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Discrete micro-scale cellular automata model for modelling phase transformation during heating of dual phase steels

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ABSTRACT

Development of the discrete two-dimensional cellular automata (CA) model for modelling phase transformation during heating of dual phase (DP) steels is the subject of the present work. The model is based on the solution of fundamental diffusion equation, which is associated with local equilibrium conditions, and takes into account growth of austenite during phase transformation driven by the grain boundary curvature. Solution of the diffusion equation is realized by the finite difference method (FDM), while further growth is controlled by the cellular automata transition rules. All the details of the developed cellular automata model are presented and discussed. Finally comparison between obtained results and experimental data is also addressed.

1. Introduction

Materials for automotive and aerospace industries require strict measures regarding weight/strength ratio, which provide a lot of opportunities for both experimental and numerical research. As a result, fast development of modern steel grades is observed and among them one of the promising steel grades, are Advanced High Strength Steels (AHSS) [1]. These steel grades have significantly lower weight/strength ratio, which give considerable impact on efficiency in the field of automobile and aerospace applications. The Dual Phase (DP) steels are a good representation of mentioned AHSS steel grades. Elevated properties of the DP steels are related with properly designed microstructure morphologies obtained during complex thermomechanical operations involving e.g. cold rolling and annealing. Phase transformation during heating and cooling are the main phenomena, which control final properties. Much attention in this process was paid only to the transformation of austenite into ferrite phase during cooling as this is the last stage controlling the morphology. However, due to its significant effect on the final microstructure, transformation during heating recently also attracts attention of many researchers. It was proven that the transformation to austenite during heating affects many properties (e.g. grain size, grain distribution, concentration of alloying elements etc.), which are crucial for the kinetics of transformation during subsequent cooling. Eventually combination of these two stages have significant impact on

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product mechanical properties e.g. hardness, strength and formability.

Unfortunately reduction in time and research costs, limits the experimental analysis, which eventually redirects attention towards numerical modelling as an efficient tool supporting experimental investigation. However, when detailed information regarding morphology and carbon distribution across the microstructure is required, conventional models based on Avrami type equations cannot be used. The solution is application of the discrete numerical methods taking into account explicitly microstructure morphology [2]. One of the solutions to simulate explicit microstructural evolution both during heating and cooling is the cellular automata (CA) method. The CA is a collection of regular grids or cells, where each cell has a finite number of states. Changes in the cell states depend only on the governing set of transition rules defined by the user. Each cell changes its state based on the state of neighbouring cells and the cell itself from the previous time step. The main advantage of the cellular automata over other methods is that it can handle large computational domain size, which means more accurate results. The cellular automata model is always based on several components: (1) *n*-dimensional space, which is composed of similar cells, (2) finite states, which are assigned to each cell, (3) appropriate neighbourhood, e.g. von Neumann, Moore etc., and (4) transition rules for each cell. Recently, the CA method was applied to many microstructural evolution based simulations e.g. reaustenitization [3], recrystallization [4,5] or austenite to ferrite transformation [6,7].

Thus, the objective of the present work is to create the cellular automata model for phase transformation during heating controlled by the solution of diffusion equation and grain boundary curvature. Both mechanisms play a significant role during evolution of microstructure in continuous annealing process. Developed model is part of an overall model of the DP steel manufacturing cycle focused on modelling static recrystallization, transformation model during heating, and transformation model during cooling. That is why, initial microstructure for the current model consists of ferrite and pearlite phases obtained from ferrite static recrystallization model with the help of the Digital Material Representation method [8–10]. In the present work, the driving force of phase transformation is obtained by both carbon diffusion using explicit FDM and grain boundary curvature. The pearlite dissolution, ferrite transformation to austenite and grain enlargement during heating were included in the work to obtain realistic results. Finally, results from the model will be further used as an input microstructure to the CA model for phase transformation during cooling.

Details of the developed CA model of ferrite to austenite transformation are presented in the subsequent sections.

2. Process of continuous annealing of DP steels

The DP steel plates are produced by hot rolling and laminar cooling, or by cold rolling and intercritical annealing. The latter process is considered in the present paper, while former technology was modelled in earlier works [11].

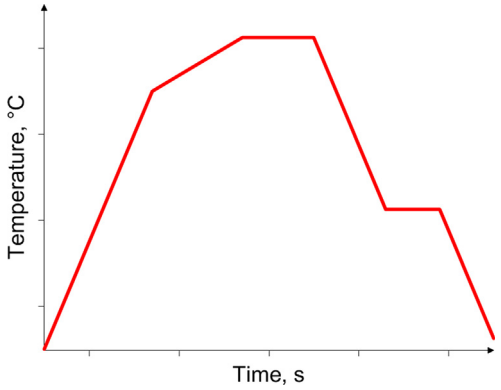

Fig. 1 – Typical thermal cycle for manufacturing of DP steels.

Conditions of the cold rolling process of the DP steels are similar to typical conditions used for carbon-manganese steels. As a result, the two-phase microstructure is obtained during continuous annealing after cold rolling [12] according to thermal cycle as presented in Fig. 1.

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 during cold rolling. During the heating, before annealing, recrystallization of ferrite takes place. The 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 influences the final structure [13].

Numerous papers dealing with the continuous annealing process can be found in the scientific literature, e.g. modelling of ferrite recrystallization kinetics [12]. Systematic discussion of annealing process can be found in [14–16]. Correlation between thermal cycle parameters and properties of the DP steels and transformations during cooling are also discussed in scientific literature, respectively [14,15]. Recapitulation of these works can be found in [16]. The influence of accelerated cooling for hot rolled DP steel strips was investigated [8]. Less attention was paid to the simulation of transformation of heating to the intercritical temperatures. Simulation of intercritical annealing using finite element solution of the diffusion equation to predict carbon segregation during transformation of the ferritic+pearlitic microstructure into austenite is presented in [17]. This problem is also discussed in further sections of the present work and application of the CA model to simulate this transformation is presented.

3. Phase transformation during heating

Initial microstructure of the DP steel after cold rolling and recrystallization contains ferrite and pearlite phases, thus the mechanisms associated with austenitization are pearlite