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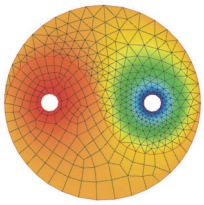

APPLICATION OF THE DIFFUSION EQUATION TO MODELING PHASE TRANSFORMATION DURING COOLING OF PEARLITIC STEEL

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Abstract

Exploitation properties of rails are formed by controlled heat treatment of the head of the rail carried out after rolling. Complex cooling schedules have to be applied to obtain required microstructure and properties of rail steels. Design of these cooling schedules should be supported by numerical simulation. This, however, requires advanced phase transformation models which are able to predict not only average parameters of the microstructure but also morphology of the pearlite and carbon distribution in this structural component. Therefore, numerical model of pearlitic transformation is proposed in this work. The model was based on the solution of the carbon diffusion equation. The boundary conditions were determined assuming local thermodynamic equilibrium. Location of the interface in each time step was predicted from the condition of mass conservation. The created model allowed determining of the interlamellar spacing and carbon distribution in austenite for different cooling cycles. The results of analysis can be used to predict the strength and hardness of the steel.

Key words: rails, pearlitic steel, pearlitic transformation, numerical modelling, diffusion

1. INTRODUCTION

Growing demand of the rail industry for new material solutions that meet the operation conditions imposed by a technical progress was the motivation for this research. Continuous changes in work conditions for rails are associated with increasing train speeds and axle loads, as well as increasing rail traffic volumes.

The government plan for development of rail transport in Poland by 2030 assumes the creation of infrastructure adjusted to the needs of high-speed trains. Implementation of this plan involves the construction of rail lines which would meet contemporary requirements using the highest quality steels for rails. The new generation rails should be characterized by improved fatigue strength, abrasive wear strength, fracture toughness and good weldability.

Medium-carbon steels with normal or increased manganese content are used in the production of rails. These are mainly pearlitic steels. Their properties are strongly dependent on the morphology of pearlite, which can be formed by heat treatment through processes such as tempering or isothermal annealing (Kuziak & Zygmunt, 2013; Aaronson et al., 2010; Herian & Aniołek 2010). The parameters of microstructure which determine the properties of rail steel are: the interlamellar spacing, pearlite colony size and pearlite grain size. With a decrease of the interlamellar spacing, strength and hardness of steel increases, as well as the abrasion and fatigue resistance. Reducing the size of colony and particle results in improved ductility of the perlitic steel. The main goal of this work is to determine the relationship between the parameters of heat treatment and properties of the finished product. The numerical tool proposed in the present work should supply

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information concerning the interlamellar spacing and carbon distribution in the pearlite and should support development of the optimal process of rails manufacturing. To reach this goal numerical model of pearlitic transformation was based on the solutions of the diffusion equation in 1D and 2D domains. The boundary conditions are determined assuming local thermodynamic equilibrium. According to the equilibrium diagram obtained for the tested steel, the content of carbon in austenite, ferrite and cementite was 0.73%, 0.02%, and 6.67% respectively.

2. MODEL OF THE AUSTENITE TO PEARLITE TRANSFORMATION

2.1. Physical basis

The main goal of the heat treatment of rails is to obtain a fine structure of pearlite. Rapid cooling of rails after rolling promotes fragmentation of the structure, but it can also lead to an occurrence of unfavorable components of degenerated pearlite and bainite. For this reason, the heat treatment should be conducted in a controlled manner.

The processes of heat treatment of rails are carried out either in the rolling line or off-line. In the former case the rails are cooled directly after rolling from the temperature of purely austenitic microstructure. In the latter case, the rail must be heated to a temperature of austenite, maintained at that temperature until the uniform distribution is obtained and only then accelerated cooling can be performed. The methods of heat treatment have been continuously improved during last three decades (Ackert & Nott, 1987; Sahay et al., 2009; Pohanka & Kotrbacek, 2012). The method of cyclic cooling of the rail head in the aqueous solution of the polymer mixture, which was presented by Kuziak and Zygmunt (2013) and investigated experimentally by Kuziak et al. (2014), was used as an example in the present work.

Pearlitic transformation begins when cooling temperature drops below Ar_1 . This temperature depends on the chemical composition. Pearlitic steel containing 0.71%C, 1.1%Mn, 0.31%Si, and 0.13%Cr was considered. A part of the phase equilibrium diagram determined using ThermoCalc software is shown in figure 1. Austenite-perlite transformation starts after Ar_1 temperature is exceeded, which in case of this steel, is equal to 722°C.

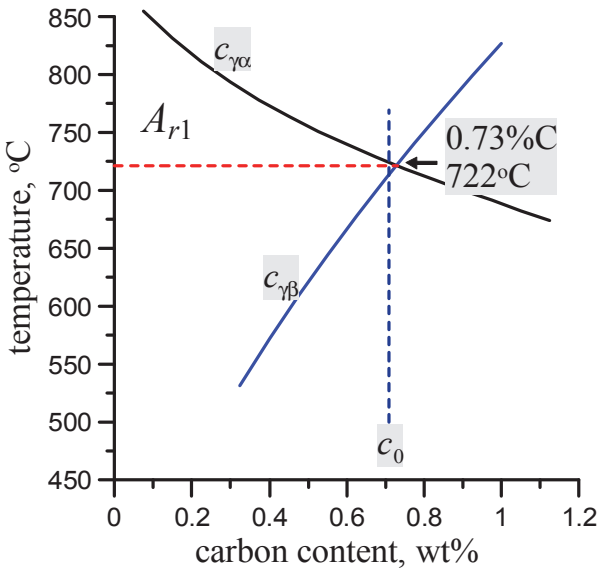

Fig. 1. *A part of the phase equilibrium diagram determined using ThermoCalc software, c_0 - carbon concentration in steel, $c_{\gamma\alpha}$ - carbon content at the austenite-ferrite boundary, $c_{\gamma\beta}$ - carbon content at the austenite-cementite boundary.*

The driving force of transformation is the difference in free energy of austenite and mixture of ferrite and cementite. Two processes occur during the transformation of austenite to pearlite. The first is diffusion of carbon and the second is reconstruction of the crystallographic lattice. The rate of transformation is controlled by the diffusion of carbon atoms, and the crystallographic change occurs as readily as the redistribution of carbon is allowed.

Typical structure of pearlitic steel is shown in figure 2. One grain of pearlite usually consists of few pearlite colonies. Within each colony plates of ferrite and cementite have the same crystallographic orientation.

In the eutectoid steels phase transformation begins from cementite nucleation at the austenite grain boundaries or at undissolved cementite particles, as well as at ferrite grains. The studies show that the rate of pearlite nucleation increases linearly with time and decreases with temperature. According to Hillert concept we can observe the orientation relationship between the ferrite in pearlite and the parent austenite, resulting in a partially coherent interface.

Formation of pearlite colony occurs by sidewise growth and front growth. In the first case (figure 3a) carbon diffuses from austenite containing 0.71%C to cementite, with 6.67% of carbon content.

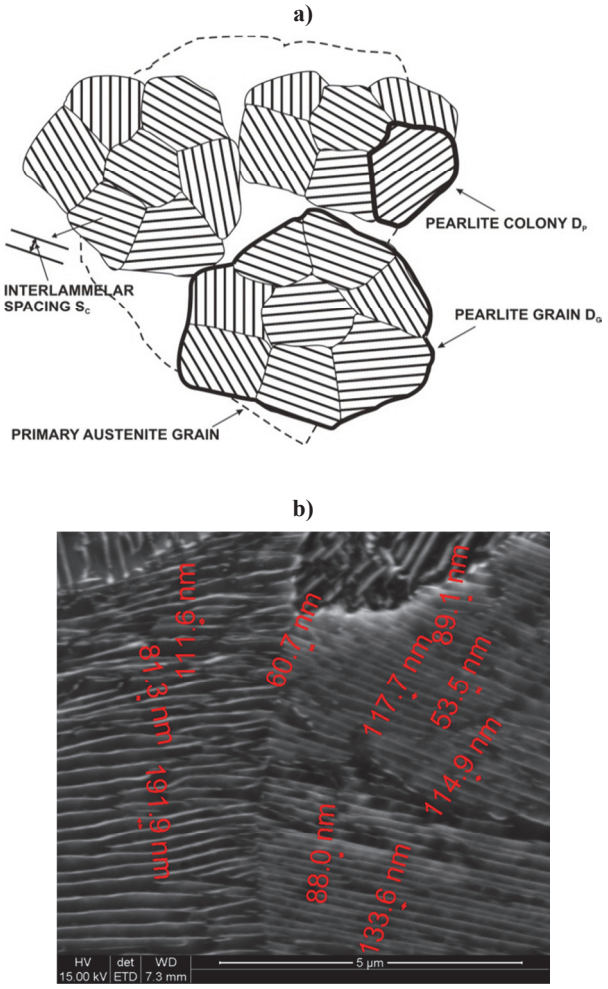

Fig. 2. *Schematic representation of structure of pearlitic steels (a) and microstructure of this steel (by courtesy IMŻ Gliwice) (b).*

When the area around the cementite plates becomes poor in carbon then austenite begins transformation into ferrite. The growth of ferrite plate causes pushing carbon to austenite and increasing its concentration until the composition required to form cementite is reached. The whole cycle is repeated until the disappearance of the austenitic phase. The plates of both phases grow inside the austenite grains. The thickness of the ferrite plates is about seven times greater than that of cementite plates. This mechanism was a basis of the model developed in the present work.

Front growth of pearlite colony (figure 3b) occurs by the carbon diffusion from austenite. The atoms of carbon of the area encircled by a dotted line join the plates of ferrite and cementite according to the arrows direction.

2.2. Review of numerical models

In parallel with the experimental research, numerical simulations that allow the determination of the relation between the parameters of heat treatment, parameters of the structure and properties of the rails were developed. The models should be capable to perform simulation of temperature distribution at the cross section of the rail during the cooling and should be integrated with the simulation of phase transformations occurring in this time.

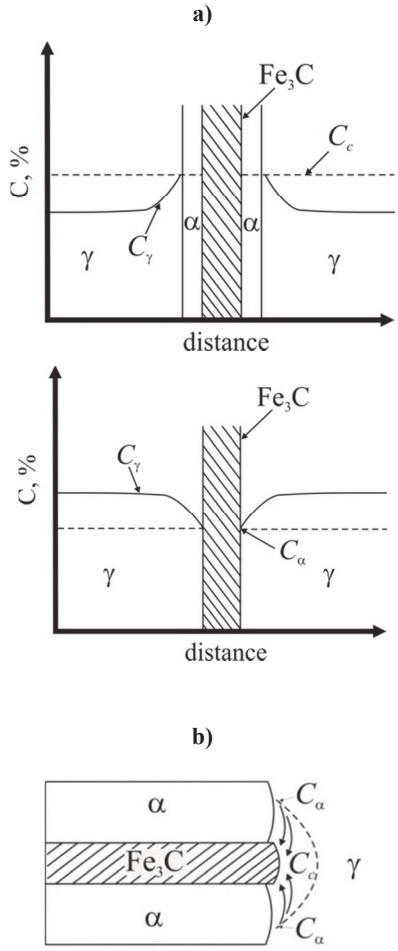

Fig. 3. *Schematic representation of the growth of pearlite colonies: a) sidewise growth, b) front growth.*

Among the commonly used models those based on mixed-mode approach should be distinguished. Such solutions can be found in the works (Pandit & Bhadeshia, 2011; Offerman et al., 2003). In case of these models, the criteria of maximum growth rate or maximum rate of entropy production is used to determine the interlamellar spacing. Adaptation of the first criterion is synonymous with implementation of Hillert-Zener assumption according to which the growth rate of pearlite is directly proportional to the difference in the carbon concentration in ferrite and cementite phases and inversely proportional to the distance between the plates. Such an approach based on the phase filed method can be found in (Nakajima et al., 2006).

The model presented in the first paper allows simulation of sidewise growth of pearlite colonies for isothermal conditions. Interlamellar spacing is assumed constant for the given undercooling. The obtained results differed noticeably from the results of experiments. In the paper (Offerman et al., 2003) only the growth rate of pearlite colonies for assumed interlamellar spacing was determined.

Papers (Pandit & Bhadeshia, 2011; Offerman et al., 2003) describe models which take into account both processes occurring at the interface i.e. volume carbon diffusion and interface mobility. However, relying on the criteria which determine the distance between the plates of cementite, it is not possible to specify the size of this important parameter. In addition, there is no experimental verification that would confirm the validity of the assumptions.

In the paper (Capdevila et al., 2002) JMAK equation (Johnson-Mehl-Avrami-Kolmogorov) was used to describe the kinetics of pearlite transformation. This solution allows to determine the change of pearlite phase volume fraction for different cooling cycles. Developed at AGH finite element model of cooling combined with phase transformations model based also on JMAK equation was presented by Pietrzyk & Kuziak (2012). Optimization task for rail cooling formulated with this model is described by Szeliga et al. (2014). The analysis of the literature showed that although there is a detailed theoretical description of the phenomena occurring during the transformation of pearlite, only few of numerical models were created due to the complexity of the problem. In addition, the existing solutions do not allow the identification of the most important parameter, i.e. the distance between the plates of cementite, which would affect the mechanical properties of pearlitic steels.

2.3. Details of implementation

The model proposed in this work is based on the assumption that carbon diffusivity is the main controlling parameter during the pearlitic phase transformation. Movement of carbon atoms is described by the second Fick law:

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

where: c – local carbon concentration, D – coefficient of carbon diffusion, T – temperature, t – time.

Numerical solution assumes that the initial structure is pure austenite with carbon content of 0.71%. The first plate of cementite is created when the carbon concentration increases locally to 6.67%. This plate grows until the content of carbon in a distance greater than 3.5 times the thickness of the plate falls below c_b (0.4%, 0.1%, 0.05%C), then two new cementite plates are nucleated. Given values of c_b were assumed in this paper as the primary approach. In the future these values will be determined by an inverse analysis.

Both during the nucleation and the growth of plates the condition, resulting from the conservation of mass, must be complied. The initial and boundary conditions at the interface are:

$$c(x,y,0) = c_0$$

$$c(\xi,t) = 0.02$$

$$\frac{\partial c}{\partial \mathbf{n}}(x,y,t) = 0,\ (x,y) \in \Gamma_1,\ \Gamma_2 \text{ – edges of the solution domain} \tag{2}$$

where: c_0 – carbon content in austenite, ξ - edge of cementite, $\mathbf{n}$ – unit vector normal to the surface.

In the presented model the diffusion coefficient was introduced as a function of carbon concentration and temperature. The relationship derived by Agren (1986) on the basis of measured values and presented in the work of Wells et al. (1950) was used. This relationship gives good results for the entire range of temperature Ar_3-Ar_1, which was reported in the paper by Vasilyev et al. (2012). The influence of alloying elements on the carbon diffusion was not included in the model:

$$D = 4.53\times10^{-7}\left[1 + y_c(1-y_c)\frac{8339.9}{T}\right] \exp\left[-\left(\frac{1}{T} - 2.221\times10^{-4}\right)(17767 - 26436\, y_c)\right] \tag{3}$$

where: $y_c = x_c/(1-x_c)$, x_c is the molar fraction of carbon.

The explicit finite difference method was used to solve equation of diffusion (1). The finite difference scheme for the equation of the diffusion in1D and 2D system is given by:

$$c_{j,k+1} = \left(1 - 2\frac{D\Delta t}{\Delta x^2}\right)c_{j,k} + \frac{D\Delta t}{\Delta x^2}\left(c_{j-1,k} + c_{j+1,k}\right) \tag{4}$$

$$c_{i,j,k+1} = \left(c_{i,j,k}\right)\left(1 - 2\frac{D\Delta t}{\Delta x^2} - 2\frac{D\Delta t}{\Delta y^2}\right)$$
$$\left(c_{i+1,j,k} + c_{i-1,j,k}\right)\frac{D\Delta t}{\Delta x^2} + \qquad (5)$$
$$\left(c_{i,j+1,k} + c_{i,j-1,k}\right)\frac{D\Delta t}{\Delta y^2}$$

where: $k = 1,2,\ldots, n,n+1$, Δt – time step, Δx – linear step.

3. RESULTS

Numerical simulations of austenite to pearlite phase transformation were performed for rail steel 900A with a composition given in section 2. Carbon distribution in the front of cementite plate, the thickness of which varies from 0.02 µm to 0.1 µm, is presented in figure 4. Interlamellar spacing is seven times greater than thickness of cementite plate. At the beginning of the transformation, when the undercooling is small, fast carbon diffusion from austenite to cementite occurs and the steepest gradient of the concentration is observed for the thinnest plate.

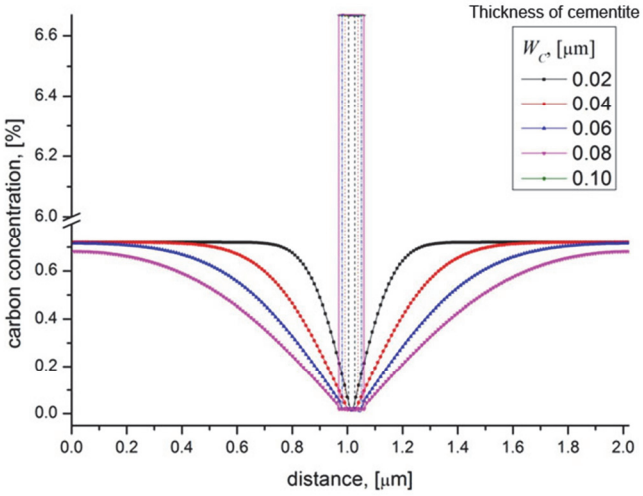

Fig. 4. Profile of carbon concentration during the growth of cementite plate.

The results of the numerical simulation of the cementite plates growth during the whole transformation are presented in figures 5 and 6. Two new plates appeared symmetrically when the content of carbon at a distance greater than 3.5 times the thickness of the plate falls below 0.1%. The increase of the cooling rate causes the decrease of interlamellar spacing. The greatest distance equal to 0.7 µm was obtained at the cooling rate of 0.1°C/s. During cooling at a rate of 0.5 and 0.7°C/s the interlamellar spacing in the structure was between 0.56 and 0.14 µm.

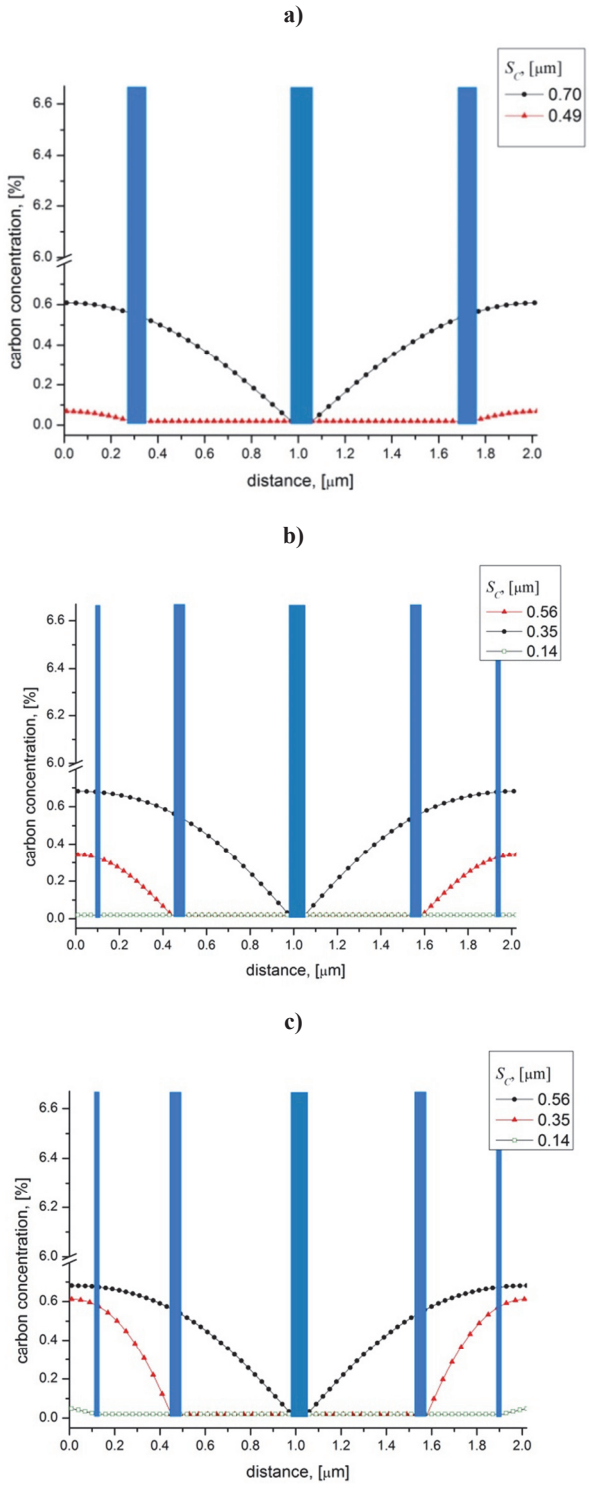

Fig. 5. Growth of cementite plates during cooling at the rate of 0.1°C/s (a), 0.5°C/s (b) and 0.7°C/s (c).

Diffusion occurs slowly at larger undercooling (lower temperature). Therefore, significant decrease in the concentration of carbon occurs only around the cementite plates which favors thickening of plates. In the rest of austenite, carbon concentration varies slightly thus preventing formation of new

ferrite and cementite plates. Faster nucleation of cementite plates can be induced by controlling value of c_b, as shown in figure 6.

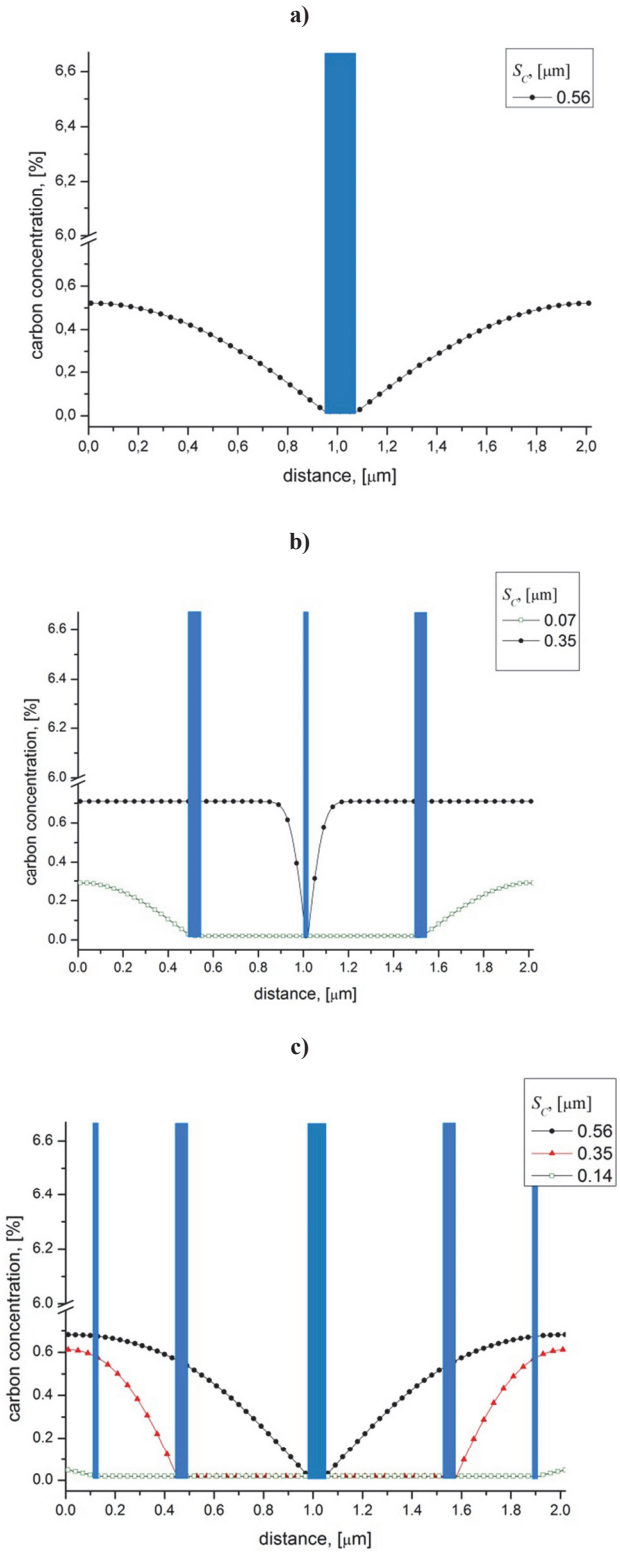

Fig. 6. Carbon distribution and distance between cementite plates for different carbon concentration condition c_b: a) 0.4, b) 0.1, c) 0.05%C.

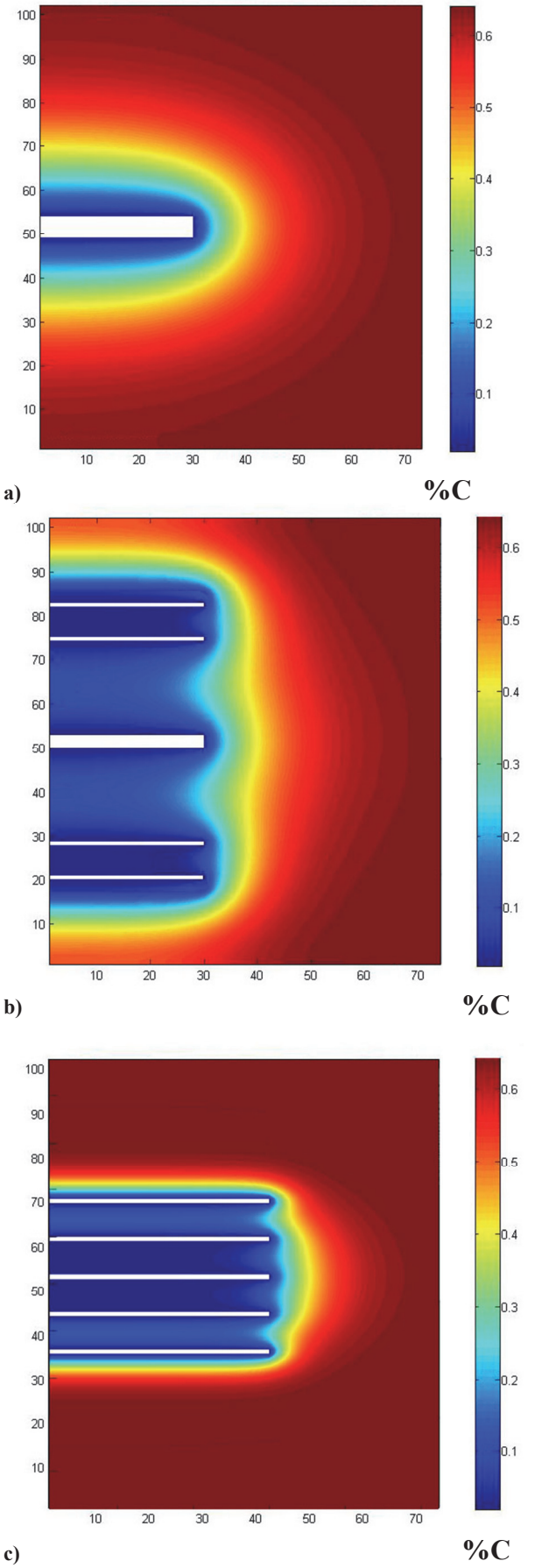

Fig. 7. Growth of pearlite colonies during cooling at the rate of 0.1°C/s (a), 0.5°C/s (b) and 0.7°C/s (c).

Simulations in 2D domain were performed for three cooling rates: 0.1, 0.5, 0.7°C/s and for one condition of c_b = 0.1%. Symmetry was assumed during occurrence of nucleation and growth of the plates. Sidewise growth of pearlite was analyzed, while front growth was not considered. Growth of pearlite colonies during cooling at various cooling rates is shown in figure 7. Using lower cooling rate we get thicker plates of cementite and greater interlamellar spacing. The least distance equal to 0.7 μm was obtained at the cooling rate of 0.7°C/s. During cooling at a rate of 0.1° C/s only thickening of the plate takes place, whereas the nucleation of new cementite is not possible due to the slow diffusion.

The result analysis confirmed good qualitative behavior of the model. The presented results show that the model is capable to predict variations of carbon concentrations in steel during cooling, as well as distribution of interlamellar spacing. Further research will focus on the two aspects. The first is the identification of parameters which were assumed in calculations. This should give good quantitative accuracy of the model. The second, is the future research on the application of this model in formulating the predictions of the exploitation properties of pearlitic steels.

These properties, i.e. strength and hardness, are strongly dependent on the interlamellar distance S_c. This effect has been explained on the basis of a dislocation pile-up mode, whereby dislocations occurring in piled-up groups give rise to internal stress-fields. In general, the relationship between the interlamellar distance and strength is well described by the Hall–Petch equation, but the solution proposed by (Brown & Ham, 1971) is also used to determine mechanical properties of pearlitic steels.

4. SUMMARY

The development of a numerical model of austenite to pearlite phase transformation is a complex task. Both saturation of carbon from the austenite and pushing carbon in front of the growing ferrite plate occur during the formation of pearlite colonies. This paper presents the preliminary concept of the numerical model based on the solution of the carbon diffusion equation. The model created opportunities to describe the mechanism of growth of cementite and ferrite plates during cooling of rail steels. Created model has a capability to determine changes of the carbon distribution and, in consequence, to predict the size of interlamellar spacing. Performed simulations confirmed qualitatively good accuracy of the model. Simulations showed reduced interlamellar spacing with increasing cooling rate. This model will be used in the future to predict the exploitation properties of pearlitic steels.

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MOŻLIWOŚCI ZASTOSOWANIA ROZWIĄZANIA RÓWNANIA DYFUZJI DO MODELOWANIA PRZEMIANY FAZOWEJ PODCZAS CHŁODZENIA STALI PERLITYCZNEJ

Streszczenie

Własności wytrzymałościowe szyn kształtowane są na drodze kontrolowanego procesu obróbki cieplnej główki szyny prowadzonej po procesie walcowania. Aby uzyskać wymaganą mikrostrukturę i własności stali należy zastosować złożone cykle cieplne. Zaprojektowanie tych cykli powinno być wspierane numerycznym modelowaniem, co wymaga zastosowania zaawansowanych modeli przemian fazowych. Modele takie powinny przewidywać nie tylko średnie parametry mikrostruktury, ale także morfologię perlitu i rozkład stężenia węgla. W pracy przedstawiono model przemiany perlitycznej zachodzącej podczas kontrolowanego chłodzenia. Model ten oparto na rozwiązaniu równania dyfuzji z ruchomą granicą międzyfazową. Warunki brzegowe modelu wyznaczono na podstawie lokalnej równowagi termodynamicznej. Model pozwolił na określenie wielkości płytek cementytu i ferrytu, oraz rozkładu stężenia węgla w austenicie dla różnych cykli chłodzenia. Otrzymane wyniki mogą posłużyć do określenia twardości i wytrzymałości stali.

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