

NUMERICAL MODEL OF PEARLITE - AUSTENITE TRANSFORMATION

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Abstract

The diffusional transformation of pearlite to austenite takes place when the iron alloy with a matrix containing pearlite is heated to a temperature above A_{c1} . Development of the transformation contains two stages. The first stage is the formation of austenite nuclei. The second stage involves the growth of the austenite nuclei up to the moment of a complete transformation of the pearlite into austenite. The transformation rate depends on the parameters of the initial microstructure and also on the temperature transformation. Among parameters of the initial structural the most important are: the thickness of a cementite and a ferrite plate (called interlamellar distance) and the size of the pearlite colony. Following the Roosz at al. [1] a numerical model of the pearlite-austenite transformation has been developed. It allows for the calculation of the time of the transformation at an assumed temperature as well as to determine the TTT diagram for the assigned temperature range. The developed computer program also enables to calculate the CHT diagram. The results of modeling the transformation showed a strong influence of the size of pearlite colony and interlamellar distance on the transformation kinetics. Decrease of the interlamellar distance reduces the time needed to end of the transformation. Verification of the derived model using published data was done.

Keywords: Pearlite, TTT diagrams, CHT diagrams, modelling of phase transformations

1. INTRODUCTION

Computer simulations in materials science allow using mathematical models to reproduce industrial processes and analysing the characteristics of the materials tested in a manner analogous to the actual process [2-12]. Obtaining the desired microstructure of alloys of iron with carbon, and hence the relevant mechanical properties, requires the optimization of technological parameters of the process. Because of that it seems advisable to use the computer techniques that are currently being cheap and effective way to optimize, for modeling and analysing phenomena taking place during the phase transformation of iron-carbon alloys. During heating of the iron-carbon alloy with a pearlitic microstructure to a temperature above A_{c1} the diffusional transformation of pearlite to austenite occurs. The mechanism for this transformation involves the nucleation and growth of austenite grains. According to the literature [13-18], the grain size and homogeneity of the resulting austenite, as a starting point for the final microstructure after heat treatment are essential. The rate of pearlite-austenite transformation depends largely on the microstructure parameters of the starting material (interlamellar distance and pearlite colony size) and on the degree of superheat of pearlite above the A_{c1} temperature during the isothermal heating or on heating rate for continuous heating. In this work, using developed computer program the analysis of the effect of these parameters on the rate of transformation of pearlite - austenite under isothermal conditions and in a continuous heating was carried out. The aim of presented work was to develop the computer program for analysis of the kinetics of the pearlite - austenite transformation during isothermal and un-isothermal conditions.

2. MODEL OF PEARLITE - AUSTENIT TRANSFORMATION

2.1 Numerical model

According to the literature we can differentiate between 3 groups of models, describing the transformation of pearlite to austenite [14-25]:

- diffusion mechanism of the transformation taking place between the plates of ferrite, cementite and austenite,
- a diffusion field in the growing austenite grain at the front face plates of ferrite and cementite,
- Avrami's equation (Johnson - Mehl - Avrami's equation) of the dependence of a fraction of the transformed austenite on the time.

In this work the third of mentioned models was used and adapted. The numerical model was based on Roosz model [1]. In this model it is assumed that the microstructure consists from pearlite colonies of similar shape and size. The shape of the pearlite colonies is described by truncated octahedron with its edge equals to a_p , μm . The parameter colony is also interlamellar distance between ferrite and cementite plates- σ_0 , μm .

During pearlite- austenite transformation the austenite nuclei can appear only on cementite Fe_3C / ferrite (α) interphase. Three different ferrite/cementite interfaces are found in purely pearlitic steel:

- the whole interface of ferrite and cementite platelets,
- the line of intersection of the platelets with the surfaces of pearlite colonies,
- the points of intersection of the platelets with the edges of pearlite colonies.

The numerical model of the austenite-pearlite transformation describes the Avrami equation, expressing the influence of the rate of nucleation, J , $1 / (\text{mm}^3 \text{s})$, austenite grain growth rate, V_w , mm/s and the transformation time, t , s at a given temperature, T , $^\circ\text{C}$ on a fraction of the volume, V_V , resulting austenite:

$$V_V = 1 - \exp\left(-\frac{\pi}{3} J G^3 t^4\right) \quad (1)$$

However, at a rate of heating of pearlite, V , $^\circ\text{C} / \text{s}$, the fraction V_V conversion function of time is described by equation [18]:

$$V_V = 1 - \exp\left(-\int_{A_{c1}}^T \frac{4}{3} \frac{\pi J G^3}{V^4} \Delta T^3 dT\right) \quad (2)$$

where $\Delta T = T - A_{c1}$, T - current temperature, $^\circ\text{C}$, A_{c1} , the equilibrium temperature for pearlite - austenite transformation .

Roosz et al [1] on the basis of investigations of transformation kinetics under isothermal conditions, provided that the pearlite colonies undergoing transformation are in the shape of truncated octahedron, presented equations describing the basic parameters of the equation (1), J and G as a function of overheating ΔT , also dependent on the parameters of starting microstructure pearlite: edge length, a_p and pearlite interlamellar distance σ_0 . These equations have the form:

$$J = \frac{1.378 \cdot 10^{-12}}{[(a_p)^2 \sigma_0]^2} \exp\left(-\frac{25.38}{\Delta T}\right) \quad (3)$$

$$G = \frac{7 \cdot 10^{-11}}{\sigma_0^2} \exp\left(-\frac{29.7}{\Delta T}\right) \quad (4)$$

Based on these equations, we can calculate time of the start and end of transformation at a given temperature, T . Typically, as the start is assumed time at which $V_V = 0.01$, and the end time - the time after which $V_V = 0.99$. On the basis of equations (1) and (2) can also be calculated TTT charts, describing the transformation kinetics under isothermal conditions. Using equation (2) and equations (3) and (4) we can also calculate the time transformation in the heating conditions with a known constant speed, as well as a CHT diagram that describes the kinetics of transformation in an un-isothermal condition. In developed computer program for calculation of the integral in equation (2) the Simpson method is used [26].

2.2 Characteristics of computer program

The present mathematical model of pearlite to austenite transformation the computer program P_G3D was developed. The input data for the program are:

- temperature range of transformation (T_d , T_g , °C) and the number of calculation points (np),
- edge length of the pearlite colonies (a_p , μm),
- the interlamellar distance (σ_0 , μm),
- minimum (V_d , °C / s) and maximum (V_g , °C / s) heating rate and the number of rate steps (nv)
- minimum (t_{min} , s) and maximum (t_{max} , s) transformation time and time step (d_{time}).

The developed program allows calculation of the transformation kinetics in the case of isothermal heating (TTT module), and in the case of continuous heating (module CHT).

Developed computer program allows the calculation of TTT and CHT diagrams for eutectoid steel, as well as the calculation of the relationships between austenite fraction and time in isothermal and un-isothermal conditions. The calculation results are stored in tabular form in separate text files. In addition, you can store graphs obtained in the form of the final charts.

Program contains two main program windows of input data: window TTT (Fig. 1a) and a window CHT (Fig. 1b). In CHT window presentation of the relationship between volume fraction of transformed austenite, V_v and temperature, for selected value of rate heating, V , is presented.

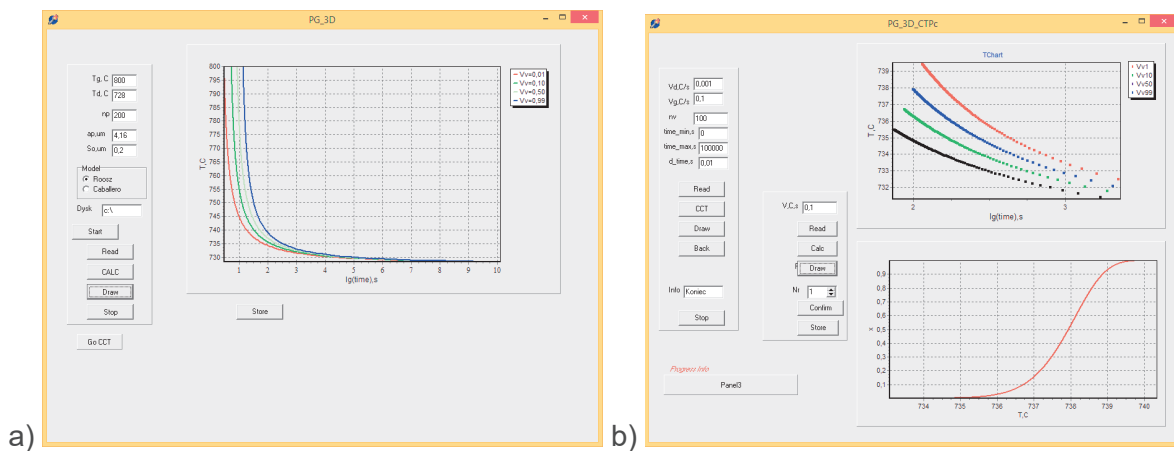


Fig. 1 Windows program PG_3D a) module TTT b) module CHT

2.3 Example of calculation

An analysis of the kinetics of transformation pearlite - austenite under isothermal and an-isothermal conditions of for eutectoid steel with given parameters of pearlite microstructure (a_p , σ_0) was carried out. The calculations were performed for two variants:

- case A: $a_p = 4 \mu m$, $\sigma_0 = 0.2 \mu m$,
- case B: $a_p = 2 \mu m$, $\sigma_0 = 0.06 \mu m$.

Simulations were performed for the transformation temperature range of 728 to 800 °C. Results of calculation of TTT and CHT diagrams are shown in Fig. 2 and 3.

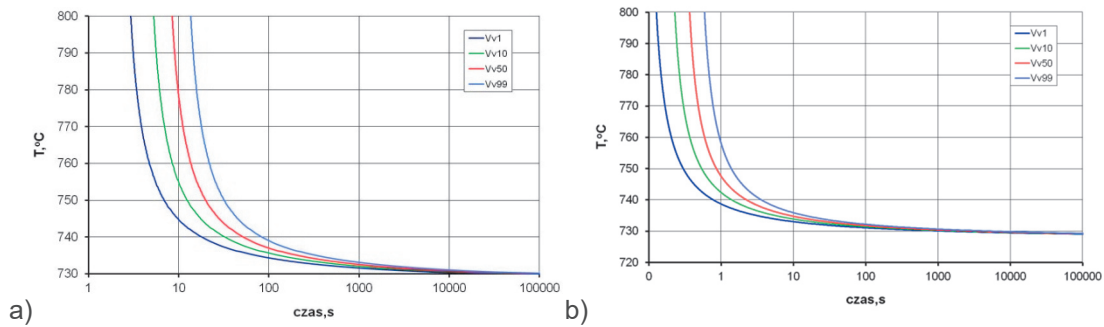


Fig. 2 TTT diagrams for pearlite parameters: a) $a_p = 4 \mu m, s_o = 0,2 \mu m$, b) $a_p = 2 \mu m, \sigma_o = 0.06 \mu m$

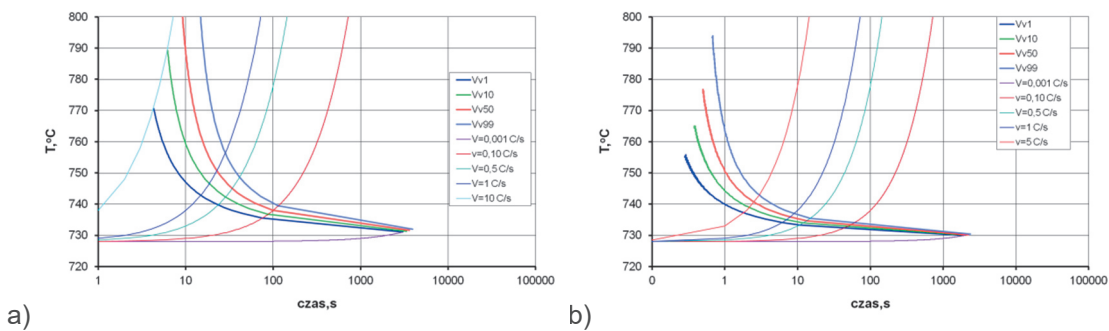


Fig. 3 CHT diagrams for pearlite parameters: a) $a_p = 4 \mu m, s_o = 0.2 \mu m$, b) $a_p = 2 \mu m, \sigma_o = 0.06 \mu m$

Data presented in **Fig. 2** and **3** describe the relationships between temperature and time for different level of transformation expressed by volume fraction, V_V , of transformed austenite: 0.01, 0.10, 0.50, and 0.99 (times $t_{0.01}, t_{0.10}, t_{0.50}, t_{0.99}$). As we can see on the charts TTT and CHT, the start time and the end time of the transformation decrease with increasing temperature transformation. These times also decrease with decreasing the pearlite colonies size and interlamellar distance. At isothermal conditions (**Fig. 1**) at a temperature $T = 760 \text{ }^\circ\text{C}$, $t_{0.01}$ are 7 times and 0.7 s, and the times $t_{0.99}$ are equal 20 and 0.9 s for case A and B, respectively. From data presented in **Fig. 2** we can conclude that with increasing heating rate the temperatures for start and end of transformation increase, while decreasing the start, $t_{0.01}$ and end, $t_{0.99}$, times decrease. Comparison of the position of transformation curves in the graphs TTT and CHT indicate their shift to the right for longer times for CHT diagram. Verifying of the model for calculation of the kinetics of pearlite - austenite transformation was carried out using experimental data Caballero at all. [18]. These data include results of measurements of the volume fraction of transformed austenite V_V as function of temperature for two heating rate: 0.5 $^\circ\text{C/s}$ and 5 $^\circ\text{C/s}$ Parameters of the initial pearlite microstructure were: $a_p = 4.16 \mu m$ and $\sigma_o = 0.2 \mu m$. Comparison of calculation results with the experimental data are shown in Fig.4a.

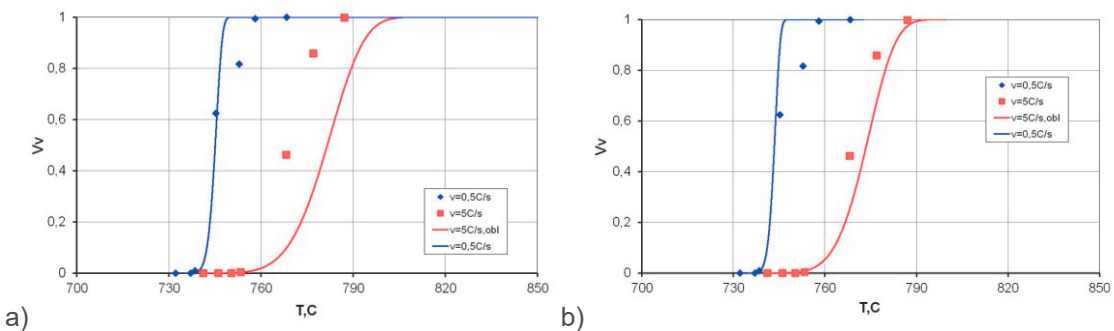


Fig. 4 Experimental and calculated kinetics results for the formation of austenite inside pearlite under different heating rates, using: a) Roosz et al. equations, b) Caballero et al. equations with modification

As we can see, the results of calculations for the heating rate $V = 5 \text{ }^\circ\text{C} / \text{s}$ are shifted to longer times compared to the experimental results.

Second calculations of relationships $V_v = f(T)$ were carried out using equations for J and G modified by Caballero et al. [17]:

$$J = \frac{7 \cdot 10^{11} (a_p)^6}{[(a_p)^2 \sigma_0]^{\frac{1}{6}}} \exp\left(-\frac{25.38}{\Delta T}\right) \quad (6)$$

$$G = \frac{1 \cdot 10^{-10}}{\sigma_0^2} \exp\left(-\frac{29.7}{\Delta T}\right) \quad (7)$$

Also in this case the agreement of calculated and experimental data was unsatisfied. More satisfactory agreement between calculated and experimental results (Fig.4b) was achieved with slightly modified equation (6) in the form:

$$V_z = \frac{7 \cdot 10^{11} (a_p)^5}{[(a_p)^2 \sigma_0]^{\frac{1}{6}}} \exp\left(-\frac{25.38}{\Delta T}\right) \quad (8)$$

4. DISCUSSION AND CONCLUSIONS

The paper presents the model and the computer program to analyze the kinetics of the pearlite transformation - austenite under isothermal and un-isothermal conditions and calculation of TTT as well as CHT diagrams for eutectoid carbon steel. The calculation results confirmed the strong influence of the pearlite parameters (edge colony length a_p , interlamellar distance, σ_0) on the kinetics of transformation. Along with decreasing size of the pearlite colonies and interlamellar distance increases transformation rate at a given temperature. This is mainly due to the increase in the rate of nucleation of austenite grains. This process is a heterogeneous nucleation and with decreasing parameters of pearlite - size a_p and σ_0 - increases the number of preferential nucleation sites for austenite. In Roosz model it was assumed that the nucleation of austenite grains occurs in the corners of a substantially pearlite colonies. Experimental verification of the model based on experimental data Caballero et al. [18] showed, however, that derived by Roosz et al. [1] equations, describing the transformation parameters J and G are not universal. This shows that in the process of nucleation of austenite, except the corners of colonies are also involved other less privileged places: the line of intersections of the platelets with surfaces of pearlite colony as well as the cementite - ferrite interfaces. The proportion of these sites will increase with the increase of the transition temperature, because with temperature increases the driving force for transformation - the difference in the free energy between austenite and mixture of ferrite and cementite. Therefore, this model requires further investigations on the effects of pearlite parameters and temperature on the pearlite - austenite transformation progress – in order to ensure satisfied agreement between calculated and experimental results.

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