Application of the Mixed-Mode Model for Numerical Simulation of Pearlitic Transformation

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The multiscale model of pearlitic transformation, including the finite element solution of the second Fick's equation with moving boundary in the microscale and Fourier equation in the macroscale, is presented in this paper. According to the mixed-mode approach, both the volume diffusion and the interface mobility were considered. Model describes sidewise and frontal growth of cementite and ferrite plates in a single grain of the austenite. Assessment of the possibility of the developed model application to determine the key parameters in terms of strength properties of pearlitic steel, i.e., pearlite grain size and colony size as well as interlamellar spacing for various cooling conditions, was the main aim of this work. The model was validated and verified on the basis of experimental tests performed for two eutectoid steels. In practice, developed model can support design process for a technology of high-strength rods and long products manufacturing. Rails were selected as a case study in this work, and therefore, numerical simulations of accelerated cooling of the rail head were performed and the relationship between the parameters of heat treatment, parameters of the structure and properties of the finished product was determined on the basis of obtained results.

Keywords diffusion equation, mixed-mode approach, multiscale numerical model, pearlitic phase transformation, physical simulations, rails

1. Introduction

Fully pearlitic steels are of great importance in a number of extremely demanding structural applications, in a large part due to their combination of strength and toughness (Ref 1). These exceptional properties are controlled by the microstructures developed in pearlitic steels, especially interlamellar spacing, pearlite colony size and prior austenite grain size. Among many applications of pearlitic steel we can distinguish wires (Ref 2) and rails (Ref 3) investigated in the present paper. The latter application is investigated in the present paper.

Prediction of the relation between pearlite microstructural parameters and the product in-use properties is crucial for the design of the manufacturing technology. Numerical models of pearlitic transformation can support process of designing of rails manufacturing technology, which leads to costs reduction and improves the quality of finished products. The existing description of pearlitic transformation and pearlite microstructure, based on kinetics of transformation and volume fractions of phases only, is imprecise. A detailed description of the microstructure features of pearlitic steels is required to investigate the correlation between the complex microstructure and the exploitation properties. Indeed, advanced full field models based on the explicit representation of the microstructure have been recently developed and are available in the scientific literature (Ref 4, 5).

However, due to the prospective application to the industrial conditions, the models should be characterized primarily by short computation time and reasonably high accuracy, which depends on the correctness of the description of physical phenomena.

Another important feature expected from the models is universality of the solution and flexibility, which create opportunity of changing the input parameters in the wide range. Thus, a hypothesis was made that description of the heterogeneous microstructure of pearlitic steels with the approach based on the mixed-mode will allow building the model with capability to predict various parameters of the microstructure and evaluate their effect on the final product properties.

Author's earlier works (Ref 6, 7) showed that the model based on the solution of the Fick's equation is characterized by the large predictive capabilities. Improvement in this model and its adaptation to pearlitic steel were the main objectives of the present work. The particular objectives were formulated as follows:

- Accounting for the influence of the interface mobility on the kinetics of phase transformation, which should significantly improve model's efficiency.
- Assessment of the possibility of the developed model application to determine transformation kinetics and morphological parameters of the pearlitic structure
- Validation and verification of the model by comparing the results with the experimental data obtained for A900 and C80U steels.
- Performing simulations of manufacturing of pearlitic steel rails and design of the optimal technological parameters.

2. Model

2.1 Physical Background

Phase transformation of austenite into pearlite begins when temperature drops below A_1 (Fig. 1a). The driving force of this

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Fig. 1 A part of the phase equilibrium diagram, c_0 —carbon concentration in steel, $c_{\gamma\alpha}$ —carbon content at the austenite-ferrite boundary, c_γ —carbon content at the austenite-cementite boundary

process is the difference between the free energy of austenite and the free energy of the mixture of ferrite and cementite. The carbon concentration at the ferrite/austenite boundary $c_{\gamma\alpha}$ and at the austenite/cementite boundary $c_{\gamma\text{cem}}$ for steel containing x_γ is determined using extrapolation of the A_3 and A_{cm} curve, respectively. In the eutectoid steels first phase which nucleates is cementite and ferrite is the second.

Typical structure of pearlitic steel is shown in Fig. 2(a). One grain of pearlite usually consists of few pearlite colonies. Within each colony, plates of ferrite and cementite have the same crystallographic orientation. Distance between two plates of ferrite, referred to as interlamellar spacing, is about seven times greater than width of cementite plates. Pearlite typically forms heterogeneously on the austenite grain boundaries and grain corners (Fig. 2b). As the system always strives to minimize energy, and the surface tensions associated with nucleation depend on the crystallographic orientation, we can expect dependence between the orientation of the embryo and the orientation of the grain of austenite in which it grows. Meanwhile, microscopic observation shows that interface of the pearlite colony created with austenite is an incoherent high-energy interface. However, we can distinguish two different crystallographic relationships between ferrite and cementite within pearlite colony. Independent of carbon concentration and degree of undercooling, nucleation on clear austenite boundary exhibits the Pitsch/Petch relationship. Nucleation on the proeutectoid ferrite or cementite results in the formation of Bagaryatski relationship (Ref 8). Microscopic observation shows that single plates can cross austenite grain without a perceptible change in the direction. The rate of pearlite nucleation depends on the rate of cooling, the structure of austenite and its chemical homogeneity. The finer grain of austenite and the greater variation in chemical composition, the faster is nucleation. Consequently, smaller colonies are created. The increase in carbon content in austenite causes the increase in the driving force of nucleation of cementite and the decrease in the driving force of nucleation of ferrite. When the concentration of carbon decreases, the effect is reversed (Ref 9).

Fig. 2 Schematic representation of structure of pearlitic steels (a) and pearlite growth on the prior austenite boundaries and at grain corners (b)

Further growth of the pearlite phase occurs due to the movement of the interface boundary connected with the transport of carbon and alloying elements across the interface and their long-range diffusion in the austenite. This process simultaneously leads to the reconstruction of FCC austenite crystal lattice into a BCC ferrite lattice or orthorhombic lattice of cementite. The factors control the rate at which the interface moves are varied. According to Hillert's (Ref 10) theory, when the interface boundary has a high mobility and can move as fast as substitutional solutes can be redistributed, the growth is controlled by volume diffusion. This assumption was adopted in the numerical models presented in the papers (Ref 4, 11). However, if the boundary is characterized by low mobility (even at high driving forces) and long-range diffusion processes are fast, the change is controlled by the interface diffusion.

The results of experimental tests and extended theoretical analysis indicate a significant influence of interface diffusion on the kinetics of the phase transformation (Ref 12). The values of activation energy determined for the interface diffusion are more realistic, less than that for volume diffusion in austenite and greater than for volume diffusion in ferrite. This effect is particularly well seen at high temperatures. Consequently, a mixed-mode model, which takes into account both volume diffusion as well as interface diffusion, was proposed by Sietsma and van der Zwaag (Ref 13) and was further developed by Pandit and Bhadeshia (Ref 14). In the presented work, this approach was used for the creation of the numerical model of pearlitic transformation.

The classic physical models of pearlitic transformation were improved as the research methods of the microstructure progressed. Detected anomalies: such as the creation of needles, branching of plates, were attributed to elastic stress (Ref 5, 15, 16), resulting from the mismatch of the lattice near the front of the transformation. The formation of spheroidal particles (Ref 17, 18), including autocatalytic mechanisms, for metastable conditions was considered. A detailed description of the process physics not directly reflected in possibility of predicting structure parameters, including: the interlamellar spacing and the size of the pearlite colony for varying temperature conditions. In addition, the computation time prevents the use of models for designing real technological processes.

Searching for a balance between model's predictive capabilities and computing time was the main motivation for the work. Developed mixed-mode model was based on the simplified physical model of pearlite forming, assuming that such approach accelerates prediction of the final structure and mechanical properties of steel. In contrast to existing solutions, model allows to determine the interlamellar spacing for the conditions of cyclic cooling.

2.2 Existing Numerical Solutions

The models were analyzed for the possibility of describing the kinetics of pearlitic transformation and predicting the morphological parameters of the structure, which determine the

strength properties. These parameters are the interlamellar spacing and the size of the pearlite colonies.

The kinetics of the pearlitic phase transformation is correctly described by models based on the solution of JMAK equation (Ref 19-21), see, for example (Ref 22). The need to apply the Scheil additivity rule (Ref 23) to account for temperature change is the main disadvantage of this model. The alternative approach is the Leblond model (Ref 24) and its upgrades (Ref 25), in which kinetics of phase transformation is described by a differential equation with respect to time. Both models provide information about volume fraction of phases in near real time, but they require experimental identification of parameters.

On the basis of theories of growth controlled by volume diffusion and interface diffusion, two relationships to determine the size of the interlamellar spacing as a function of undercooling were created. Zener (Ref 26) assumed that the system stabilized at a spacing for which the growth rate is a maximum, and this hypothesis leads to:

$$S_c = \frac{4T_e\sigma_{\gamma\text{cem}}}{\rho Q(T_e - T)} \quad (\text{Eq 1})$$

where T_e —the eutectoid temperature, $\sigma_{\gamma\text{cem}}$ —interfacial energy per unit area of the ferrite-cementite boundary, ρ —density, Q —the heat of the transformation.

On the other hand, Puls and Kirkaldy (Ref 27) formulated the following relationship for interface diffusion-controlled growth and the maximum rate of entropy criterion:

Fig. 3 Schematic representation of the sideways growth of cementite (a), ferrite (b) and frontal growth of pearlite colony

Table 1 Parameters of the numerical model

A900 steel	C80U steel
$c_{\gamma\alpha} = 4.8513 - 0.005776T$	$c_{\gamma\alpha} = 5.612 - 0.00621T$
$c_{\gamma\text{cem}} = -1.46583 + 0.002887T$	$c_{\gamma\beta} = -1.532 + 0.00234T$
$M_B = 863.5 - 425[C] - 42.5[\text{Mn}] - 31.5[\text{Ni}]$	$M_S = 307 - 31.42c_\gamma$
$M_S = 272 - 82.9c_\gamma$	
$c_{\gamma\alpha}$ carbon content at the γ/α interface, $c_{\gamma\beta}$ carbon content at the $\gamma/\text{cementite}$ interface, c_γ carbon content in the austenite and T temperature in $^\circ\text{C}$	

Table 2 Chemical composition of the investigated steels, wt. %

Steel	C	Mn	Si	P	S	Cr	Ni	Mo	Al	Co	Cu
C80U	0.81	0.281	0.207	0.013	0.018	0.084	0.019	0.008	0.002	0.002	0.034
A900	0.7	1.1	0.34	0.016	0.018	0.36	...	0.05	0.003	...	...

(a)

(b)

Fig. 4 Microstructure of pearlite colonies observed in samples of C80U steel austenitized at (a) 820 °C, (b) 800 °C and cooled at 2 °C/min (etched in reagent of 3% nital)

$$S_c = \frac{6T_e \sigma_{zcm}}{\rho Q(T_e - T)} \quad (\text{Eq 2})$$

Experimental tests (Ref 28) confirm the better predictive capabilities of the Zener model. However, it should be noted that the above relationships can be used for isothermal conditions only.

Among the models which predict kinetics of pearlitic transformation and morphology of the final structure, model based on the Phase Field Method (Ref 5) should be distinguished. This model describes growth of pearlite colony and takes into account divergence of the plates. The interlamellar spacing is a function of temperature and time of the isothermal transformation. Meanwhile, the ability to determine the size of this parameter for variable temperature conditions is crucial due to use of the model in practice.

Taking into account continuous cooling conditions or cyclic temperature changes requires the use of more advanced models. The empirical relationship presented in (Ref 22)

allows determining the constant interlamellar spacing within each colony for weighted average temperature of the transformation:

$$S_0 = \frac{1}{a - bT_p} \quad (\text{Eq 3})$$

$$a = 129.3 - 54.4[\text{Mn}] - 4.38[\text{Cr}] - 17.5[\text{Si}]$$

$$b = 0.178 - 0.072[\text{Mn}] - 0.012[\text{Cr}] - 0.0274[\text{Si}]$$

where T_p —weighted average of temperature of pearlitic transformation in °C, [Mn], [Cr], [Si], [C]—manganese, chromium, silicon and carbon content in wt.%.

Meanwhile, due to its strong influence on the strength properties, it is necessary to determine distribution of the interlamellar spacing in the whole volume. Such a possibility is provided by models based on the solution of the diffusion equation. In addition, that model allows determining the size of the pearlite colony and distribution of carbon in the austenite.

2.3 Numerical Formulation

Model describes sidewise and frontal growth of few pearlite colonies (Fig. 3) in a single grain of austenite, in which size was determined experimentally. The concentration at the interface between austenite/cementite and austenite/ferrite corresponded to the thermodynamic equilibrium conditions for a given temperature. Sites of nucleation on the edges of the austenite grain were selected randomly. Nucleation of first and next plates of cementite resulted from the mass balance, which took into account the carbon content in cementite at 6.67 wt.% (Fig. 3a). Cementite grows until the content of carbon in the distances dx and dy (size of the step) drops below c_b (0.05%C); then, the first plates of ferrite are symmetrically created (Fig. 3b). Value of parameter c_b was determined using inverse analysis for the experimental data and sensitivity analysis. Growth of ferrite plates causes pushing carbon into austenite and increase in its concentration, which leads to creation of new plates of cementite in a distance greater than 7 times the thickness of previously created plates of cementite. The whole cycle was repeated until the disappearance of the austenitic phase. The plates stop growing after the impingement with other plates.

Growth of ferrite and cementite plates is controlled by both the volume diffusion and the interface mobility. This approach is commonly referred to as a mixed-mode model, and its use in numerical modeling of pearlitic transformation can be found in (Ref 14, 29).

Volume diffusion of carbon in the austenite is described by the second Fick's law:

$$\frac{\partial c}{\partial t} = \nabla \cdot D \nabla c \quad (\text{Eq 4})$$

where D —diffusion coefficient, c —carbon concentration, t —time.

In Eq 4, much slower redistribution of substitutional alloying elements was omitted. The initial and boundary conditions at the interfacial boundary were determined for local thermodynamic equilibrium at γ/α and $\gamma/\text{cementite}$ interfaces using ThermoCalc software. In consequence, the initial and boundary conditions were given by the following equations:

Fig. 5 The stages of pearlitic colonies formation in C80U steel during cooling at a rate of 20 °C/min from an austenitization temperature of 800 °C to room temperature (etched in reagent of 3% nital)

$$\begin{aligned} c(x, y, 0) &= c_\gamma \quad x, y \in \Omega \\ c(x, y, t) &= c_{\gamma\alpha} \quad x, y \in \Gamma_1 \\ c(x, y, t) &= c_{\gamma\text{cem}} \quad x, y \in \Gamma_2 \\ \frac{\partial c}{\partial n}(x, y, t) &= 0 \quad x, y \in \Gamma_3 \end{aligned} \quad (\text{Eq 5})$$

where c_γ —carbon concentration in austenite, $c_{\gamma\alpha}$ —equilibrium carbon concentration at γ/α boundary, $c_{\gamma\text{cem}}$ —equilibrium carbon concentration at $\gamma/\text{cementite}$ boundary, $\mathbf{n}$ —unit vector normal to the surface, Ω —solution domain, Γ_1 — $\gamma/\text{cementite}$ boundary, Γ_2 — γ/α boundary, Γ_3 —edge of the solution domain.

The austenite grain shape constituting the domain of the solution Ω was compliant with the ASTM specification. Location of the interfaces was calculated from the condition of mass conservation according to which at the time t the same amount of carbon which diffuses from ferrite must appear in the austenite, whereas cementite absorbs carbon from austenite, which leads to a local decrease in carbon concentration. Therefore, the interface velocity, corresponding to the growth rate of pearlite, depends only on the rate of the carbon redistribution ahead of the transformation front.

The volume diffusion coefficient of carbon in austenite, which is the function of temperature and average carbon concentration, was calculated using Agren (Ref 30) relationship in the form:

$$\begin{aligned} D &= 4.53 \times 10^{-7} \left[1 + y_c(1 - y_c) \frac{8339.9}{T} \right] \\ &\exp \left\{ - \left[\frac{1}{T} - 2.221 \times 10^{-4} (17767 - 26436 y_c) \right] \right\} \end{aligned} \quad (\text{Eq 6})$$

where $y_c = x_c(1 - x_c)$, x_c —mole fraction in the steel, T —temperature in K.

The Fick's Eq 4 was solved in 2D using FE method. Application of the variational principle gives:

$$\mathbf{H}\mathbf{c} + \mathbf{C} \frac{\partial}{\partial t} \mathbf{c} = \mathbf{p} \quad (\text{Eq 7})$$

where $\mathbf{c}$ —vector of nodal values of concentration, $\mathbf{H}$ —diffusion matrix, $\mathbf{C}$ —geometrical matrix, $\mathbf{p}$ —boundary conditions vector. Matrices $\mathbf{H}$, $\mathbf{C}$ and vector $\mathbf{p}$ are calculated as:

$$H_{ij} = \int_{\Omega_i} (\nabla n_i)^T D (\nabla n_j) d\Omega_j \quad C_{ij} = \int_{\Omega_j} n_i^T n_j d\Omega_j \quad p_i = 0 \quad (\text{Eq 8})$$

where n_i —shape functions in the FE method.

Assumption of the quasi-stationary state during time step Δt and application of the Galerkin time integration scheme yields the final set of equations:

$$\hat{\mathbf{H}}\mathbf{c} = \hat{\mathbf{p}} \quad (\text{Eq 9})$$

where

$$\hat{\mathbf{H}} = \left[2\mathbf{H} + \frac{3}{\Delta t} \mathbf{C} \right] \quad \hat{\mathbf{p}} = \left[-\mathbf{H} + \frac{3}{\Delta t} \mathbf{C} \right] \mathbf{c}_i \quad (\text{Eq 10})$$

Solution of Eq 9 allows to calculate distribution of the carbon concentration $\mathbf{c}$ in the austenite grain at the end of the time step Δt when this distribution at the beginning of the time step $\mathbf{c}_i$ is known.

At each time step, the carbon concentration profile in the austenite was calculated by the solution of the second Fick's law (4) and on the basis of this solution the interface concentration c_γ^{int} was determined. The interface velocity was proportional to the available chemical driving force with the interface mobility (Ref 31):

$$v = M\Delta G \quad (\text{Eq 11})$$

(a)

(b)

(c)

(d)

Fig. 6 Perlitic-martensitic structure of C80U steel. Microstructure of samples austenitized at 800 °C and cooled at: (a) 1 °C/s, (b) 2 °C/s, (c) 5 °C/s, (d) 10 °C/s (etched in reagent of 3% nital)

$$M = M_0 \exp\left(\frac{Q}{RT}\right) = \frac{d^4 v_D}{kT} M^* \exp\left(\frac{Q}{RT}\right) \quad (\text{Eq 12})$$

where M —interface mobility, ΔG —driving force for the phase transformation calculated using ThermoCalc, Q —the activation energy, R —the gas constant, d —the jump distance across the interface, v_D —Debye frequency, k —Boltzmann constant, M^* —fitting parameter equal 0.8.

The driving force ΔG was proportional to the deviation from the equilibrium concentration:

$$\Delta G = \chi (c_{\gamma}^{\text{int}} - c_{\gamma\alpha}) \quad (\text{Eq 13})$$

where c_{γ}^{int} —carbon content at γ/α and $\gamma/\text{cementite}$ interface.

Process of diffusion evolves until equilibrium is reached in terms of carbon composition and phase fraction. The mixed-mode character is quantified by the parameter S , according to which if $S = 0$ phase transformation is diffusion controlled, whereas $S = 1$ means interface-controlled solution (Ref 32).

$$S = \frac{c_{\gamma}^{\text{int}} - c_{\gamma\alpha}}{c_{\gamma}^{\infty} - c_{\gamma\alpha}} \quad (\text{Eq 14})$$

Fig. 7 Perlitic-martensitic structure of C80U steel. Microstructure of samples austenitized at 820 °C and cooled at 2 °C/s (etched in reagent of 3% nital)

Table 3 Parameters of the heat treatment of C80U steel

Temperature of austenitization, °C	Rate of cooling, °C/s	Tempering temperature, °C	Time of cooling, s	Volume fraction of austenite, %	Volume fraction of pearlite, %	Standard deviation
800	0.16	730	420	91.87	8.13	0.50
		720	480	83.35	16.65	5.12
	0.083	740	720	97.57	2.43	0.71
		730	840	88.60	11.40	3.55
		720	960	69.7	30.3	5.85
		695	1260	62.03	37.97	2.68
	0.033	740	1800	96.15	3.85	5.92
		730	2100	83.65	16.35	4.63
		720	2400	76.63	23.37	4.02
		710	2700	42.96	57.04	2.34
	0.016	695	3120	8.84	91.16	2.26
		740	3600	85.85	14.15	2.03
		730	4200	59.49	40.51	5.99
		720	4800	34.88	65.2	7.77
820	0.033	740	2400	96.79	3.21	0.94
		720	3000	74.39	25.61	5.18
		705	3450	3.96	95.94	1.87

All parameter values used in the developed model are listed in Table 1. Equilibrium carbon concentrations for investigated steels were determined using ThermoCalc software, while temperatures of bainite start B_s and martensite start M_s were calculated on the basis of dilatometric tests.

3. Experiments

Experiments were performed to supply data for verification and validation of phase transformation models (C80U steel) and assessment of their applicability to simulate processes of rails manufacturing (A900 steel). Chemical composition of the investigated steels is given in Table 2.

3.1 Investigation of the Phase Transformation Kinetics

The main goal of this part of experimental tests was to provide results, which will enable to evaluate correctness of the model in terms of prediction of the volume fraction of pearlite. Experiment concerned cold-worked tool steel C80U, in which pearlitic structure guarantees high strength and high utility properties, including hardness, abrasion resistance and durability. Tests were performed for various cooling rates and two temperatures of austenitization: 800 and 820 °C. The progress of the transformation was stopped by quenching in water—phase of austenite was represented by martensite. The metallographic analysis was performed to determine transformation kinetics. Microstructure of steel is shown in Fig. 4. The stages of pearlitic colonies formation during cooling at a rate of 20 °C/min are presented in Fig. 5.

In the first set of experimental tests, the cementite mesh method was used to determine average size of prior austenite grains which amounted to 34.8 μm for temperature of austenitization equal 800 °C and 39.2 μm for 820 °C. In the second set, the tests samples were heated to the austenitization temperature of 800 °C and then were cooled at various rates in the range 2÷10 °C/s to the room temperature. The samples were prepared using a standard metallographic technique. Selected microstructures showing perlite colonies on the background of martensite are presented in Fig. 6 and 7. It is

seen that the volume fraction of pearlite decreases with the increase in cooling rate (Table 3). Volume fractions of phases were determined using digital image analysis.

Further investigations allowed determining the influence of austenitization temperature on the phase fraction in the final structure. For this purpose, the samples were heated to a temperature of 820 °C and cooled at 2 °C/s. Analysis of the microstructures showed a smaller volume fraction of perlite than for cooling at the same rate from 800 °C. Selected microstructures of pearlite colonies are presented in Fig. 4. The average interlamellar spacing determined on the basis of the tests was about 0.9 μm.

3.2 Investigation of the Interlamellar Spacing of Pearlite

The verification of correctness of developed numerical model in determining the interlamellar spacing of the perlite was carried out based on the results of the experimental tests which were performed at the Institute for Ferrous Metallurgy in Gliwice, Poland. The research concerned the process of accelerated cooling of high-strength rails in the air and polymer mixture. The main goal of the heat treatment of rails was to obtain a fine structure of pearlite in the whole cross section of the head, which guarantees the best mechanical and exploitation properties. Rapid cooling after rolling of rails promotes fragmentation of the structure, but it can lead to an occurrence of unfavorable components of degenerated pearlite and bainite. The precise selection of parameters of the heat treatment is therefore a key task.

Experiment, which details were presented in (Ref 33), was performed for the steel 900A with the chemical composition given in Table 2. The research involved the physical simulations of the process of continuous cooling of the rail head at the rate of 0.25, 0.5 and 5 °C/s. The measured interlamellar spacing was, respectively, 0.143, 0.129 and 0.094 μm. Selected microstructures are shown in Fig. 8.

4. Results of Numerical Simulation

The scope of numerical simulations was convergent with the range of experimental tests presented above.

Fig. 8 Microstructure of A900 rails after cooling at the rate of: (a) 0.25 °C/s, (b) 0.5, (c) 5 °C/s

Fig. 9 Stages of pearlite creation: (a) growth of cementite and (b) growth of ferrite and cementite

4.1 Kinetics of the Phase Transformation

Numerical simulations of the kinetics of the pearlitic transformation were performed for steel C80U with a composition given in Table 2. Subsequent stages of pearlitic transformation are shown in Fig. 9. One can observe absorption of carbon from the austenite by growing plate of cementite (Fig. 9a). Decrease in carbon content to a level of $c_b < 0.2\%C$ leads to nucleation and growth of ferrite. During sideways and frontal growth of ferrite, carbon is pushed into the austenite (Fig. 9b).

Growth of pearlite colonies during cooling at various rates from the temperature of austenitization equal 800 and 820 °C is shown, respectively, in Fig. 10 and 11. The volume fraction of pearlite corresponded to 20, 50 and 80% of the progress of phase transformation. The nucleation sites were chosen randomly. The nucleation rate increases with increasing overcooling below A_{c1} . At lowest cooling rate of 1 °C/s, the thicker plates of cementite and greater interlamellar spacing equal to 0.87 μm were observed. The smallest interlamellar spacing equal 0.52 μm was obtained for cooling rate of 10 °C/s. According to the assumed boundary conditions, absorption of carbon from the austenite by growing plate of cementite was noticeable. Meanwhile, during sideways and frontal growth of

Fig. 10 Results of simulations of pearlite growth during cooling at the rate of (a) 1 °C/s, (b) 2 °C/s, (c) 5 °C/s and (d) 10 °C/s. Temperature of austenitization 800 °C. The volume fraction of pearlite corresponding to 20, 50, 80% of phase transformation. Steel C80U

ferrite carbon was pushed to austenite. The steepest gradient of the carbon concentration was observed for the thinnest plate.

Kinetics of pearlitic transformation, which was represented by the changes in pearlite volume fraction with time, is presented in Fig. 12. Dashed lines created by extrapolation of experimental results, marked by filled symbols, have the S-type shape. Results of simulations presented by open symbols

remain within the margin of error, what confirms the correctness of the model.

On the basis of results of numerical simulation performed for cooling at 5 °C/s and presented in Fig. 12, graphical representation of microstructure with 50% pearlite content was created (Fig. 13), which enables discussions on the kinetics and mechanism of phase transformation.

Fig. 11 Results of simulations of pearlite growth during cooling at the rate of 2 °C/s. Temperature of austenitization 820 °C. Volume fraction of pearlite corresponding to 20, 50, 80% of phase transformation. Steel C80U

Fig. 12 Kinetics of phase transformation for constant cooling rates in the range of 0.016-0.16 °C/s, temperature of austenitization: (a) 800 °C, (b) 820 °C. The volume fraction of pearlite as function of time (filled symbols—results of experimental tests, open symbols—results of numerical simulations)

4.2 Interlamellar Spacing of Pearlite

The main task of the developed model was a correct prediction of the size of the interlamellar spacing. Simulations of pearlite growth during continuous cooling and cyclic temperature changes were performed.

In the first case, rails made of A900 steel were cooled with the rates of 0.25, 0.5 and 5 °C/s. Stages of pearlite creation are

Fig. 13 Numerical visualization of C80U steel microstructure after cooling at the rate of 5 °C/s

shown in Fig. 14. Nuclei of cementite were formed randomly at the edges of austenite, and their number increased with the degree of undercooling. The ferrite nucleated symmetrically when the carbon concentration fell below 0.1. The growth of pearlite led to the saturation of carbon to the level of $0.02 \pm 0.22\%$. The smallest interlamellar spacing equal to 0.11 μm was obtained for the highest rates of cooling 5 °C/s, whereas the pearlite with the largest thickness of plates 0.154 μm was created for the cooling equal 0.25 °C/s. The results of simulations compared with the results of experimental tests confirm the correctness of the solution (Fig. 15).

Further numerical simulation concerned accelerated cooling of the rail head by a cyclic immersion in the polymer solution. The developed model included the finite element (FE) solution for heat transport in the macroscale and the solution of mass transport in the microscale. Single-point models were solved at each Gauss point of the FE mesh, while mixed-mode models were used in three points located in the main axis of the cross section of the rail head. The model assumes the heat transfer coefficient equal to 1700 W/m²K for temperatures exceeding 700 °C and reaching 2400 W/m²K at 300 °C. At lower temperatures, coefficient decreases and reaches 1200 W/m²K at the ambient temperature. Other parameters such as conductivity, density and specific heat were introduced as functions of temperature.

Process of cyclic cooling of the rail head was simulated according to the schedules shown in Table 4. The input to the model was the temperature distribution at the exit from the last rolling stand calculated in (Ref 34).

Fig. 14 Results of simulations of pearlite growth during continuous cooling at the rate of 0.25, 0.5 and 5 °C/s. Steel A900

Fig. 15 Interlamellar spacing in pearlite created during continuous cooling at the rate of 0.25, 0.5 and 5 °C/s. Steel A900

Table 4 Schedule of rail head cooling

Time, s						
I						
Air	10	20	10			25
Solution		15	15	20		
II						
Air	10	15	15			25
Solution		30	10	20		

Results of simulation of cyclic cooling according to schedules I and II for 3 points located at a distance of 2.5,

12.5, 25 mm from the surface of the rail head are presented in Fig. 16. In both cases, at the point 1, which was situated close to the surface of the rail head, cyclic increase and decrease in temperature were observed, while at points 2 and 3 temperature decreases continuously. Cyclic cooling in the polymer solution and heating due to the latent heat leads to the formation of temperature fields characterized by different symmetries than at the exit from the last rolling stand.

After the cycle I, which was characterized by a shorter total time of cooling in the polymer mixture, temperature reaches 540 °C at the surface area and 600-675 °C in the center of the rail head. At the cross section of the rail head, we can observe four symmetrical temperature fields: 520.3-543.6 °C, 543.6-566.9 °C, 566.9-590.2 °C and 590.2-613.5 °C. Cycle II allows to get lower temperatures in the whole volume of the rail head, i.e., 490 °C at the surface area and 535-624 °C in the center of the rail head. Temperature fields range from 477.8 to 504.6 °C close to the surface to 531.5-692.6 °C in the center of the head. Obtained time-temperature profiles were used as entry data in the developed model of pearlitic transformation.

Results of simulations are presented in Fig. 17. The smallest interlamellar spacing equal to 0.21 μm was obtained for time-temperature profile according to cycle II at point 1 located close to the head surface. This distance at point 2 reached average value of 0.28 μm. The largest interlamellar spacing equal to 0.42 μm was obtained for point 3, in which pearlite transformation occurred at the highest temperatures.

5. Conclusions

Numerical model based on the solution of the Fick's equation was presented in this paper. Model describes sidewise and frontal growth of cementite and ferrite plates in a single grain of austenite. Rate of growth of plates was limited by

Fig. 16 Temperature distribution at the rail head (left) and time-temperature profiles (right) in the cooling cycles I (a) and II (b)

Fig. 17 Interlamellar spacing in pearlite created during cyclic cooling in the polymer mixture. Steel A900

volume carbon diffusion in austenite and interface mobility. The state of thermodynamic equilibrium was assumed.

The predictive capabilities of the model in terms of correct determination of kinetic and morphological parameters of the structure shaped in variable temperature conditions were analyzed. The results of numerical simulations in relation to results of experimental data allowed drawing the following conclusions:

- The presented mixed-mode model of pearlitic transformation, despite some simplification, is useful in technological applications, which was confirmed experimentally.
- The model allows the prediction of volume fraction of pearlite, interlamellar spacing and distribution of carbon concentration in the austenite. In consequence, the model has a capability to predict strength and utility properties of pearlitic steels, including hardness, abrasion resistance and durability depending on the manufacturing parameters.
- Developed model correctly predicts the kinetics of pearlitic phase transformation. Discrepancies between calculations and measurements were within error ranges. On the other hand, model is computationally costly. The duration of the simulation of one thermal cycle is about 4 h. For comparison, solution based on the JMAK equation gives a real-time response. In this aspect, the model based on the solution of the Fick's equation is not a competitive tool.
- The FEM calculation in the area with a high-concentration gradient required the use of adaptive mesh refinement.
- Capability of the mixed-mode model to design an optimal rail cooling cycle was confirmed.

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