

Numerical model of phase transformation of steel C80U during hardening

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Abstract

The article concerns numerical modelling of the phase transformations in solid state hardening of tool steel C80U. The transformations were assumed: initial structure – austenite, austenite – perlite, bainite and austenite – martensite. Model for evaluation of fractions of phases and their kinetics based on continuous heating diagram (CHT) and continuous cooling diagram (CCT). The dilatometric tests on the simulator of thermal cycles were performed. The results of dilatometric tests were compared with the results of the test numerical simulations. In this way the derived models for evaluating phase content and kinetics of transformations in heating and cooling processes were verified. The results of numerical simulations confirm correctness of the algorithm that were worked out. In the numerical example the simulated estimation of the phase fraction in the hardened axisymmetrical element was performed.

Keywords: Heat treatment; Phase transformation; Mathematical and numerical modelling

1. Introduction

The correct prediction of the final proprieties after hardening process is possible after defining the type and the property of the nascent microstructure of the steel element in the process of heating and then the cooling. It is essential for the correct prediction of the final properties to define the type and the property of the microstructure formed in the process of heating, and then cooling of the thermally treated steel-element. To achieve this, it is necessary to establish equations describing: phase transformations during the heat treatment [1-5]. In the past the kinetics of phase transformations was determined only by curves of the cooling and a suitable transformations graph. At present the simulation of this phenomena based on the theory of the nucleation and the growth of grains [6-8]. The last decade saw strong evolution of numerical methods whose aim to a greater or smaller extent was to design processes of heat-treatment. Every work dealing with this topic should contain thermal,

microstructural and stress analysis. Special emphasis put on the development of this branch of numerical methods is inspired by the industry, which demands tools improving heat-treatment processes because of modern technologies and costs reduction trends. Nowadays models of heat-treatment processes are being developed to include similar phenomena in processes of hot forming, such as: forging, rolling, welding etc. [6]. On the basis of the current state of knowledge on heat-treatment and data on mathematical and numerical modelling of these phenomena, a model of hardening of the tool steel was designed. Presented model includes the phase transformations in the solid state during heating and cooling at elements made with the steel C80U.

2. Phase transformations in the solid state during hardening process

In the model of phase transformations graphs of continuous heating (CHT) and cooling (CCT) are used [2,4,9]. The phase fraction transformed during continuous heating (austenite) is calculated in the model using the Johnson-Mehl and Avrami formula and [3,4,10,11]:

$$\eta_{\underline{A}}(T, t) = 1 - \exp(-b(t_s, t_f) (t(T))^{n(t_s, t_f)}) \quad (2.1)$$

where: $b(t_s, t_f)$ and $n(t_s, t_f)$ are coefficients calculated assuming the initial fraction (η_s) and the final fraction (η_f).

Coefficients b and n are calculated using the formula (2.1) and on condition that the part of the nascent phase equals " η_s " during " t_s " and " η_f " in time " t_f ". Formulas for these coefficients have a form:

$$n(t_s, t_f) = \frac{\ln(\ln(\eta_s)/\ln(\eta_f))}{\ln(t_f/t_s)}, \quad b(t_s, t_f) = \frac{-\ln(\eta_f)}{(t_s)^n} \quad (2.2)$$

where: $t_s = t_s(T_s)$, $t_f = t_f(T_f)$, and from the assumption: $\eta_s=0.01$, $\eta_f=0.99$.

The phase fraction during cooling, i.e. the pearlite fraction or the bainite fraction are calculated using the formula:

$$\eta_{(\cdot)}(T, t) = \beta \left(1 - \exp(-b(t(T))^n) \right) \quad (2.3)$$

$$\beta = \eta_{(\cdot)}^{\%} \eta_{\underline{A}} \text{ for } \eta_{\underline{A}} \geq \eta_{(\cdot)}^{\%} \text{ or } \beta = \eta_{\underline{A}} \text{ for } \eta_{\underline{A}} < \eta_{(\cdot)}^{\%}$$

where: $\eta_{(\cdot)}^{\%}$ is the maximum phase fraction for the established of the cooling rate, estimated on the ground of the continuous cooling graph, $\eta_{\underline{A}}$ is the fraction of austenite created in the process of heating.

The fraction of the martensite is calculated using the Koistinen and Marburger formula [10]:

$$\eta_M(T) = \beta \left(1 - \exp(-k(M_s - T)^m) \right) \quad (2.4)$$

where: m is the constant chosen by means of experiment; for examined steels it is accepted that $m = 1$, whereas the constant „ k ” is calculated based on the condition that the transformation below the temperature M_s and the finishes temperature M_f . For steel C80U the constant k equals: $k \approx 0.008$ [4,5].

The increment of the isotropic strain generated by temperature change and structural strains in the processes of heating and cooling are calculated using formulas [4,5]:

$$d\varepsilon^{Tph} = \sum_{i=1}^{i=4} \alpha_i \eta_i dT - \text{sgn}(dT) \sum_{j=1}^{j=4} \varepsilon_j^{ph} d\eta_j \quad (2.5)$$

where: $\alpha_i = \alpha_i(T)$ are thermal expansion coefficients of: austenite, bainite, martensite and pearlite, $\text{sgn}(\cdot)$ is a sign function,

ε_1^{ph} is an isotropic strain accompanying the conversion of the initial structure into austenite, whereas $\varepsilon_j^{ph} = \varepsilon_j^{ph}(T)$ ($j=2,3,4$) are isotropic strains from phase transformations of: austenite into bainite, martensite or austenite into pearlite fraction.

3. Experimental verification of the presented model

The purpose of the dilatometric research was to analyse phase transformations during heating and continuous cooling of steel C80U. Dilatometric research was done in the Institute for Ferrous Metallurgy in Gliwice by means of a dilatometer DIL805 produced by Bähr Thermoanalyse GmbH.

During the research critical temperatures A_{C1} and A_{Cm} at fast heating (100°C/s) were defined. Also austenite phase transformations of the examined steel during simulated cycles of cooling (construction of the CCT graph) were studied. Particular components of the examined steel: 0.84C, 0.19Mn, 0.21Si, 0.006P, 0.003S, 0.11Cr, 0.08Ni, 0.03Mo, and 0.14Cu (%) remain within the range of admissible values defined by a suitable standard (PN-85/H-93002). Cylindrical samples $\phi 4/2 \times 10$ mm and $\phi 4/3 \times 10$ mm (for the velocity of cooling $\geq 50^\circ\text{C/s}$) were used.

Heating to austenization temperature (1100°C) was carried out in the vacuum with the velocity of 100°C/s, the heating (the austenization time) equaled 2 seconds, at the cooling of samples was carried out at different rate: 300, 200, 150, 100, 50, 30, 20 and 10°C/s. For the established heating rate the temperatures of the beginning (A_{C1}) and the end of austenization (A_{Cm}) were equal: 784 and 852±4°C respectively, whereas equilibrium temperatures A_{C1} and A_{Cm} for this steel equal ~740 and ~760 °C respectively [9].

After dilatometric tests the examination of the microstructure of samples, and measurement of their microhardness were carried out. Microsections of cross-sections of samples were etched with nital. The microstructures were observed and the pictures were recorded by means of the optical microscope Axiovet 25, manufactured by Zeiss, and a digital camera. A description of the obtained microstructures of the considered steel depending on the rate of cooling are presented in the paper [4].

Using temperature curves, diagrams of individual dilatometric tests, fraction phases were assessed based on the examination of microstructures and measurements of the microhardness, the CCT graph of steel C80U was constructed (cf. [2,5]). Basing on this graph, as well as on the CCT graph of steel C80U found in literature [9], the CCT graph was shifted so that it could be used for numerical simulation of phase fraction and phase kinetics. The graph shift results from the assumption present in the numeric algorithm that the calculation of the cooling process begins at the point when the temperature $T(t_{cool}=0) = 810^\circ\text{C}$. While calculating the phase fraction the time of the cooling is counted from the moment of the intersection of the temperature curve of the cooling with a line $T=810^\circ\text{C}$, i.e it is assumed that $t_{cool}=0$ at the moment of the intersection [4,5,9].

The coefficient of thermal expansion for pearlitic structure of the steel C80U depends not linear on the temperature (see. Fig. 1),

and an approximation of this coefficient using the square function of the form was applied:

$$\alpha_p = -1.2955 \cdot 10^{-11} T^2 + 2.5232 \cdot 10^{-8} T + 3.7193 \cdot 10^{-6} \quad (3.1)$$

Based on comparisons of experimental and simulator dilatometric curves for the examined steel, values of thermal expansion coefficients and isotropic structural strains of each micro-constituents were determined. They equal: 22, 10, 10 and $14.5 (\times 10^{-6})$ [1/K] and 1.9, 4.5, 8.7 and $1.5 (\times 10^{-3})$ for austenite, bainite, martensite and pearlite respectively [4,5].

In order to verify the model of phase transformations test-numerical simulations were carried out. Results of these simulations and appropriate comparisons to the experiment results are presented in picture 1.

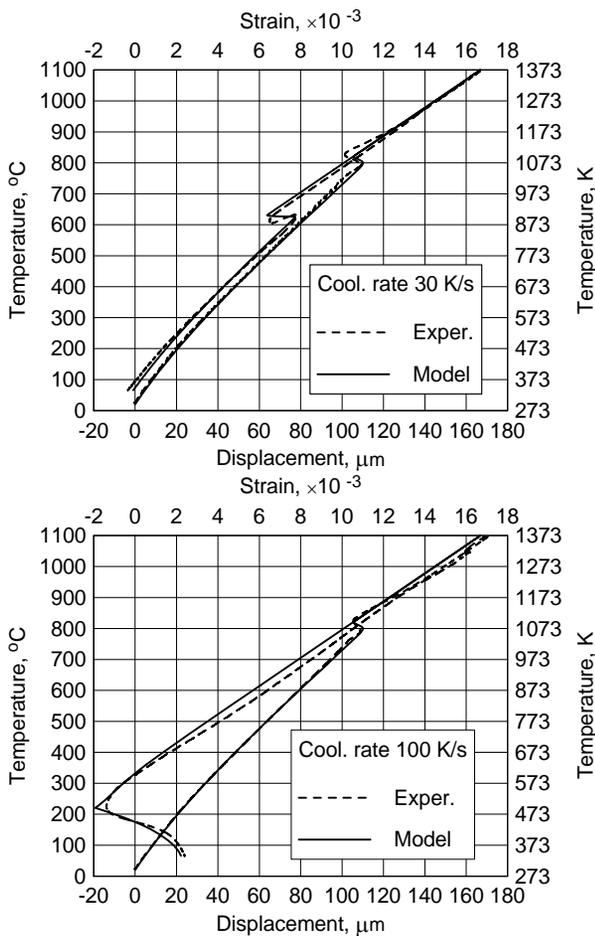


Fig. 1. Experimental and simulated dilatometric curves

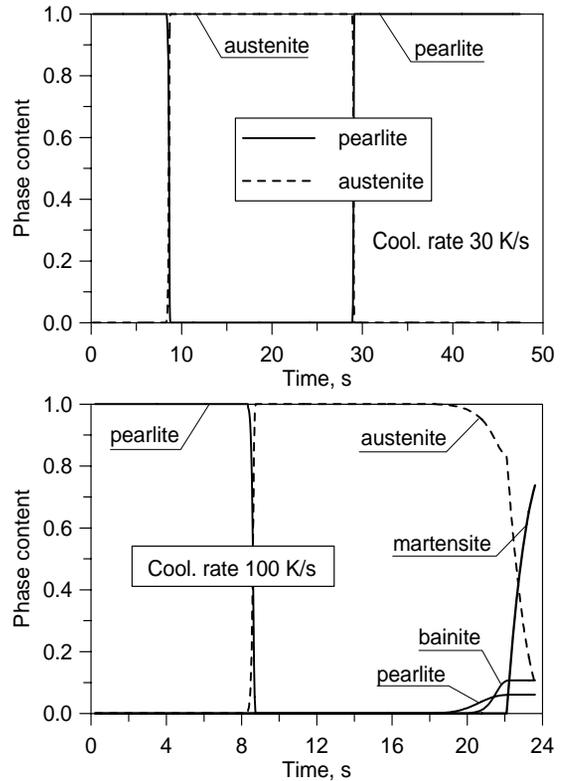


Fig. 2.. Kinetic of transformations

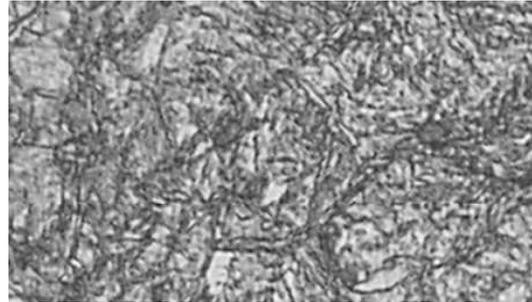


Fig. 3. Microstructure of investigated steel after cooling, zoom $\times 500$, cooling rate 100 K/s

4. Simulated estimation of the phase contents in the hardened element

The axisimmetrical object with the size $\phi 30 \times 60$ mm underwent hardening simulation. The thermophysical coefficients for the conductivity equation were assumed on the basis of the data in the paper [12]. After heating it had an even temperature equalling 1100 K and the output structure was austenite.

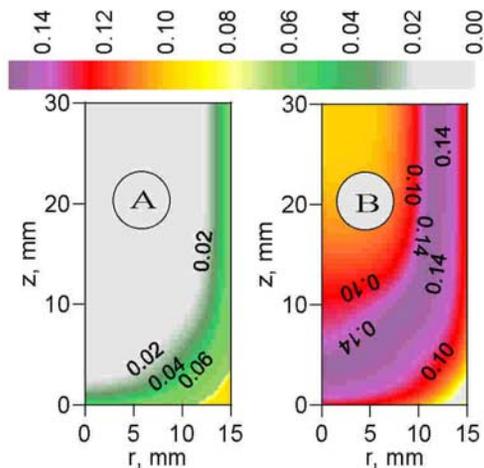


Fig. 4. Distributions of the retained austenite and bainite

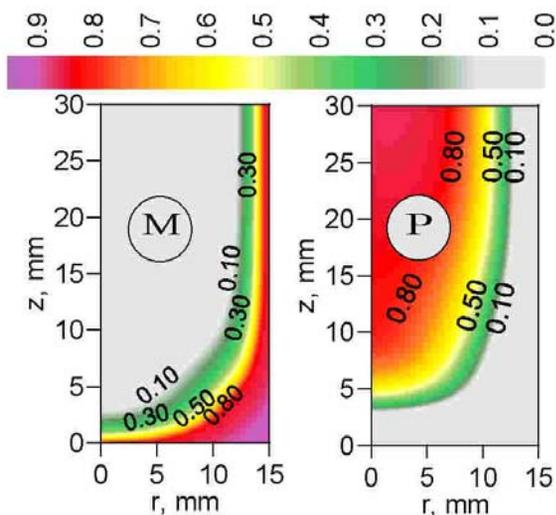


Fig. 5. Distributions of the martensite and pearlite

The cooling was modelled with the Newton condition [4,13]. The temperature of the cooling medium equalled 300 K. The heat transfer coefficient (from the external surface) was assumed equal 4000 [W/(m² K)] (cooling in the fluid layer [14]). The equation conductivity are solved by FEM [4,13].

Distributions of the simulated fractions in the microstructure after hardening of the object are presented in figures 4 and 5.

5. Conclusions

The results of the verification of the phase transformations model are satisfactory and confirm the correctness of the designed model of phase transformations for the carbon tool steel (figs. 1÷3). Having analysed the results of the object hardening simulation after full austenitizations it can be noticed that the hardened layer is comparable to the one obtained after deep inductive heating (figs. 4 and 5) [3,4]. However when cooling in

the fluid layer is performed more superficial deposition of the martensite is obtained and a slightly bigger deposition of the bainite in superficial layers can be observed.

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