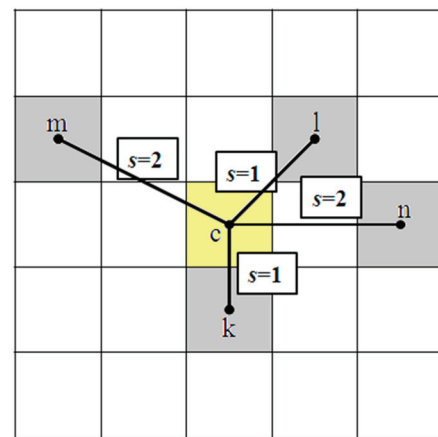
Fig. 3. The Neumann boundary conditions for solute gradient in the first Fick's law for two dimensional CA space, at the interface cell.

2.9. Elimination of artificial anisotropy on 2D CA grid

In several previous cellular automaton models of two-dimensional grain growth (Zhang et al., 2003; Lan et al., 2004; Zheng et al., 2012), hexagonal cells were applied to avoid artificial anisotropy. However, the square cell grid is more easy to implement and integrate with FDM solution. Moreover, it is simple to extend it to cubic cells for 3-dimensional modeling.

Unfortunately, application of the square cell grid leads to an intrinsic problem of artificial anisotropy

in representing grains in the microstructure when all cells for the Moore neighborhood are treated equally. To simplify a description, it is assumed that cells which are not perpendicular to the sides of central cell in the Moore neighborhood, will be called "corner cells". If the calculations of grain growth at "corner cells" are included with equal weight as other neighbors, a tendency towards evolution in directions of "corner cells" is observed. One of the causes of this behavior is connected to the fact that "corner cells" have bigger distance from centers of gravity to the central cell than other neighborhood cells. To eliminate this problem the "corner cells" should have limited impact on the state of central cell in which the growth of new phase is calculated. For this model, a simple approach was developed in which neighboring cells are weighted by a coefficient Θ . For example in figure 4(a) the Moore neighborhood is shown of the central cell c with distance $s = 2$ to cell m .



(a)

| | | |
|-------------------|--------------|--------------------|
| $F_{Top-Left}$ | F_{Top} | $F_{Top-Right}$ |
| F_{Left} | F_{Center} | F_{Right} |
| $F_{Bottom-Left}$ | F_{Bottom} | $F_{Bottom-Right}$ |

(b)

Fig. 4. Definition of effective neighboring cells (a); scheme of the Moore neighborhood (b).



In this model, the determination of the normal vector $\vec{n} = (n_x, n_y)$ is performed similarly as in works (Burbelko, 2004; Marek, 2006). Coordinates n_x and n_y of normal vector can be calculated in the following way:

$$n_x = \frac{-\delta F_x}{\sqrt{(\delta F_x)^2 + (\delta F_y)^2}} \quad (24)$$

$$n_y = \frac{-\delta F_y}{\sqrt{(\delta F_x)^2 + (\delta F_y)^2}} \quad (25)$$

where:

$$\delta F_x = F_{Top-Right} + F_{Right} + F_{Bottom-Right} - F_{Top-Left} - F_{Left} - F_{Bottom-Left} \quad (26)$$

$$\delta F_y = F_{Bottom-Left} + F_{Bottom} + F_{Bottom-Right} - F_{Top-Left} - F_{Top} - F_{Top-Right} \quad (27)$$

where: F_{index} – is the value of volume fraction of growing phase and is taken from neighboring cells as is presented in figure 4(b). The cell with attribute F_{Center} is the cell to which the normal vector is determined.

The weight coefficient Θ is the reciprocal of the normalized distance from the neighbor cell to the central one (cell in question) and is determined as follows:

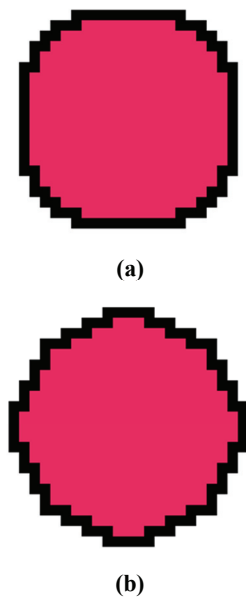


Fig. 5. Comparison of growth of one ferrite nuclei for simulation: (a) without inclusion of the weight coefficient Θ ; (b) with inclusion of the weight coefficient Θ .

$$\Theta = \frac{1}{|\vec{n}|} = \frac{1}{\sqrt{(n_x)^2 + (n_y)^2}} \quad (28)$$

Figure 5(a) shows the growth of one ferrite nuclei during simulation without inclusion of the weight coefficient. In this case, the artificial anisotropy can be observed. Simulated result in figure 5(b) presents that artificial anisotropy can be eliminated by using weight coefficient Θ and the growth of single ferrite grain is more consistent with the assumption of homogeneous interfacial energy of nucleus taken in the calculation.

3. INITIAL MICROSTRUCTURE REPRESENTATION SETTING

A simulation of the austenite to ferrite phase transformation requires a creation of starting microstructure. For two-dimensional simulations, this microstructure can be obtained using DMR scheme. A ferrite–austenite aggregate is a starting microstructure prior to cooling of the DP steel from intercritical temperature ranges. This kind of microstructure is created in the CA grid by digitising a picture of real microstructure. Digitising procedure consists of:

- 1) Taking a picture of selected area of a sample (see figure 6(a)), for which the structure is described in section 2.4.
- 2) Manual depiction of each phase (see figure 6(b)) using a Metllo[®] software (Szala, 2009).
- 3) Generating grain boundaries with Metllo[®] procedures (see figure 6(c)).
- 4) Loading of the two images from steps ii and iii to the program with CA model. Subsequently, conversion of these images to the CA grid and creation of uniform microstructure with phases and boundaries is performed (see figure 6(d)).
- 5) Generating ferrite grains in the CA grid based on marked phases and boundaries.
- 6) Generating γ - α interface cells between austenite and ferrite grains and as a result the initial microstructure in the two-dimensional CA grid is ready for the simulations of the phase transformations.
- 7) The domain size (CA grid dimension) is a result of a recalculation of the marker length, in pixels and micrometers, from the real micrograph picture, and an assumed physical side length of one cell in micrometers L_{CA} . The definition of side length of one cell in micrometers is the most important prerequisite for the proper microstructure characterization. The L_{CA} parameter deter-



mines if some details of real microstructure will be visible on the digitized microstructure in the CA grid or not. Based on DMR tests using a typical partially transformed microstructure, the physical side length of one cell is typically of the order of 0.1 μm .

performed to test the solution of carbon diffusion using the finite difference method. The initial condition was assumed as the one ferrite nuclei has been set in the middle of the CA grid and its growth was simulated during an isothermal process. Periodic conditions were adopted in the simulation.

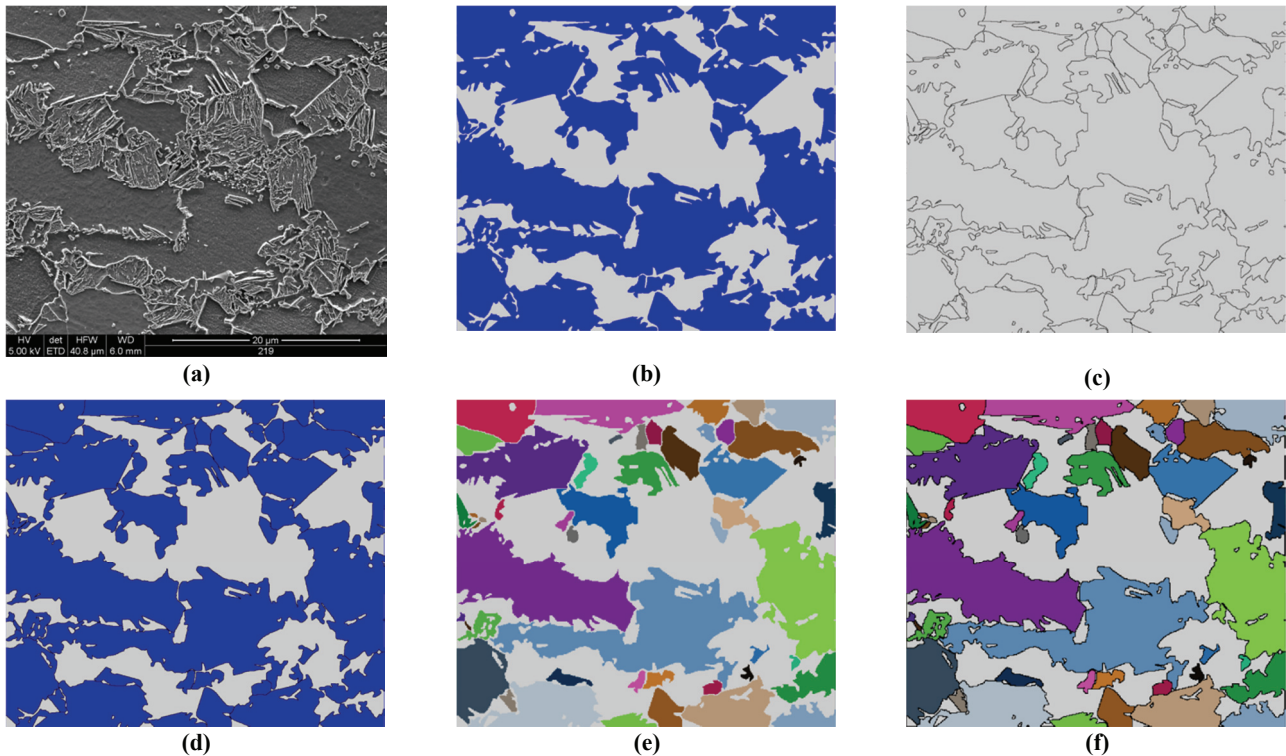


Fig. 6. Stages of the procedure for digitising micrograph of real microstructure: (a) picture of real microstructure of the sample; (b) marked phases using Metllo[®] software (blue color means ferrite phase); (c) generated grain boundaries; (d) uniform microstructure with phases and boundaries in the CA grid; (e) generated ferrite grains in the CA grid; (f) final output microstructure in the two-dimensional CA grid to simulate phase transformations.

As will be shown in our next publication, using the protocol described above, for a simple lean steel the microstructure development and the element redistribution could be very well described and no artificial microstructural features as a result of the square CA lattice were generated. A full description of the simulation results is beyond the scope of the current publication.

4. RESULTS AND DISCUSSION

The chemical composition (wt%) of the steel used in the simulations is C 0.09, Mn 1.42, Si 0.1, Ni 0.01, Cr 0.35, Mo 0.005, Cu 0.03, Al 0.053, V 0.02, Ti 0.001, Nb 0.001, P 0.011, S 0.01, B 0.0001, N 0.0005. The simulation CA grid was a square domain with 101x101 cells, and the size of a cell represented 0.1 μm in real space of the material, which corresponded to 10.1x10.1 μm^2 . The temperature distribution in the CA grid was assumed to be homogenous. In the simulation, a simple approach was

The carbon diffusion during the ferrite nucleation and growth process is one of the most important aspects of the simulations. Figures 7(a)–(c) present the results of the isothermal process simulation after 5s at temperature 790°C. The results of the simulation show that as expected the formation and growth of ferrite nucleus is assisted by the rapid rejection of carbon into surrounding austenite matrix. The carbon diffusion from the ferrite grain to the austenite matrix grain raises the carbon concentration in the vicinity of α/γ interface and as results carbon concentration profile develops in the matrix. Carbon atoms gradually diffuse from the interface surrounding into the austenite matrix interior. The process of carbon diffusion in austenite phase slows down, as a result the average ferrite growth velocity decreases at the later stage of austenite to ferrite transformation.



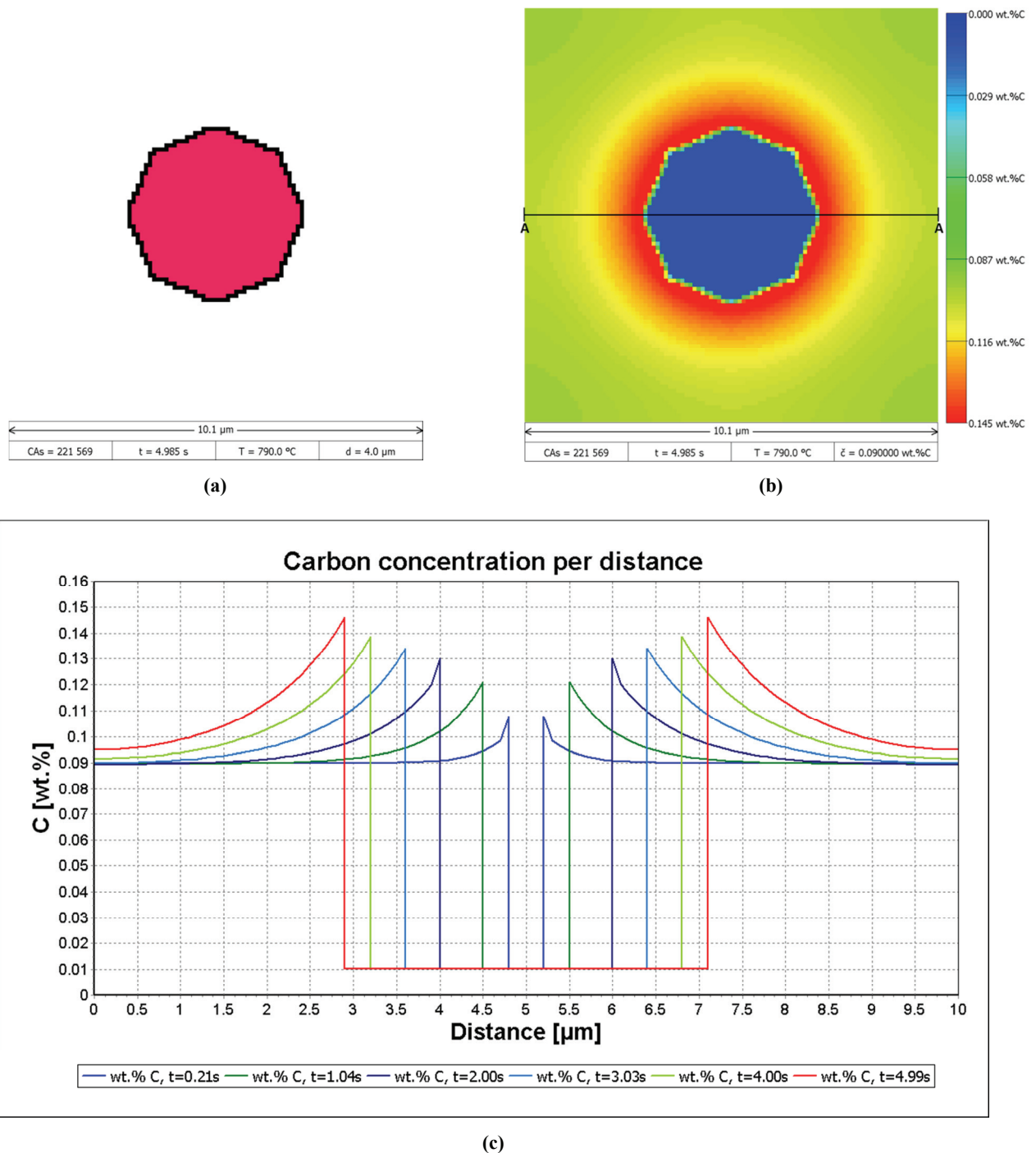


Fig. 7. Results of isothermal process simulations at 790°C after 5s for: (a) one ferrite grain growth; (b) redistribution of the carbon concentration; (c) carbon concentration distribution along the A-A line from figure 7(b).

The results obtained so far prove that solving diffusion in the CA grid with FDM and using the MM approach at sharp interface is appropriate solution to modeling of the ferrite transformation. Figure 7(c) shows that the transformation is gradually controlled from the beginning with the IC model to the DC model at later stages.

5. CONCLUSION

A two-dimensional cellular automaton (CA) model combined with the mixed-mode (MM) approach has been developed to simulate segregation of solute atoms during the phase transformation from austenite to ferrite (γ - α) in DP steels. The model is based on local equilibrium conditions and the assumption that the phase transformation is controlled by both diffusion and other phenomena oc-



curing at the interface, as formulated in the so-called mixed-mode model. The implementation and integration of the CA and MM models is described in detail. A simple and effective approach is presented to eliminate artificial anisotropy of ferrite growth when using a cubic lattice. Boundary conditions assumed in the CA model are described in detail. The method of transferring a real microstructure to the CA grid using DMR scheme has been applied and is described here in detail. The new model can handle complex and realistic microstructures as starting structures for the simulation. The solution of carbon diffusion in the CA grid using the FDM gives suitable results for growth of single ferrite grain and it will be used for simulations to more complex microstructures. A more detailed analysis of the kinetics and topology of the microstructure evolution during further cooling will be presented in a subsequent publication.

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DWUWYMIAROWY MODEL CA DO SYMULACJI ROZWOJU MIKROSTRUKTURY ORAZ SEGREGACJI WĘGLA PODCZAS PRZEMIANY FAZOWEJ AUSTENITU W FERYT PRZY ZASTOSOWANIU RZECZYWISTYCH MIKROSTRUKTUR PO CZĄTKOWYCH

Streszczenie

Model dwuwymiarowego automatu komórkowego (CA) zintegrowany z podejściem mixed-mode (MM) został opracowany do symulacji rozwoju mikrostruktury oraz segregacji węgla podczas przemiany fazowej austenitu w ferryt (γ - α), dla stali DP. Model zbudowany jest w oparciu o lokalne warunki równowagi oraz o założenie, że kinetyka przemiany kontrolowana jest równocześnie dyfuzją węgla oraz zjawiskami zachodzącymi w powierzchni rozdziału. Podejście to nazywane jest modelem mixed-mode. W pracy szczegółowo opisano implementację oraz kombinację modeli CA i MM. Zaprezentowano proste i efektywne podejście do eliminacji sztucznej anizotropii zarodka ferrytu podczas wzrostu, wynikającej z zastosowania kwadratowej siatki CA.

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