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# Sensitivity analysis of phase transformation model based on solution of diffusion equation

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ABSTRACT

Presented work is focused on modelling of the phase transformation during laminar cooling after hot rolling of dual phase steel strips. Conventional FE model describing heat transfer was used in the macroscale. The model based on the solution of the diffusion equation with moving boundary was selected to predict properties of the steel based on phase transformations which occur in microscale. Preliminary observations indicated that results depend on various parameters of the model, such as: diffusion coefficient, boundary velocity factor and cooling rate. Therefore, sensitivity analysis of the model with respect to these parameters was performed in order to enhance the predictive capabilities of the model and to simplify further solution.



## 1. Introduction

Dual phase (DP) steels are commonly used in the automotive industry and a number of car body parts responsible for safety of passengers are now made of these materials. DP steel allows for lighter construction design than in conventional steels and has a greater ability to absorb crash energy. As a result, the most important elements of the crumple zone, such as bumpers, rocker panels, side roof arches, are produced from these steels. Properties of two-phase materials depend on their structural composition. DP steel structure is a mixture of ferrite and martensite, with possible small amounts of bainite and retained austenite. Each of these components, both its shape and size and distribution of hardness, has an influence on the properties of the final product. The strength properties increase with increasing volume fraction of martensite. The presence of soft ferritic phase improves workability. Maintaining the balance between these two features is the main challenge in the design of DP steels.

Studies on the development of multi-phase steel structure have been conducted for many years [1]. Improvement of both strength and ductility has been recently obtained for austenitic steels with a high manganese content [2]. The mechanical properties of these steels are strongly dependent on the chemical composition of the hard constituents. Unfortunately, a high content of alloying elements increases the cost of production and creates problems in casting and heat treatment. For this reason researchers are still searching for new solutions for low manganese AHSS.

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DP steel strips are produced either by hot rolling and laminar cooling or by cold rolling and continuous annealing [3]. All processes have a joint influence on the final microstructure. A large number of technological parameters requires precise control, which makes the control of the manufacturing process very difficult. Therefore, numerical modelling in now commonly used to predict kinetics of phase transformations during manufacturing of DP steels.

Reasonably good results of modelling of laminar cooling and continuous annealing were obtained when a conventional model based on Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation was applied (see authors' publications [3,4]). This simple model appeared to be efficient and accurate when volume fractions of phases only are of interest. On the other hand, information concerning morphology of phases and chemical composition of hard constituents is now needed to design a new generation of DP steels. The idea of application of the solution of the diffusion equation with a moving boundary, which was proposed by Pernach and Pietrzyk [5], was applied to predict changes of carbon concentration in austenite and to determine the shape and composition of the martensite islands [6]. A similar model was developed for the transformation during heating of the ferritic-pearlitic microstructure [7]. Analysis of results obtained in [6,7] has shown that a number of coefficients in the model are difficult to determine. Therefore, in the present work, a sensitivity analysis (SA) of this model with respect to model and process parameters was performed. The objective was to enhance predictive capabilities of the model and to simplify further solution (for example multiscale simulations). One-at-a-time SA approach has been applied. Phase transformations during cooling were considered.

## 2. Existing models

The transformation of austenite to ferritic-pearlitic microstructure begins when the temperature drops below $Ae_3$. Phase transformation $\gamma$-$\alpha$ occurs by processes of nucleation and growth. In modelling, two mechanisms have to be distinguished: the reconstruction of an austenite lattice into a ferrite lattice and carbon diffusion occurring simultaneously. The progress of both processes determines the speed of the transformation. Ferrite grain growth is equivalent to the movement of the interface, which is based on mixed mode approach and described by a diffusion mechanism with the Dirichlet boundary condition dependent on the conventional interfacial mobility term.

During the transformation, the carbon content in the austenite increases and, when it achieves the equilibrium content $c_{\gamma\alpha}$ at the austenite-cementite boundary, the remaining austenite is transformed into pearlite. For faster cooling, the temperature drops below the bainite start temperature before the equilibrium content $c_{\gamma\alpha}$ is reached and bainitic transformation begins. This transformation combines features of diffusive and non-diffusive transformation. In the initial phase of the transformation bainitic ferrite is created and, after that, the remaining austenite becomes richer in carbon and is decomposed into carbides and low temperature transformation products [8]. Martensitic transformation occurs in undercooled alloys and is based on change of the crystallographic lattice without change in chemical composition. The transformation is diffusionless in the meaning of long range diffusion and the motion of the interface. Volume fraction of martensite increases with decreasing temperature and does not change with time.

Many models of phase transformations with different prediction capabilities exist. The well-known simplest methods based on thermodynamic relations and JMAK equation do not provide information about carbon distribution and concentration and do not include microstructure morphology in calculations. They provide good estimates, but not sufficient in many cases for scientific research. On the other hand, they are capable of solving problems very fast, which make them useful for online computations. More information concerning chemical composition distribution was obtained when phase field models were applied [9,10]. Sietsma [11] discussed the possibilities of application of various methods, including phase field and an alternative mixed mode approach, to simulation of phase transformation in AHSS. In these models [12,13], grain growth is controlled only by interface mobility, while the influence of boundary diffusion is omitted. As a result, we can observe a large discrepancy between the results of numerical simulations and experimental tests.

More sophisticated models like those based on cellular automata concept [14,15] provide higher prediction capabilities, but at the cost of computation time. Very limited possibilities for local grid refinement in cellular automata framework cause time of computation to be strictly dependent on the number of cells used for space discretization. Also if grid is too coarse, significant numerical errors could be introduced.

## 3. Numerical formulation

Model presented in this paper is based on the assumption that transformation is controlled only by the rate of carbon diffusion, i.e. the interface moves as fast as diffusion of carbon allows. Furthermore, the model assumes conditions of local equilibrium. The influence of interface mobility on the velocity of transformation is omitted. The first model based on the solution of the diffusion equation with a moving boundary was proposed by Pernach [5], where the finite difference method was used to solve the diffusion equation. This approach was further developed in [6,7] and a finite element code was applied. Present approach is based on implicit interface representation, which, as opposed to explicit methods, does not require direct tracking of the interface surface. The mathematical formulation is based on the solution of the second Fick's law:

$$\nabla\cdot(D\nabla c) = \frac{\partial c}{\partial t} \tag{1}$$

where $D$ – diffusion coefficient, $c$ – carbon concentration.Eq. (1) was solved with the following initial and boundary conditions:

$$\begin{aligned} c(x,0) &= c_0 \\ c(x_\xi,t) &= c_{\gamma\alpha} \end{aligned} \tag{2}$$

where $c_0$ – carbon concentration in steel, $c_{\gamma\alpha}$ – equilibrium carbon concentration at the austenite–ferrite boundary, $x$ – vector of coordinates, $x_\xi$ – position of the interface. Variational