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V.V. Kaverinskiy, A.I. Trotsan, G.A. Bagiluk, Z.P. Sukhenko

Institute for Problems in Materials Science

SIMULATION OF VOLUMETRIC AUSTENITE TRANSFORMATION

A computer mathematical model for austenite transformation process simulation was developed. The developed model can be useful for prediction of structure obtained during metal cooling. Using in the model combined heat transfer and physical kinetics solution the allocation of structure types in a sample cross section could be obtained. A simulation of structure formation during quenching of an ordinary low-carbon steel cylindrical sample was carried out. Quenching depth and parts of structure types in different distances from surface were predicted. The simulation showed that the properly quenched depth in a cylindrical sample of ordinary low-carbon steel with diameter 20 mm is about 2 – 3 mm (in water cooling conditions). Then the part of martensite significantly decline and the structure becomes consists mostly from ferrite. The model is useful for heat processing developing. Using it you can fast and with minimum of expense develop a proper tempering regime without large number of experimental.

Keywords: mathematical model, phase transformations, austenite, steel, simulation, quenching.

В.В. Каверинський, А.І. Троцан, Г.А. Баглюк, З.П. Сухенко

МОДЕЛЮВАННЯ ПРОЦЕСУ РОЗПАДУ АУСТЕНИТУ В ОБ'ЄМІ МАТЕРІАЛУ

Розроблено комп'ютерну модель, що описує процес перетворення аустеніту. Модель використовується для передбачення структури металу, що формується в процесі його охолодження. Використання комбінації рішення задачі теплопереносу з моделюванням кінетики фазових перетворень дозволяє передбачити розподіл отриманої структури по об'єму виробу. У даній роботі представлений приклад використання даної моделі для опису структуроутворення при загартуванні циліндричного зразка з низькоуглецевої сталі.

Ключові слова: комп'ютерна модель, фазові перетворення, аустеніт, сталь, моделювання, гартування.

В.В. Каверинский, А.И. Троцан, Г.А. Баглюк, З.П. Сухенко

МОДЕЛИРОВАНИЕ ПРОЦЕССА РАСПАДА АУСТЕНИТА В ОБЪЕМЕ МАТЕРИАЛА

Разработана компьютерная модель, описывающая процесс превращения аустенита. Модель используется для предсказания структуры металла, формирующейся в процессе его охлаждения. Применение комбинации решения задачи теплопереноса с моделированием кинетики фазовых превращений позволяет предсказать распределение полученной структуры по объёму. В данной работе представлен пример использования данной модели для описания структурообразования при закалке цилиндрического образца из низкоуглеродистой стали.

Ключевые слова: компьютерная модель, фазовые превращения, аустенит, сталь, моделирование, закалка.

Introduction. The austenite transformation processes play a significant role in structure and properties formation of steels [1, 2]. Austenite decomposition during steel cooling could leads to formation of a various structural types [1]. Different factors have influence on the obtained final structure. Among them are temperature and cooling rate, material composition, grains size and deformation degree [3]. Physically grounded computer simulation of these phenomena is a challenging and practically important task. This work is devoted to demonstration of implementation of the developed by us computer model of phase transformations in alloyed steels to describe the structure formation in different places of a low-carbon steel cylinder transverse section when it's cooling. The simulation includes solving of a heat exchange problem and description of the phase transformation (austenite decomposition) kinetics.

Methodology and base theory. The computer model of phase transformations [4] consists of the next modules: thermodynamic module, ferrite transformation kinetics module, pearlite transformation kinetics module, bainite transformation kinetics module, martensite transformation kinetics module. Also was created a small program for selection data sets from the calculation results. For the software realization used program languages C++ and Python.

The thermodynamics modeling is based on CALPHAD-method [5, 6]. The original special software was developed by us for this module realization. The detailed description of this module implementation is given in our work [7].

Ferrite transformation kinetics modeling is baled on works [1, 3]. Ferrite nucleation is given by equation (1):

$$J_i = C_i \cdot N_i^0(t) \frac{1}{\sqrt{T}} e^{-\frac{Q_N(Y_{AE})}{RT}} \cdot e^{-\frac{K_1(x)}{K_2(x) k_B \cdot T \cdot \Delta G_{\gamma \rightarrow \alpha}^2(T, Y_{AE})} \sigma_{eff}^3} \quad (1)$$

where: J_i – rate of ferrite nucleation by i -th process mode, $1/s \cdot m^2$; C_i - empirical factor, which takes into account the influence of a crystal lattice defects rate in the certain place on the atoms moving rate, $K^{1/2}/s \cdot m^3$; $N_i^0(t)$ - the amount of potential nucleation places by the moment; T – temperature, K; $Q_N(Y_{AE})$ – the activation energy of the $\gamma \rightarrow \alpha$ lattice rebuilding, J/mol; R – universal gas constant, J/mol·K; $K_1(x)$, $K_2(x)$ – empirical coefficients; σ_{eff} – the effective surface energy of a ferrite, $J \cdot m^2$; k_B – Boltzmann constant, J/K; $\Delta G_{\gamma \rightarrow \alpha}(T, Y_{AE})$ – change of the volumetric Gibbs energy in $\gamma \rightarrow \alpha$ transformation as a function of the chemical composition and temperature, J / m^3 .

Ferrite growth rate, controlled by the diffusion of carbon outflow, for a spherical shape ferrite grain is given by equation (2) [1, 8, 9]:

$$V_{\gamma/\alpha}^C(T, Y_{AE}) = \frac{\bar{D}_C(T, Y_{AE})}{R_a} \cdot \frac{(x_{C_\gamma}^{int} - x_C)}{(x_{C_\gamma}^{int} - x_{C_\alpha})}, \quad (2)$$

where: $\bar{D}_C(T, Y_{AE})$ - the bulk diffusion coefficient of carbon in austenite as a function of composition and temperature, averaged over the carbon concentration profile, m^2/s ; R_a – the radius of a ferrite grain, m; $x_{C_\gamma}^{int}$ - an interface molar concentration of carbon in the austenite; x_C - a current average molar concentration of carbon in the austenite; x_{C_α} - an equilibrium molar concentration of carbon in the ferrite.

The rate of the γ / α - border controlled rearrangement of the lattice described by the equation (3) from [8]

$$V_{\gamma/\alpha}^L(T, Y_{AE}) = -M_{\alpha/\gamma}^0 \cdot e^{-\frac{Q_N(Y_{AE})}{RT}} \cdot \Delta G_{\gamma \rightarrow \alpha}(T, Y_{AE}), \quad (3)$$

where: M_0 – the mobility parameter of γ / α -border, $M_0 \approx 10 \text{ m}^4/c \cdot J$; Y_{AE}^* indicates that the values calculated for the concentrations that occur directly in the transition area.

The value of the carbon interface concentration is calculated from the condition of the ferrite growth rates obtained by the equations (2) and (3) equality. Formula (2) was used to compute the effective growth rate.

The carbon diffusion coefficient in an alloyed solid solution was calculated by equation (4) from [10]:

$$D_C(T, Y_{AE}) = D_{C0} \left(1 - y_c \cdot (1 - y_c) \cdot \frac{2 \cdot \left(\left(1 - \sum_{S=X}^Z y_S \right) \cdot L_{CVa}^{Fe}(T) + \sum_{S=X}^Z y_S L_{CVa}^S(T) \right)}{RT} \right) \times e^{\left(\frac{\theta \cdot \left(\Delta U_C(y_C) + \sum_{S=X}^Z \alpha_S \cdot y_S + y_C \cdot \sum_{S=X}^Z \gamma_S \cdot y_S \right)}{R} \right)} \cdot e^{\left(\frac{\Delta U_C(y_C) + \sum_{S=X}^Z \alpha_S y_S + y_C \cdot \sum_{S=X}^Z \gamma_S \cdot y_S}{RT} \right)}, \quad (4)$$

where: D_{C0} – pre-exponential factor, depends on the crystal lattice and the average frequency of the atoms thermal vibrations, m^2/s ; $D_{C0} \approx a^2 \cdot \nu$, where a is a lattice parameter, ν – average frequency of the atoms vibrations; y_C – sublattice concentration of carbon atoms; y_S - sublattice concentration of an alloying element atoms; $L_{CVa}^{Fe}(T)$ - a temperature-dependent interaction energy of a carbon atom with its nearest vacant place in the implementations sublattice of Fe lattice, J / mol; $L_{CVa}^S(T)$ - a temperature-dependent interaction energy of a carbon atom with its nearest vacant place in the sublattice of the alloying element lattice, J/mol; R – universal gas constant, J / mol·K; T – temperature, K; θ - parameter which determines

the relationship between entropy and energy of migrations activation, K^{-1} , $\Delta U_C(y_C)$ - migrations of carbon in Fe activation energy barrier without alloying as a function of the carbon concentration, J / mol; α_S and γ_S - parameters of of others elements influence on the carbon migration activation barrier, J / mol.

The rate of pearlite colonies growth is given by equations (5, 6) from [8, 9]:

$$V_{pe}^C(T, Y_{AE}) = \frac{6.35 \cdot \bar{D}_C(T, Y_{AE})}{S_{\theta\alpha}} \cdot \frac{x_{C_\gamma}^{int} - x_{C_\gamma}/\theta}{x_{C_\theta} - x_{C_\alpha}}, \quad (5)$$

$$S_{\theta\alpha} = -\frac{4 \cdot \sigma_{\alpha/\theta}}{\Delta G_{\gamma \rightarrow \theta}(T, Y_{AE})}, \quad (6)$$

where: x_{C_γ}/θ - the concentration of carbon in a boundary section austenite/cementite carbide; x_{C_θ}

- a concentration of carbon in cementite; $x_{C_\gamma}^{int}$ - interface molar concentration of carbon in the austenite; $\bar{D}_C(T, Y_{AE})$ - a bulk diffusion coefficient of carbon in the austenite as a function of its composition and temperature, m^2/s ; $S_{\theta\alpha}$ - a half-width distance in pearlite interlamellar; $\sigma_{\alpha/\theta}$ - a specific energy of α/γ - boundary; $\Delta G_{\gamma \rightarrow \theta}(T, Y_{AE})$ - the Gibbs energy change of the cementite carbide precipitation from austenite.

Nucleation rate of bainite elements is given by formula (7) from [1, 11, 12]:

$$J_k(t, T, Y_{AE}) = C_k \cdot F_k(t) \cdot e^{-\frac{Q_B(Y_{AE}) + k_k \cdot \Delta G_{\gamma \rightarrow \alpha}(T, Y_{AE})}{R \cdot T}}, \quad (7)$$

where C_k - pre-exponential factor, empirical parameter, which depends on the mode of the process; $F_k(t)$ - parameter determining the change over the process of the number of places of bainitic elements nucleation; $Q_B(Y_{AE})$ - an activation energy of bainitic elements nucleation as a function of the chemical composition of the austenite; k_k - an amendment coefficient.

Martensitic transformation was described by the methods from of [13]. According to the indicated work, the part of austenite capable to transformation at a certain temperature is given by the equation:

$$f_M = 1 - e^{-m(M_S - T)^n} \quad (8)$$

where M_S is the temperature of the martensitic transformation start, depending on the austenite chemical composition, K; m , n - empiric parameters depending on the chemical composition [13].

More detailed information about the mathematical model essence is shown in our works [7, 14]. Also in the paper [14] some experimental verification of the model was given.

As a simulation sample was accepted a steel cylinder with diameter 20 mm. On the back side of the cylinder were set border conditions of intensive cooling (quenching in water). The heat transfer coefficient (α) was set changing from 1000 to 10000 W/mK as a function of surface temperature according to data from works [15 - 17]. The start temperature of the metal was set 1000 °C (constant across section in the initial moment). The heat transfer in the metal was described by the heat conduction equation solved by the finite elements method. Finite elements size was set 1 mm.

Studied material and its properties. The studied material was an ordinary low-carbon steel with composition given in table 1.

Table 1.

Composition of the material accepted in the simulation (wt. %)

Fe	C	Mn	Si	Ni	Cr	Mo	Cu
base	0.1	0.5	0.2	0.02	0.02	0.02	0.02

Physical needed for heat transfer calculation properties were accepted temperature depending. The temperature dependences of thermal conductivity, density and heat capacity were taken from [18].

The initial average austenite grain size was set 40 μm . Calculated values of the equilibrium critical points for this steel are: $A_1 = 728.7\text{ }^\circ\text{C}$, $A_2 = 902.1\text{ }^\circ\text{C}$.

Results and discussion. Because of different and nonlinear cooling rates in a sample transverse section there occur different conditions of the austenite transformation process. As a result there is a structure type change along the sample radius. On figure 1 the simulated cooling curves corresponding to points along the radius (from the surface to center) are shown.

Steels of the current type are known as poorly hardened when quenching and as ones which have low stability of supercooled austenite. But they could be quenched, for instance after surface carburization or carbonitriding. Another aspect is when such steel undergoes fast cooling during some other technical processing. And information about the structure obtained not only in the surface but in the bulk is also important technological issue.

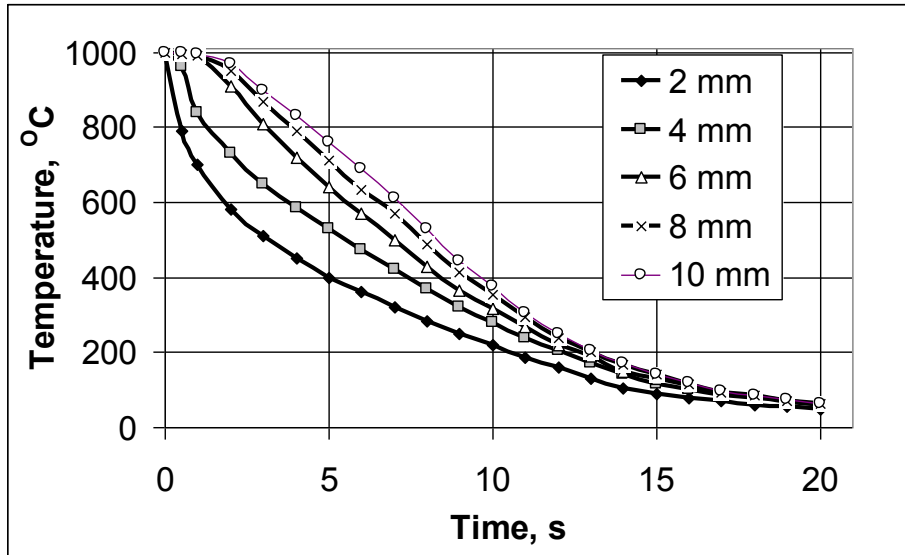


Fig. 1. Simulated cooling curves in different distances from the surface of the sample

For each of the shown cooling curves simulation of austenite transformation process was performed. This involved to obtain a map of structure types in the sample transverse section. Figure 2 shows the simulated results of structure type distribution in the sample transverse section.

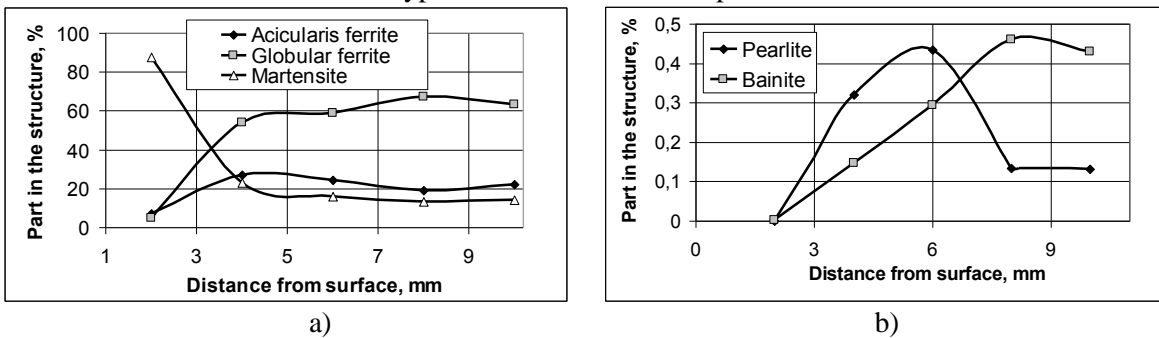


Figure 2. Results of structure formation simulations across the sample transverse section: a) ferrite and martensite; b) pearlite and bainite

As it was expected, this steel sample after water cooling will have structure with high martensite level only near surface. At the distance 4 mm from the surface the part of martensite according to simulation results will just about 20 %. So only first 2 mm from the surface could be properly quenched in this sample. The structure at this distance and further become more ferritic. The part of martensite decline but more slowly than at the first 4 mm. The parts of pearlite and bainite are small everywhere, they are less than 0,5 %. At the distance after 6 mm and further the part of pearlite become decline. Part of bainite grows from the surface to center. Such behavior could be caused by nonlinear shape of cooling curves. So we have bainite part increasing. This is most facilitated by more complete ferrite transformation at higher temperatures which leads to increasing of carbon content in austenite. This increasing of carbon content promotes pearlite and bainite formation (that needs higher carbon).

The simulation shows that quenching of such sample leads to surface hardening which is important for cementation or carbonitriding processing. And the most of bulk metal will have ferrite structure which is more plastic and less brittle but little hardened by some amount of martensite.

Conclusions. Analyzing the above, we can draw the following conclusions:

1. A computer mathematical model which can predict structure formation in steels during cooling process was developed. The model can predict allocation of structure types in bulk using combined heat transfer and physical kinetics solution.

2. Operability of the developed model was demonstrated by simulation of a low-carbon steel sample quenching. The simulation predicted the distribution of martensite in the cross section, so the depth of quenching could be estimated. The simulation showed that the properly quenched depth in a cylindrical sample of ordinary low-carbon steel with diameter 20 mm is about 2 – 3 mm (in water cooling conditions). Then the part of martensite significantly decline and the structure becomes consists mostly from ferrite.

3. The model is useful for heat processing developing. Using it you can fast and with minimum of expense develop a proper tempering regime without large number of experimental.

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