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OPTIMIZATION OF THE HEAT TREATMENT PROCESS TO OBTAIN THE REQUIRED DISTRIBUTION OF MECHANICAL PROPERTIES IN THE RAIL HEAD OF PEARLITIC RAILS

OPTYMALIZACJA PROCESU OBRÓBKI CIEPLNEJ W CELU UZYSKANIA POŻĄDANEGO ROZKŁADU WŁAŚCIWOŚCI MECHANICZNYCH W GŁÓWCE SZYNY ZE STALI PERLITYCZNYCH

The paper presents metallurgically based approach allowing the design of the parameters of the pearlitic rail head heat treatment to obtain the targeted mechanical properties. The described solutions enable predicting the progress of phase transformations, final microstructure and mechanical properties distribution in the pearlitic rail subject to heat treatment. It also allows the optimization of the cooling conditions to obtain a strictly defined distribution of mechanical properties in the rail head. The program is developed as a result of research activities performed in the HyPremRail R&D project. The core of the program consists of the phase transformations model which is implemented in the numerical code based on the FEM for heat transfer calculations. The model predicts the pearlite nodule and colony size as well as cementite interlamellar spacing. Using these parameters, strength properties distribution in the rail can be predicted, since the phase transformations model is combined with the Fourier heat transfer equation. To perform the numerical simulations, the boundary conditions for heat treatment should be defined. On the contrary, using inverse analysis, the program can provide the cooling conditions allowing obtaining defined mechanical properties distribution in rail head.

Keywords: pearlitic microstructure, phase transformations, mechanical properties, heat treatment of rails, numerical modelling

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Artykuł przedstawia matematyczny model oparty na wiedzy metaloznawczej, umożliwiający zaprojektowanie parametrów obróbki cieplnej główki szyny ze stali perlitycznej w celu uzyskania pożądanych właściwości mechanicznych. Dzięki implementacji modelu w programie komputerowym opartym na metodzie elementów skończonych możliwe jest śledzenie postępu przemian fazowych w trakcie obróbki cieplnej główki szyny o strukturze perlitycznej, a w efekcie końcowym również przewidywanie parametrów mikrostruktury finalnej oraz właściwości mechanicznych szyny. Drugą funkcją programu jest określenie warunków obróbki cieplnej powodujących uzyskanie założonego rozkładu właściwości mechanicznych w główce szyny obrabianej cieplnie. Prezentowane podejście oraz program komputerowy opracowano w ramach prac związanych z realizacją projektu badawczo-rozwojowego "HyPremRail". Po zadaniu warunków chłodzenia program realizuje lokalnie obliczenia odległości między płytkami cementytu, wielkości ziarna i kolonii perlitu w oparciu o opracowany model przemian fazowych, posługując się rozwiązaniem MES równania Fouriera, a następnie przelicza wartości uzyskanej odległości międzypłytkowej na twardość, granicę plastyczności i wytrzymałość na rozciąganie. Przeprowadzenie obliczeń wymaga zdefiniowania warunków początkowych i brzegowych procesu obróbki cieplnej. Z kolei zagadnienie optymalizacji parametrów procesu w celu uzyskania korzystnego rozkładu właściwości mechanicznych w obszarze główki rozwiązywane jest za pomocą metody obliczeń odwrotnych.

<u>Słowa kluczowe:</u> mikrostruktura perlityczna, przemiany fazowe, właściwości mechaniczne, obróbka cieplna szyn, modelowanie numeryczne

1. INTRODUCTION

Over last decades, a constant progress has been taken place in the rail transportation sector, which involves not only the improvement of its organization, but also the implementation of technological solutions complying with the strict safety requirements and regulations imposed on natural environment protection. Growing requirements stemmed from the constant development of rail transport, specifically focused on the increase of train speed and application of greater axle loads due to an increase in the weight of materials carried by rail transport. One of the main priorities as regards to global railway development is the construction of fast rail networks in Europe and other countries throughout the world.

The rail transport capacities depend strongly on the track's parameters. The most important comprise: car stability, geometry of the contact with running wheel, and possibility to sustain greater loads. For these reasons, an intensive research aimed at designing of new method of pearlitic rails head hardening process giving rise to substantial reduction of the interlamellar spacing of cementite lamellae and the size of pearlite colony has been launched at IMZ [1-5]. Pearlite microstructure with small distance between the cementite lamellae (around 0.08-0.12 µm) is characterized by the high wear resistance, high fatigue strength and resistance to the development of rolling contact and fatigue damages, as compared to the pearlite microstructure after the natural slow air cooling of rails after hot rolling, characterized by lamellar spacing within the range of 0.2-0.3 µm. Reduction of the distance between cementite lamellae results in an increase of pearlite strength/ hardness. Simultaneously, it results in thinning of cementite lamellae, thus increasing plasticity of this phase.

2. METALLURGICAL MODEL OF THE RAIL HEAD HARDENING PROCESS

Rails currently used in rail transport are mainly manufactured of pearlitic steel. According to the standard EN 13674-1:2011+A1:2017, it is admissible to manufacture railway rails of 9 grades of pearlitic steel (including 4 grades designed for rails production with heat treatment).

In the rails production process, pearlitic structure is developed below the $A_{\rm el}$ temperature, which is around 727°C, during cooling from the austenite stability range of temperatures to ambient temperature. The most important parameter characterizing pearlite microstructure is the spacing between cementite lamella. Schematic definition of this parameter is given in Fig. 1, presenting the interrelation



Fig. 1. Determining the actual distance between the cementite lamellae in pearlite $S_0 = L/2$ [2]

Rys. 1. Schemat ilustrujący procedurę wyznaczania rzeczywistej odległości między płytkami cementytu w perlicie $S_0 = L/2$ [2]

between the actual distance between the cementite lamellae – S_0 , interlamellar spacing in the plane of observation – S, and the mean linear intercept of cementite lamellae – L.

Pearlitic transformation involves the nucleation and growth process of pearlite nuclei. Nucleation primarily occurs at corners, edges and surfaces of austenite grain boundaries. The resulting microstructure is composed of pearlite nodules which are sheared by pearlite colonies (Fig. 2). Typically, there are several colonies in pearlite nodules, characterized by the same orientation of the pearlite lamellae within each colony. High- or low angle boundaries are developed between neighboring pearlite colonies. Such pearlite microstructure is formed when austenite grains before the transformation are relatively large (> 20 μ m), and pearlitic transformation occurs at slight supercooling with respect the temperature $A_{\rm el}.$ For smaller austenite grains and considerable supercooling of austenite at the beginning of transformation, the size difference between the nodes and pearlite colonies disappears. In such a case, only colonies are visible in the microstructure and the perlite is called colonial. Differences between nodular and colonial pearlite are presented at Fig. 2 along with the definition pearlite nodule (D_p) and colony size (D_c) . As it is the case of interlamellar spacing, an average size of nodule and colony can be determined with the mean intercept method. In this paper, pearlite and colony size is represented by means of mean equivalent diameter.



Fig. 2. Morphological types of pearlite: (a) nodular pearlite, (b) colonial pearlite and definition of the pearlite nodule size (D_p) and colony size (D_c) ; D_γ in Fig. 2a refers to the prior austenite grain size Rys. 2. Typy morfologiczne perlitu: (a) perlit ziarnisty, (b) perlit kolonialny; na rys. 2a zdefiniowano wielkość ziarna perlitu (D_p) , wielkość kolonii perlitu (D_c) i wielkość ziarna pierwotnego austenitu (D_γ)

Parameters of pearlitic microstructure can be connected with the chemical composition of steel and temperature at which austenite transforms to pearlite. As the temperature of transformation decreases, interlamellar spacing also decreases. On the other side, the total elongation reaches its maximum value when the transformation takes place at around 550°C [1, 5]. The interlamellar spacing after transformation at 550°C typically is within the range of 0,07–0,11 μ m, and the average size of pearlite colony is around 5–7 μ m.

Effect of the chemical composition of steel on kinetics of pearlitic transformation has been investigated by Kuziak [1]. The developed model takes into account the incubation period and growth of pearlite grains. Incubation period is described by the following equation:

$$\tau = \frac{KT \exp\left(\frac{Q}{RT}\right)}{(T_0 - T)^{w}} \tag{1}$$

where K parameter depends on the content of elements in steel:

$$K = 2.6 - 1.44C - 2.95C^{2} + 0.69Mn + 1.5Mn^{2} + + 13.9Cr + 65.5Cr^{2}$$
(2)

T is the temperature in the absolute scale, T_0 is the equilibrium temperature below which the transformation starts, *Q* is the activation energy of 114 500 J/mol, while values of the remaining coefficients are: n = 1.96, m = 1.94, w = 4.65.

Equation (1) makes it possible to calculate temperature of the start of pearlitic transformation during continuous cooling of the rail with the application of Sheil's principle [6]:

$$\int_{0}^{t} \frac{dt}{\tau} = 1 \tag{3}$$

Equation (2) shows that increase of carbon content increases the temperature of the start of pearlitic transformation during continuous cooling, whereas manganese and chromium lowers this temperature. JMAK equation describes the kinetics of the growth of the pearlitic nuclei:

$$X(t)_{p} = 1 - \exp\left[-b(T)\left(\frac{t^{n}}{D_{\gamma}^{m}}\right)\right]$$
(4)

$$\ln[b(T)] = -2.546 \cdot 10^{-4} T^2 - 0.279 T - 72.23$$
 (5)

Spacing of cementite lamella in pearlite is also described in the publication [1] with the following equation:

$$\frac{1}{S_0} = A - B(\langle T_P \rangle - 273)$$
(6)

where: $\langle T_{\rm p} \rangle$ is the mean temperature of pearlitic transformation in Kelvins, which during continuous cooling is calculated with the following equation:

$$\left\langle T_{\rm p} \right\rangle = \frac{\int T dX(t)_{\rm p}}{\int dX(t)_{\rm p}} \tag{7}$$

where *A* and *B* coefficients depend on the chemical composition of steel in the following way:

$$A = 129.28 - 54.373Mn - 4.378Cr - 17.5Si$$

$$B = 0.1783 - 0.0723Mn - 0.0121Cr - 0.0274Si$$
(8)

Mathematic model of pearlitic transformation developed by Kuziak also makes possible to predict both the pearlite nodule size (D_p) and pearlite colony size (D_c) using the following equations:

$$D_{\rm p} = \frac{600 \left[1 - \exp(-0.016D_{\gamma})\right]^{0.6}}{(T_0 - \langle T_{\rm P} \rangle)^{1.2}} \tag{9}$$

$$\frac{1}{D_{\rm C}} = 0.857 - 0.001189(\langle T_{\rm P} \rangle - 273) \tag{10}$$

The most important parameter characterizing pearlite microstructure is spacing between cementite lamellae. This parameter has influence on strength properties of pearlite. In publication [1], proof stress and ultimate tensile strength of pearlite is linked with the so-called average free path (χ) for dislocation motion in ferrite lamellae:

$$R_{0.2} [\text{MPa}] = 259 + 0.087 \chi^{-1}$$
(11)

$$R_{\rm m} [{\rm MPa}] = 773 + 0.058 \chi^{-1} + 122Si$$
 (12)

where:

$$\chi = 2(S_0 - t) \tag{13}$$

$$t = 0.15S_0C$$
 (14)

where Si and C is, respectively, silicon and carbon contents in steel.

Vickers hardness in the developed model is calculated using the following equation:

$$HV_{\rm p} = c + \frac{d}{S_0} \tag{15}$$

Dependence of the average free path and tensile strength on temperature, calculated with eq. (11) – (14) is presented in Fig. 3.



Fig. 3. Dependence of the average free path in pearlitic ferrite and tensile strength on temperature of pearlitic transformation for steel with the chemical composition: 0.7% C, 1.1% Mn and 0.25% Si Rys. 3. Zależność średniej drogi swobodnej w płytkach ferrytu w perlicie i wytrzymałości na rozciąganie od temperatury przemiany dla stali o składzie chemicznym: 0.7% C, 1.1% Mn i 0.25% Si

Temperature of pearlitic transformation in naturally cooled rails is within the range of 690–670°C, which allows to achieve tensile strength in the range of around 850–900 MPa. To achieve strength higher than 1200 MPa, temperature of pearlitic transformation should be shifted to below 560°C.

The most important parameters to achieve high ductility of pearlitic structure comprise the prior austenite grain size and pearlite colony size. Equations (9) and (10) show that pearlite nodule size depends on the size of austenite grain and temperature at which pearlitic transformation occurs. Furthermore, the size of pearlite colony depends only on the temperature of the transformation. These relations are presented in Fig. 4 based on the calculations performed using equation (9) and (10). Dependence of the pearlite nodule size on temperature of the transformation is presented for two austenite grain sizes, i.e. 20 and 60 μ m.



Fig. 4. Effect of the transformation temperature on the pearlite nodule and colony size

Rys. 4. Wpływ temperatury przemiany perlitycznej na wielkość ziarna i kolonii perlitu

Fig. 4 shows that when pearlitic transformation occurs in fine grain austenite, reduction of transformation temperature results in equal size of nodule and pearlite colony. In such a situation, steel structure contains pearlite colonies only and such pearlite is called a colonial pearlite by Garbarz and Pickering [7].

When the transformation occurs at temperature in the range of 550–500°C, the structure contains, besides lamellar pearlite, degenerated pearlite or bainite. When austenite transformation occurs at temperature below 500°C, bainite is present in the microstructure [6]. Increase in the content of degenerated pearlite and bainite in the structure reduces rail ductility. To achieve proper mechanical properties of rails, parameters of head hardening of rails should be adjusted in such a way that pearlitic transformation in the head occurs within the range of 570–530°C [4, 5].

3. NUMERICAL SIMULATIONS OF RAIL HEAD HARDENING PROCESS

Process of heat treatment after hot rolling is simulated using authors FE program [8] with phase transformation and mechanical properties models solved at each Gauss integration point of the FE mesh. In this paper, the program capability to optimize this process is demonstrated. In the case of heat treatment of pearlitic steel rails, the goal of the optimization should be obtaining the following rail's head requirements [5]:

- small interlamellar spacing of cementite in pearlite
- lack of bainite in the microstructure
- high level of the hardness (HV > 350)
- lack of the fast hardness drop from the head running surface to the head centre.

Criteria connected with low interlamellar spacing, lack of bainite in the microstructure and high level of the hardness are not conflicting. On the contrary, requirement of uniform hardness distribution is in conflict with the high level of this property. Therefore, the objective function in the process of optimization is divided into two separate objectives:

$$\Phi = \sqrt{\sum_{i=1}^{n_{gp}} (w_s S_{0i}^2 + w_f F_{bi}^2) + w_{HV}} \sum_{i=1}^{n_{gp}} \left(\frac{HV_i - HV_{ave}}{HV_{ave}}\right)^2 \quad (16)$$

where:

- $n_{
 m gp}$ number of Gauss integration points in the rail head,
- $HV_{\rm ave}$ average hardness at the cross section of the rail head,
 - $F_{\rm b}$ bainite volume fraction,

 $w_{\rm s}, w_{\rm f}, w_{\rm HV}$ – weights.

Two cases are considered for the sake of the model capability presentation in this paper, namely:

Variant I: obtaining maximum hardness close to the running surface of the 60E1 rail,

Variant II: obtaining uniform hardness distribution in the cross section of the 60E1 rail.

It is assumed that the goals of the optimization will be achieved by applying five cycles of cyclic cooling of the rail head in the bath of aqueous solution of polymer substances. The times of cooling in air (A) and cooling in polymer solution (P) obtained in the course of the optimization are given in Table 1.

Table 1. Parameters of the cyclic head hardening process obtained in the process of the optimization using authors computer tool [s] Tabela 1. Parametry cykli procesu obróbki cieplnej główki szyny

otrzymane w procesie optymalizacji za pomocą opracowanego narzędzia komputerowego [s]

Variant	Α	Р	Α	Р	Α	Р	Α	Р	Α	Р
Ι	98	35	22	10	22	14	35	8	35	6
II	98	27	21	13	26	23	28	28	34	8

For the sake of obtained results presentation, nodal points are defined in Fig. 5. The hardness values, cementite interlamellar spacing and average pearlitic transformation temperature obtained in the simulation of the rail head hardening process according to variants I and II are shown in Fig. 6.



Fig. 5. Definition of the nodal points in the cross section of 60E1 rail Rys. 5. Definicja położenia punktów węzłowych w przekroju główki szyny 60E1

One can see from the performed calculations that the cementite interlamellar spacing and hardness can be correlated with the mean transformation temperature expressed by equation (7). A comparison of the calculated progress of pearlitic transformation as a function of time at point A and C for both variants is shown in Fig. 7.



Fig. 6. Results of the simulations of the 60E1 rail head hardening process for points A, B, C, D according to Variant I and II: a) hardness, b) cementite interlamellar spacing, c) average pearlitic transformation temperature

Rys. 6. Wyniki symulacji procesu umacniania główki szyny 60E1 dla punktów A, B, C, D zgodnie z Wariantem I i II: a) twardość, b) odległość między płytkami cementytu, c) średnia temperatura przemiany perlitycznej



Fig. 7. Progress of the pearlitic transformation as function of time at point A (a) and point C (b). Solid line – Variant I, dotted line – Variant II Rys. 7. Postęp przemiany perlitycznej w funkcji czasu w punktach A (a) i C (b). Linia ciągła – Wariant I, linia kreskowana – Wariant II

It is seen from Fig. 7 that the pearlitic transformation at point A is completed earlier for Variant II of cooling. However, it is completed later for point B for this variant.

4. VERIFICATION OF THE RESULTS OF NUMERICAL SIMULATIONS

The obtained results are verified in the course of experiments conducted at the Process Simulation Department with the application of the in house constructed device for the semi-industrial simulations of rail head hardening process (Fig. 8). The device allows for the computer controlled cyclic immersion and emergence of the rail's head after austenitization in the laboratory furnace. Using this device, the Variant I and II of heat treatment is executed using 4% aqueous solution of polymer substances. In Fig. 9, the results of hardness measurements represented by the averaged values of 5 measurements at the location corresponding to points A, B, C, D marked in Fig. 5 are shown.

The obtained results are in good agreement with the results of the simulations obtained by the developed numerical model (Fig. 6). The hardness values can by justified by the microstructure analysis. For example, Fig. 10 presents the obtained microstructures at point A after applying both variants of heat treatment. Mean interlamellar spacing between cementite lamella after Variant I of cooling is 0.102 μ m while after Variant II is 0.123 μ m.



Fig. 8. General view of the device used for the physical simulation of rail head hardening process by immersion method (a), a holder for the rail (b)

Rys. 8. Ogólny widok urządzenia do półprzemysłowej symulacji procesu obróbki cieplnej główki szyny metodą zanurzeniową (a), uchwyt z szyną (b)



Fig. 9. Results of the Vickers hardness measurements at points A, B, C, D defined in Fig. 4, after applying Variant I (a) and Variant II (b) of cooling

Rys. 9. Wyniki pomiaru twardości Vickersa w punktach A, B, C, D zdefiniowanych na rys. 4, po zastosowaniu Wariantu I chłodzenia (a), Wariantu II chłodzenia (b)





Fig. 10. Pearlitic microstructures obtained at point A after applying Variant I (a) and Variant II (b) of cooling Rys. 10. Mikrostruktura perlityczna w punkcie A otrzymana po zastosowaniu obróbki cieplnej zgodnie z Wariantem I (a) i Wariantem II (b)

5. SUMMARY

The metallurgical model has been presented allowing for the prediction of pearlitic transformation kinetics and the resulting microstructure and mechanical properties during continuous cooling. In the HyPremRail project, a dedicated computer tool has been developed not only allowing the numerical predictions of the phase transformations during the pearlitic rail head hardening process, but also capable of adjusting the cooling conditions to obtain assumed hardness distribution in the head. It is done by performing the inverse analysis with objective function accounting for the hardness values defined at nodal points. The developed computer tool capability is validated in the course of laboratory experiments conducted in semi-industrial unit for the simulation of rails head hardening process by means of cyclic cooling of the head in aqueous polymer solution and in still air.

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