CELLULAR AUTOMATA MODEL OF CARBONITRIDES PRECIPITATION PROCESS IN HSLA STEELS

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Abstract

Cellular Automata (CA) model of carbo-nitride precipitation in micro-alloyed 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 high strength low alloyed steels (HSLA) the micro-alloying elements: Ti, Nb, V are added in order to control their microstructure and mechanical properties. Cellular Automata 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. Numerical tests confirmed qualitatively good predictive capabilities of the model.

Keywords: Cellular automata, carbo-nitrides, micro-alloyed steels

1. INTRODUCTION

Precipitation of compounds has played crucial role in controlling of properties of alloys. The High Strength Low Alloyed (HSLA) steels were developed by numerous research. 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 carbo-nitrides precipitation in microalloyed steels is considered works of Dutta & Sellars [1], Dutta et al. [2], Dutta et al. [3]. The models allow calculate kinetics of precipitation and stereological parameters of precipitates as a function of processing parameters. In the present paper the simplified model accounting for one alloying elements [4] is used in Cellular Automata (CA) method to precipitation reaction in industrial processing. The main advantage of the model is simulation of the microstructure image for given chemical composition of steel and parameters of technological process.

2. CARBONITRIDES PRECIPITATION PROCESS IN HSLA STEELS

The micro-alloying elements such as: Ti, Nb, V are added into high strength low alloyed steels (HSLA) 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 - carbo-nitrides [5]. The composition of carbo-nitrides depends on the composition of steel as well as on the temperature. For calculation of the chemical composition of austenite as well as the composition and volume fraction of carbo-nitrides the thermodynamic models were developed [4, 6-9]. They are based on the regular solution model for stoichiometric phases developed by [9]. In steel containing one of the micro-alloying elements (Ti, Nb, V) the carbo-nitride described by chemical formula MC_yN_{1-y} is formed, where *y* means atomic fraction of carbon in carbo-nitride. The austenite and carbo-nitride composition, as well as molar fraction of carb-onitride, is described by the system of equations:

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

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

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

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

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

where: symbol of element X_a, - element content in steel in atomic fraction, symbol of element in bracket, $[X_a]$ - atomic fraction of element dissolved in austenite, L_{CN}^{M} - parameter of mixing (-4260 J / mol [4]), 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 carbo-nitride 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 [4]. Some models describing the kinetics process of binary compounds carbides or nitrides precipitation. In such simplified thermodynamic model is applied, in which the possibility of the mutual dissolution of carbide and nitride forming by micro-alloying elements is neglected and in calculation of kinetic of carbide precipitation the effect of nitrogen is considered as equivalent increase of carbon by nitrogen [1]. 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 carbo-nitrides in HSLA steels are described in [10, 11]. Some of these information was used in the present work do develop the transition rules for the Cellular Automata model.

3. CELLULAR AUTOMATA MODEL

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 [12]. 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 [13], where in the 2D case each cell is surrounded by either four or eight neighbouring cells, respectively. Each cell in the CA space is characterised by its state and by values of internal variables. The cells interactions within the CA space are based on the knowledge defined while studying a particular phenomenon. In every time step, the state of each cell in the lattice is determined by the previous states of its neighbours and the cell itself on a basis of a set of precisely defined transition rules:

$$Y_{i,j}^{t+1} = \begin{Bmatrix} if\ (\Lambda) \Longrightarrow newstate \\ else \Longrightarrow Y_{i,j}^{t} \end{Bmatrix} \quad (6)$$

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:

$$\Lambda = \Lambda\left(Y_{i,j}^{t}, Y_{k,l}^{t}, \boldsymbol{p}, \boldsymbol{q}\right) \quad (7)$$

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 Cellular Automata model of precipitation are based on the knowledge of experts, scientists, experimental observations, and available literature knowledge.

3.1. Cellular Automata model of carbonitrides precipitation process

It is very hard to find any information in publications about modelling of precipitation using the Cellular Automata. In 1995 Karapiperis [14] 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 carbo-nitride precipitates.

3.2. 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 micro-alloying 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:

$$Y_{i,j}^{t+1} = \begin{Bmatrix} if\ (\Lambda) \Longrightarrow P \\ else\ \Longrightarrow\ Y_{i,j}^{t} \end{Bmatrix} \tag{8}$$

where:

$$\Lambda = Y_{i,j}^{t} \equiv \gamma\ \wedge\ \rho_{i,j} > \rho_{cr}\ \wedge\ l_{(0,1)} < P_{N1} \tag{9}$$

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} [15]).

Micro-alloying 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:

$$\Lambda = Y_{i,j}^{t} \equiv \gamma\ \wedge\ \rho_{i,j} > \rho_{cr}\ \wedge\ Y_{k,l}^{t} \equiv P\ \wedge\ l_{(0,1)} < P_{N2}\ \wedge\ [MA]_{i,j} > [MA]_{cr}\ \wedge\ \Delta r > d \tag{10}$$

where: P_{N2} - 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.

4. RESULTS

Numerical tests were performed to evaluate model's predictive capabilities. Steel containing 0.15 % C, 0.04 % Nb and 0.008 % N subjected to heat treatment austenitization at 1200 °C with following holding at T for τ time with different strain was considered. Since precipitates are few orders of magnitude smaller than the austenite grain size, generation of the initial microstructure was limited to initiation of the input parameters. The results presented below (**Figure 1**) were obtained for the 250 × 250 cells, while the dimension of a single cell was 1 nm.

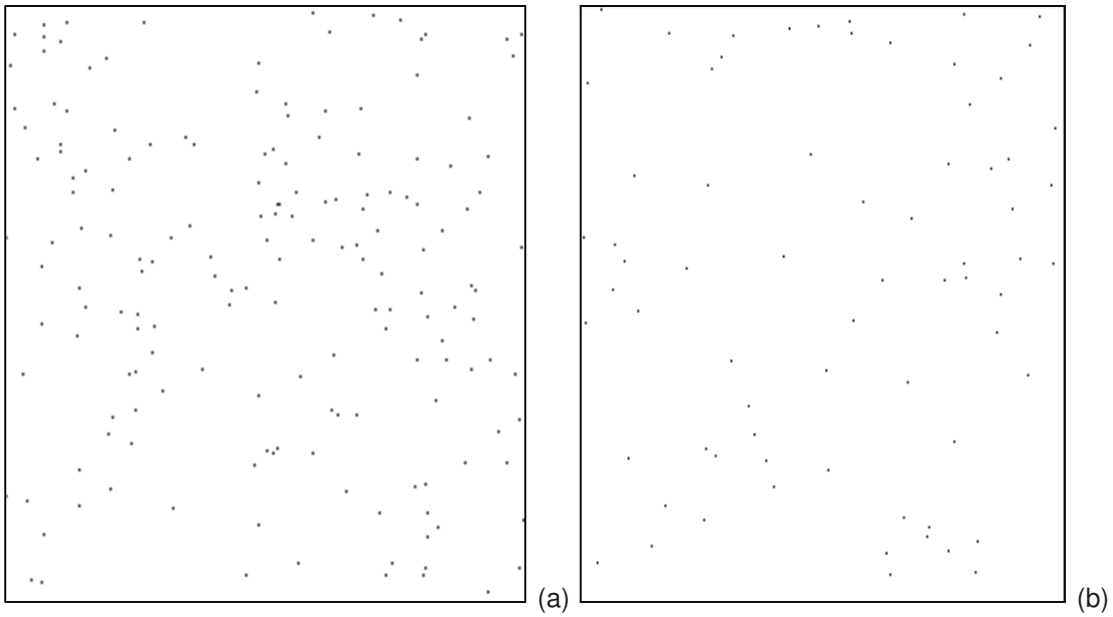

Figure 1 Comparison of simulated microstructures with precipitations of carbonitrides in HSLA steel after heat treatment: austenitization at 1200 °C with following isothermal holding at 850 °C (a) and 960 °C (b) for 120 sec

Precipitation is thermally activated process and strong influence of the temperature is expected. Solubility of niobium in iron decreases rapidly with a decrease of the temperature. Therefore, sensitivity of the model to temperature was investigated next. Changes of niobium content and radius of precipitates for steel subject to a strain of 0.01 at various temperatures are presented in **Figure 2** and **Figure 3.**

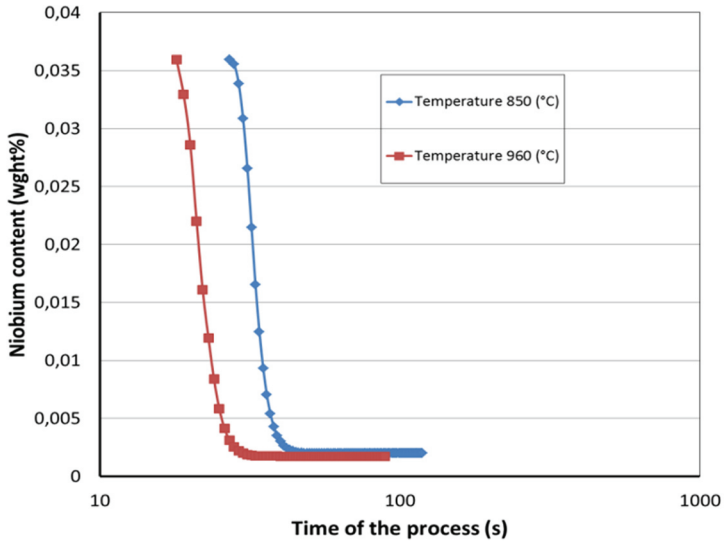

Figure 2 Calculated changes of dissolved niobium content, [Nb] for various temperatures

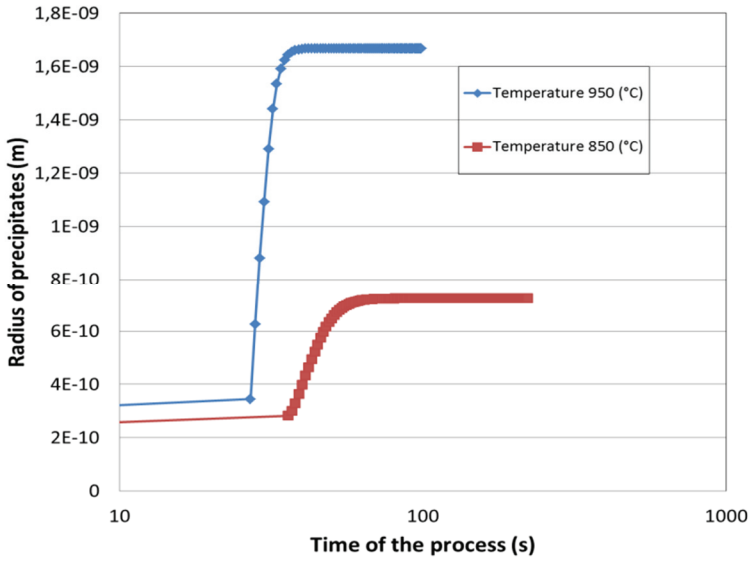

Figure 3 Calculated changes of radius, r, of precipitates for various temperatures

5. CONCLUSION

A proposition of the Cellular Automata model for the analysis of the precipitation of carbo-nitrides in HSLA steels was presented in the paper. Transition rules for nucleation and growth of precipitates were formulated. Performed numerical tests have shown that model reproduced qualitatively well process of precipitation. Predictions of kinetics of precipitation and changes of the average size of precipitates and dependence of these parameters on strains and temperature agreed with tendencies observed in experiments. The model needs further development, which should include:

- Identification of such parameters as critical dislocation density, the size distribution of precipitation and its effect on mechanical properties of steel, probabilities P_{N1} and P_{N2} in equations (9) and (10).
- Accounting for the effect of recrystallization after deformation.
- Validation of the model by a comparison of predictions with the experimental data.

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