Accounting for random character of nucleation in modelling of phase transformations in steels

Łukasz Poloczek[1], Roman Kuziak[1], Jakub Foryś[2],
Danuta Szeliga[2], Maciej Pietrzyk[2]

[1] Łukasiewicz Research Network – Upper Silesian Institute of Technology,
ul. K. Miarki 12, 44-100 Gliwice, Poland
[2] AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland
lukasz.poloczek@imz.lukasiewicz.gov.pl,
roman.kuziak@imz.lukasiewicz.gov.pl,
jakubforys@student.agh.edu.pl,
szeliga@agh.edu.pl, maciej.pietrzyk@agh.edu.pl

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1. Introduction

There is a continuous search for construction materials that combine high strength with good formability, as well as a high strength-to-density ratio. Steels have met these requirements for many decades. Modern multiphase steels, which were developed in the last decades of the 20th century, benefit from the best features of phases they are composed of. Advanced numerical models, which can predict heterogeneity of the microstructure are needed to gain knowledge on distributions of microstructural features and to design thermal-mechanical cycles allowing to obtain optimal microstructure and resulting properties. Hypothesis was put forward in [1] that application of the stochastic internal variables to the modelling of multiphase steels will allow to build the model with the capability to predict various features of heterogeneous microstructures.

Following this motivation, we developed the stochastic model, which describes evolution of the dislocation density and the grain size during multistage hot deformation. Analysis and optimization of the numerical parameters of the model are described in [2] while its description, identification, validation and application are presented in [3]. This model calculates histograms of the dislocation density and the grain size after multi-step hot deformation. On the other hand, the properties of the products are obtained by control of the phase transformation during cooling after hot forming. Therefore, the objective of our work is to extend the model by including phase transformations, accounting for the random character of nucleation of a new phase.

Literature review shows that the stochastic models were widely used to describe random nucleation during phase transformations. However, majority of the approaches consider nucleation in the microstructure represented explicitly (full-field models). Probabilistic approach was used in the Cellular Automata models [4], as well as in the Monte Carlo method, see review in [5]. Our objective is to avoid costly computations in the microstructure represented explicitly and to develop a mean-field model based on a statistical description of the phenomena occurring in the microstructure. In the case of steels, this model must be based on the non-classical nucleation theory, which occurs in a diffusional growth where diffusion field gives rise to reduced nucleation probability around growing nuclei [6]. This aspect is considered in the present work.

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2. Model and results

In the model under development, equilibrium state of the metallurgical system is described by the thermodynamics. The phase transformation model predicts changes of the state of the system between the two equilibrium states during the transient process. The equilibrium is represented by the Fe-C phase equilibrium diagram. Development of the stochastic phase transformation model for diffusion-controlled transformations is our objective. The models, which account for the probability of both nucleation and growth, can be encountered in the scientific literature, but they are based on the explicit representation of the microstructure [7] and are computationally expensive. Moreover, several published models deal with the solidification process [8] or solid-state phase transformations in other materials than steels [9]. Thus, in the first approach we focus on modelling of random character of the nucleation only and the deterministic model is used to describe growth of the new phase.

2.1. Nucleation

An initial step of transformations in solids is that of nucleation. To model nucleation, one must specify nuclei location in space as well as how nuclei appear as a function of time. In the JMAK theory, there are two nucleation modes [5]: 1) Classical theory, which assumes that the thermodynamic properties of a nucleus are uniform and the same as the equilibrium bulk counterparts within the nucleus.; 2) Non-classical nucleation theory of Cahn and Hilliard, which is based on the diffuse-interface description of the interfaces. In this theory a coalescence of subcritical clusters and stepwise nucleation is introduced [10].

For years a stochastic character of nucleation was accounted for in the modelling of phase transformations and the JMAK approach based on Poisson statistics was used. Although most of the published papers deals with the crystallization process, solid-state transformations are addressed in some publications, as well. Early papers were focused on collecting a large set of nucleation data [11]. In the homogeneous Poisson Point Process no correlation among nuclei is present and in the case of steels the probability of nucleus to appear depends on undercooling below A_{e3}, state of the austenite, etc. Thus, assuming Poisson homogenous nucleation, the probability that the nucleus of the new phase occurs in the time $\Delta t = t_{i+1} - t_i$ is:

$$\begin{aligned} &\mathbf{P}[\xi(t_i)=0] = \begin{cases} p(t_i) & if\ p(t_i)<1 \\ 1 & otherwise \end{cases} \\ &\mathbf{P}[\xi(t_i)=1] = 1-\mathbf{P}[\xi(t_i)=0] \end{aligned} \tag{1}$$

In Equation (1) $p(t_i)$ is a function, that bounds together the probability that the material point becomes a critical nucleus in a current. Assuming Poisson homogenous nucleation the following equation was used:

$$p(t_i) = b_1 D_\gamma^{-b_2} \rho^{b_3} (A_{e3} - T)^{b_4} \tag{2}$$

where: D_γ – grain size, ρ – dislocation density, b_1, b_2, b_3, b_4 – coefficients.

Our objective was to introduce non-Poisson statistics, which account for the interaction between existing grains of a new phase and a new nucleus. The solution is based on the method of the critical region [12]. Additionally, in the case of the austenite decomposition, carbon is pushed out from the ferrite grains and carbon content in the austenite c_γ increases. Thus, probability of nucleation in the neighbourhood of the new ferrite grains is decreased. The idea of this stochastic approach to modelling

austenite-ferrite transformation is shown in Figure 1a. The effect of microchemical bands, which occur during the solidification process [13], is the next factor, which we considered. The independent variables in the model were the width of the high manganese enriched band w and the distance between the bands d. The improved model accounts for a difference in the nucleation rate and the grain size between high and low manganese bands. Thus, equation (2) is revised to the following form:

$$p(t_i) = [b_{1\max}(1-\xi) + b_{1\min}\xi]D^{-b_2}\rho^{b_3}(A_{e3}-T)^{b_4}[1-X_f(t_i)]\left[\frac{c_0}{c_\gamma(t_1)}\right]^{b_5} \tag{3}$$

where: $\xi = w/d$ – relative thickness of the high manganese band, $b_{1\min}$, $b_{1\max}$ – coefficients.

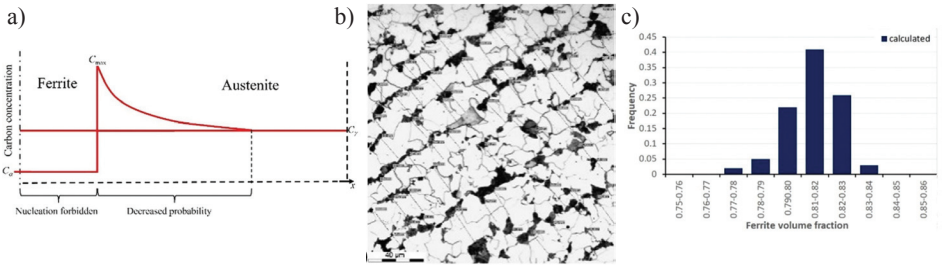

Figure 1. Carbon distribution as a function of the distance from the centre of the ferrite grain and the idea of the stochastic approach to the nucleation model based on the method of the critical region (a) and image of the microstructure with high and low manganese bands (b).

2.2. Results and conclusions

The stochastic model predicts distributions (histograms) of such parameters as volume fractions of phases and size of ferrite grains. Simulation of cooling of the flat rod was performed and the calculated histogram of the ferrite volume fraction is shown in Figure 1c. Measured average ferrite volume fraction was 0.82. It was concluded that: The model does not require explicit representation of the microstructure, which allows to decrease the computing times radically; ii) The model predicts distribution of the microstructure features in a statistical way. It allows to calculate distributions (histograms) of the microstructural features accounting for the state of the microstructure prior to transformations, including the effect of the microchemical bands.

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