

NUMERICAL ANALYSIS OF MICROSTRUCTURE AND STRESS GENERATED BY HEAT TREATED OF STEEL ELEMENTS

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Abstract

In work the presented numerical models of steel hardening processes take into account thermal, mechanical phenomena and phase transformations. In the model of phase transformations, in simulations heating process continuous heating was applied, whereas in cooling process continuous cooling of the steel at issue. The phase fraction transformed (austenite) during heating and fractions during cooling of ferrite, pearlite or bainite are determined by Johnson-Mehl-Avrami formulas. The theoretical model of phase transformations was then verified by experiments. The nascent fraction of martensite is determined by Koistinen and Marburger formula or modified Koistinen and Marburger formula. The stress and strain fields are obtained using the solution of the Finite Elements Method of the equilibrium equation in rate form. The thermophysical constants occurring in constitutive relation depend on temperature and phase composite. For determination of plastic strain the Huber-Misses condition with isotropic strengthening was applied whereas for determination of transformation plasticity a modified Leblond model was used. A satisfactory agreement was found.

Keywords: Hardening, phase transformations, numerical simulations, stress

1. INTRODUCTION

Today an intense development of numerical methods supporting designing or improvement of already existing technological processes are observed. The technologies mentioned above include also steel thermal process comprising hardening. Efforts involving thermal processing numerical models aim to encompass an increasing number of input parameters of such a process. Predicting of final properties of the element undergoing hardening is possible after determination of the type and features of the microstructure to be created, accompanying such technology of product quality improvement.

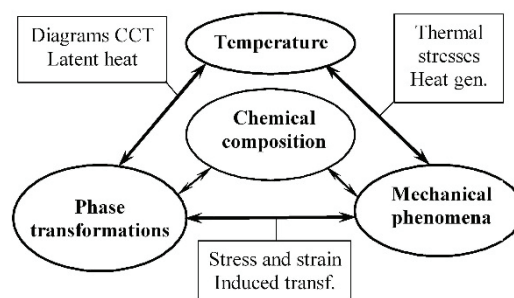


Fig. 1 Scheme of correlation of the hardening phenomena

For this to be achieved, it is necessary to take into account, first of all, thermal phenomena and phase transitions in the numerical model (**Fig. 1**). As a consequence of analyzing of the thermal processing results many mathematical and numerical models were obtained. The results of the numerical simulations of the phenomena mentioned above are dependent on the precision in calculation of the instantaneous temperature and solid-state phase kinetics, the latter significantly affecting and the microstructure final. Therefore accuracy of the solid-state phase transformations model for each steel grade is very important here. Phase

transformations numerical models exploiting isothermal heating and cooling curves can be applied with respect to several carbon steel grades if the isothermal heating and cooling curves are adequately moved. However, the values of the curve move should be confirmed by the results of experimental research conducted for this specific or a similar steel grade.

2. TEMPERATURE FIELDS

Temperature fields are obtained with solved of transient heat equation (Fourier equation) with source unit:

$$\nabla \cdot (\lambda \nabla(T)) - C \frac{\partial T}{\partial t} = -Q_v \quad (1)$$

where: $\lambda = \lambda(T)$ is the heat conductivity coefficient [W/(mK)], $C = C(T) = \rho(T)c(T)$ is effective heat coefficient, c - specific heat [J/(kgK)], ρ - thickness [kg/m³], Q_v is intensity of internal source [W/m³] (this can also be the phase transformations heat).

Superficial heating investigation in model by boundary conditions Neumann (heat flux q_n), however cooling are modelling by boundary conditions Newton with depend on temperature coefficient of heat transfer:

$$-\lambda \frac{\partial T}{\partial n} \Big|_{\Gamma} = q_n = \alpha^T(T) (T|_{\Gamma} - T_{\infty}) \quad (2)$$

In heating simulation on surfaces except heating source, also radiation through overall heat transfer coefficient was taken into account:

$$-\lambda \frac{\partial T}{\partial n} \Big|_{\Gamma} = q_n = \alpha_0 \sqrt[3]{T|_{\Gamma} - T_{\infty}} (T|_{\Gamma} - T_{\infty}) = \alpha^* (T|_{\Gamma} - T_{\infty}) \quad (3)$$

where: $\alpha^T(T)$ is heat transfer coefficient, α_0 is heat transfer coefficient experimental determine, Γ is surface, from witch is transfer heat, T_{∞} is temperature of medium cooling.

3. PHASE TRANSFORMATIONS

In the model of phase transformations take advantage of diagrams of continuous heating and cooling. In both case the phase fractions transformed during continuous heating (austenite) is calculated using the Johnson-Mehl and Avrami formula or modified Koistinen and Marburger formula (in relations on rate of heating):

$$\underline{\eta}_A(T, t) = 1 - \exp(-b(t_s, t_f) (t(T))^{n(t_s, t_f)}) \quad (4)$$

$$\underline{\eta}_A(T, t) = 1 - \exp\left(-\ln(\eta_s) \frac{T_{sA} - T}{T_{sA} - T_{fA}}\right), \dot{T} \geq 100 \text{ K/s} \quad (5)$$

where: $\underline{\eta}_A$ is austenite initial fraction nescent in heating process, T_{sA} is temperature of initial phase in austenite, T_{fA} - is final temperature this phase.

The coefficient $b(t_s, t_f)$ and $n(t_s, t_f)$ are obtain with (4) next assumption of initial fraction ($\eta_s=0.01$) and final fraction ($\eta_f=0.99$) and calculation are by formulas:

$$n(t_s, t_f) = \frac{\ln(\ln(0.01)/\ln(0.99))}{\ln(t_f/t_s)}, \quad b(t_s, t_f) = \frac{-\ln(0.99)}{(t_s)^n} \quad (6)$$

Pearlite and bainite fraction (in the model of phase transformations upper and lower bainite is not distinguish) are determine by Johnson-Mehl and Avrami formula [1].

$$\eta_i(T, t) = \chi \left(1 - \exp(-b(t(T))^n)\right) \quad (7)$$

The nascent fraction of martensite is calculated using the Koistinen and Marburger formula.

$$\eta_M(T) = \chi \left(1 - \exp \left(\ln(0.01) \frac{M_s - T}{M_s - M_f} \right) \right) \quad (8)$$

or modified Koistinen and Marburger formula [3,4,7]:

$$\eta_M(T) = \chi \left(1 - \exp \left(- \left(\frac{M_s - T}{M_s - M_f} \right)^m \right) \right) \quad (9)$$

where

$$\chi = \eta_{(c)}^{\%} \eta_{\underline{A}} \text{ for } \eta_{\underline{A}} \geq \eta_{(c)}^{\%} \text{ and } \chi = \eta_{\underline{A}} \text{ for } \eta_{\underline{A}} < \eta_{(c)}^{\%} \quad (10)$$

$\eta_{(c)}^{\%}$ is the maximum phase fraction for the established of the cooling rate, estimated on the ground of the continuous cooling graph, m is the constant chosen by means of experiment. For considered steel determine, that $m = 3.3$ if the start temperature of martensite transformations is equal $M_s = 493$ K, and end this transformations is in temperature $M_f = 173$ K [2].

Increases of the isotropic deformation caused by changes of the temperature and phase transformation in the heating and cooling processes are calculated using the following relations:

- heating

$$d\varepsilon^{Tph} = \sum_{\alpha=1}^{\alpha=5} \alpha_{\alpha} \eta_{\alpha} dT - \varepsilon_A^{ph} d\eta_A \quad (11)$$

- cooling

$$d\varepsilon^{Tph} = \sum_{\alpha=1}^{\alpha=5} \alpha_{\alpha} \eta_{\alpha} dT + \sum_{\beta=2}^{\beta=5} \varepsilon_{\beta}^{ph} d\eta_{\beta} \quad (12)$$

where: $\alpha_{\alpha} = \alpha_{\alpha}(T)$, are coefficients of thermal expansion of: austenite, bainite, ferrite, martensite and pearlite, respectively, ε_A^{ph} is the isotropic deformation accompanying transformation of the input structure into austenite, whereas $\varepsilon_{\beta}^{ph} = \varepsilon_{\beta}^{ph}(T)$ are isotropic deformations from phase transformation of: austenite into bainite, ferrite, martensite, or of austenite into pearlite, respectively. These values are usually adopted on the basis of experimental research conducted on a heat cycle simulator.

Heat of phase transformations take into account in source unit of conductivity equation (1) calculate by formula:

$$Q = \sum_k H_k^{\eta_k} \dot{\eta}_k \quad (13)$$

where: $H_k^{\eta_k}$ is volumetric heat k- phase transformations, $\dot{\eta}_k$ is rate of change fractions k- phase.

The methods for calculation of the fractions of the phases created referred to above were used for carbon tool steel represented by C80U steel. CCT diagrams for this steel grade are presented in the **Figs. 2, 3**. After analysis of the above diagrams it can be noticed that steel under consideration does not contain ferrite but can contain remnant cementite. The curves of CCT diagrams are introduced into a relevant module of phase fraction determination with supplementary information regarding maximum participation of each phase.

However, in the model based upon the diagrams of continuous cooling relevant ranges determine the paces of cooling evaluated to the time when the temperature achieves the transformation starting curve.

In order to confirm the accuracy of the phase transformation model dilatometric tests were carried out on the samples of the steel under consideration. The model was verified by comparing the dilatometric curves received for different cooling paces with simulation curves. On the basis of the analysis of the results a slight move of CCT diagram was made in order to reconcile the initiation time of the simulation transformation and the times obtained in the experimental research (**Fig. 3**). These moves were presented, for example, in the studies. On the basis of the analysis of simulation and dilatometric curves the values of the thermal expansion

coefficient ($\alpha(\cdot)$) and isotropic structural deformations of each structural component were specified. These coefficients are: 22, 10, 10 and 14.5 ($\times 10^{-6}$) [1/K] and 0.9, 4.0, 8.5 and 1.9 ($\times 10^{-3}$). It was adopted that 1,2,3,4 and 5 refer to austenite, bainite, martensite and pearlite, respectively. Exemplary comparisons of the simulation and experiment results are displayed in the **Fig. 4**. The transformation kinetics corresponding to the established speeds of cooling was presented in the **Fig. 5**.

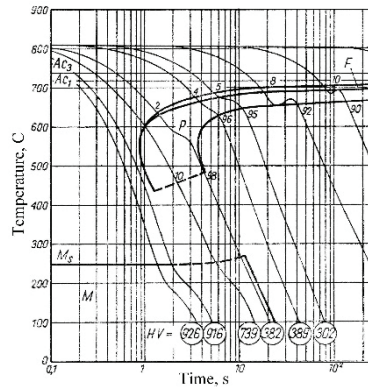


Fig. 2 Diagram CCT for steel C80U

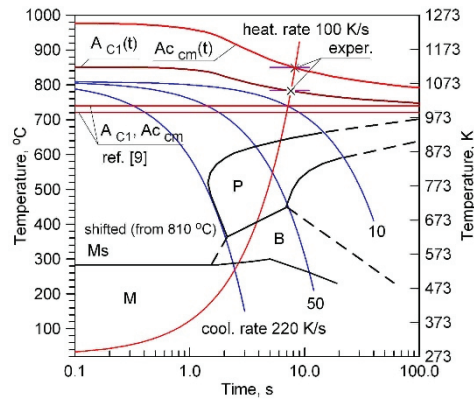


Fig. 3 Shifted diagram CCT with CHT curves for considered steel

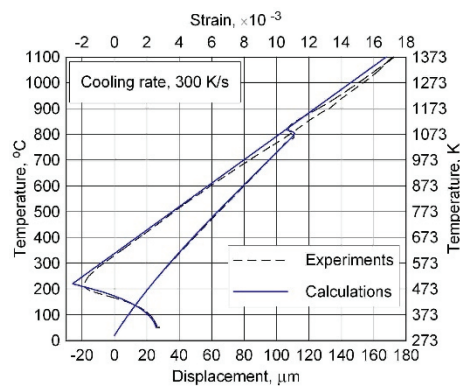
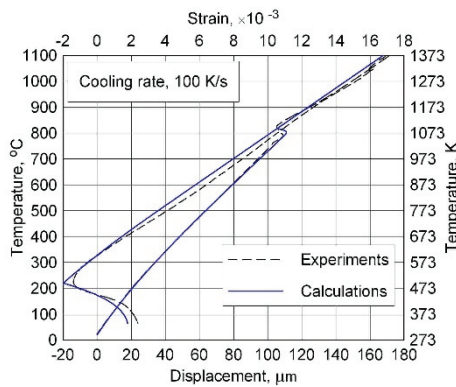


Fig. 4 Experimental and simulating dilatometric curves

Coefficient of thermal expansion the pearlite structure for considered steel is dependent on temperature (**Fig. 4**), approximate this coefficient by square function. Analysis results from the model notice, that advantageous, is use in modelling of phase transformations the CCT graph for considered group steel. Accuracy results, particularly in range rate cooling are obtain in which forming also bainite (**Fig. 5**).

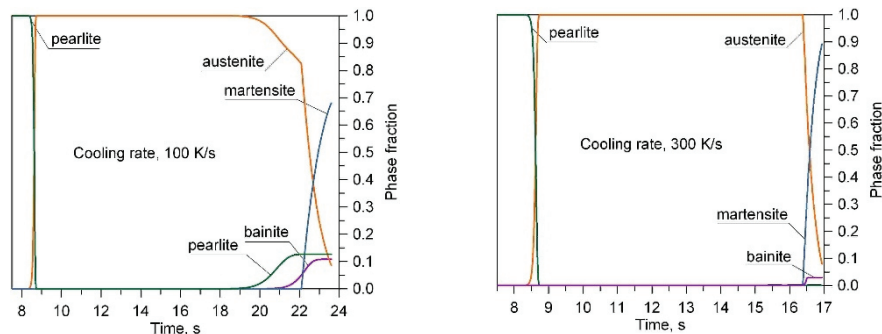


Fig. 5 Kinetics of phases for the fixed rates cooling

4. STRESSES AND STRAINS

In the model of mechanical phenomena the equations of equilibrium and constitutive relationship accept in rate form [3]:

$$\nabla \dot{\sigma}(x_\alpha, t) = \mathbf{0}, \quad \dot{\sigma} = \dot{\sigma}^T, \quad \dot{\sigma} = \mathbf{D} \circ \dot{\varepsilon}^e + \dot{\mathbf{D}} \circ \varepsilon^e \quad (14)$$

where: $\sigma = \sigma(\sigma_{\alpha\beta})$ is stress tensor, $D = D(\nu, E)$ is tensor of material constant (isotropic material), ν is Poisson coefficient, $E = E(T)$ is Young's modulus depend on temperature, whereas ε^e is tensor of elastic strain.

Assumption additives of strains, total strain in environment of considered point are equal:

$$\varepsilon = \varepsilon^e + \varepsilon^{Tph} + \varepsilon^{tp} + \varepsilon^p \quad (15)$$

where: ε^{Tph} are isotropic temperature and structural strain, ε^{tp} are transformations plasticity, whereas ε^p are plastic strain.

To mark plastic strain the non-isothermal plastic law of flow with the isotropic strengthening and condition plasticity of Huber-Misses were used. Plasticize stress is depending on phase fraction, temperature and plastic strain [4]:

$$Y(T, \eta, \varepsilon_{ef}^p) = Y_0(T, \eta) + Y_H(T, \varepsilon_{ef}^p) \quad (16)$$

where: $Y_0 = Y_0(T, \eta)$ is a yield points of material dependent on the temperature and phase fraction,

$Y_H = Y_H(T, \varepsilon_{ef}^p)$ is a surplus of the stress resulting from the material hardening.

5. EXAMPLE

As it has been already mentioned, the simulations of hardening were subject the fang lathe of cone (axisymmetrical object) made of tool steel. The superficial heating (surface hardening) the section of side surface of cone was modelling Neumann boundary conditions taken Gauss distributions of heating source. The cooling simulated by flux results from the difference of temperature among side surface and cooling medium (Newton condition). The temperature of cooling medium is equal 300 K. The coefficient of thermal conductivity was constant and was equal $\alpha_T = 4000$ [W/(m²K)]. The cooling performed to obtain by object ambient temperature, and final of structures. Obtained results of simulations were presented on the **Figs. 6, 7**.

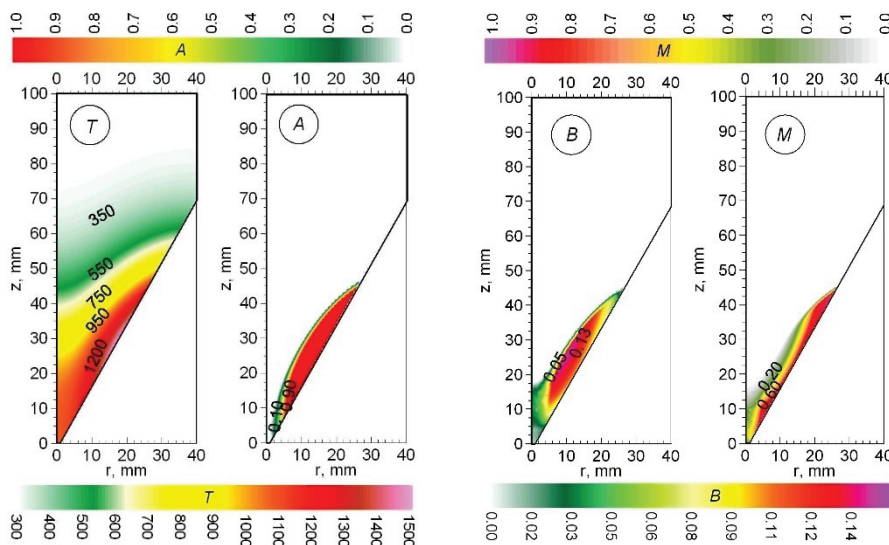


Fig. 6 Distributions: temperature a) and **Fig. 7** Zones: bainite a) and martensite b) after heating austenite b) after quenching

As it has been already mentioned, using of CCT diagrams within the cooling rate ranges wherein three transformations are observed: pearlitic, bainitic and martensitic, guarantees more precise results. The results of verification simulation of phase transformation kinetics (**Fig. 5**) prove that application of CCT diagrams enables good precise determination of fractions and kinetics of newly-created phases depending on the cooling rate.

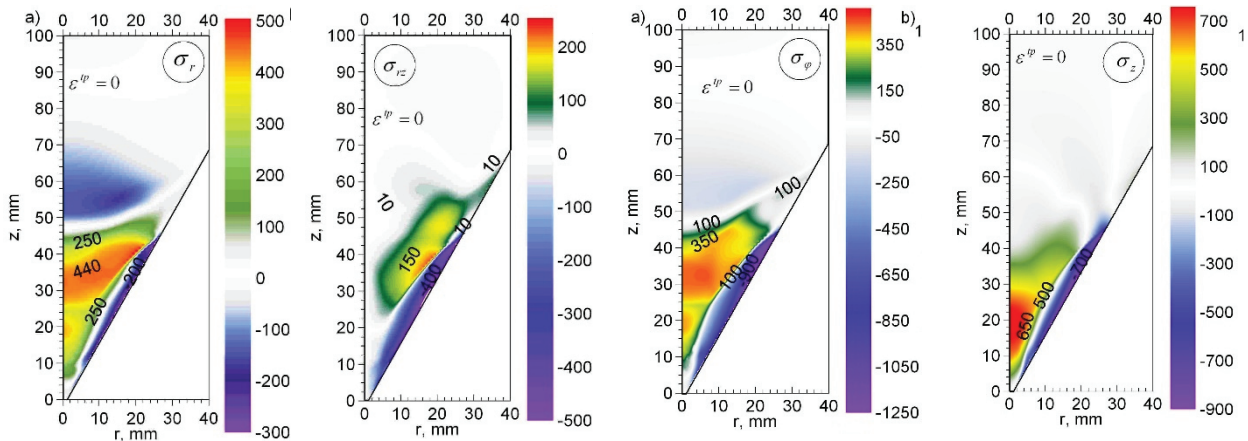


Fig. 8 Distributions of radial, circumferential, tangential and axial stresses

The simulations provide to very valuable distribution of temperature and good area of austenite deposition were obtained (**Fig. 6**). The hardened area after cooling appeared very beneficial, as well, which means that it is very well situated. The structure of the area after hardening is very good.

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