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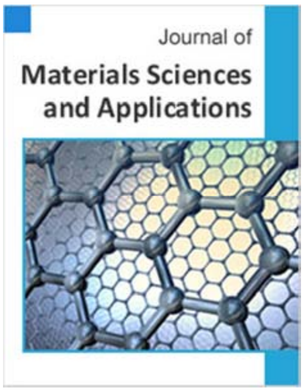

About Computer Simulation of Austenite Transformation in Bulk

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Abstract

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.

1. Introduction

The processes of austenite transformation play a significant role in structure and properties formation of steels [1, 2]. Austenite decomposition during steel cooling or isothermal processes could leads to formation of a various number of structural types [1]. The obtained final structure depends on set of different factors among which are temperature and cooling rate, material composition, grains size and pre-deformation degree [3]. Mathematical modeling and physically grounded computer simulation of these phenomena is a challenging and practically important task. And the issue is not only right physical and mathematical description of a transformation process itself but also implementation of the model application to the processes occurs in real materials and products. Thus this work is devoted to demonstration of implementation of the previously developed by us computer model of phase transformations in alloyed steels to describe the structure formation in different places of a low-carbon steel bar transverse section when it's cooling. The simulation includes solving of a heat exchange problem and description of a thermodynamics and kinetics of the phase transformation (austenite decomposition).

2. 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):

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

where: J_i – rate of ferrite nucleation by i-th process mode, 1/s ·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·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 γ → α 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/·m^2; k_B – Boltzmann constant, J/K; $\Delta G_{\gamma\to\alpha}(T, Y_{AE})$ – change of the volumetric Gibbs energy in γ→α 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]:

$$V^C_{\gamma/\alpha}(T,Y_{AE}) = \frac{\overline{D}_C(T,Y_{AE})}{R_\alpha}\cdot\frac{(x^{int}_{C_\gamma} - x_C)}{(x^{int}_{C_\gamma} - x_{C_\alpha})}, \quad (2)$$

where: $\overline{D}_C(T,Y_{AE})$ - 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_α – the radius of a ferrite grain, m; $x^{int}_{C_\gamma}$ - 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]:

$$V^L_{\gamma/\alpha}(T,Y_{AE}) = -M^0_{\alpha/\gamma}\cdot e^{-\frac{Q_N(Y_{AE})}{RT}}\cdot\Delta G_{\gamma\to\alpha}(T,Y_{AE}), \quad (3)$$

where: M_0 – the mobility parameter of γ / α-border, $M_0 \approx 10$ m^4/c·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]:

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

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; $L^{Fe}_{CVa}(T)$ - a temperature-dependent interaction energy of a carbon atom with its nearest vacant place in the implementations sublattice of Fe lattice, J / mol; $L^S_{CVa}(T)$ - 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]:

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

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

where: $x_{C_\gamma/\theta}$ - 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; $\overline{D}_C(T,Y_{AE})$ - 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; $\Delta G_{\gamma\to\theta}(T,Y_{AE})$ - 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]:

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

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].

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.

3. Experimental Verification of the Model

An experiment was carried out to verify the developed model. The chemical composition of the steel sample and the average grain size of austenite in it are given in Table 1. The initial average austenite grain size of the sample steel was 40 μm.

Table 1. The steel composition of in the verification experiment (wt.%).

C	Si	Mn	Cr	Ni	Mo	Cu	Fe
0.050	0.290	1.32	0.16	2.19	0.27	0.36	base

Figure 1 compares the austenite transformation curves obtained using the computer model (a) and the experimental data (b) for cooling rates of 10 and 45 deg/s.

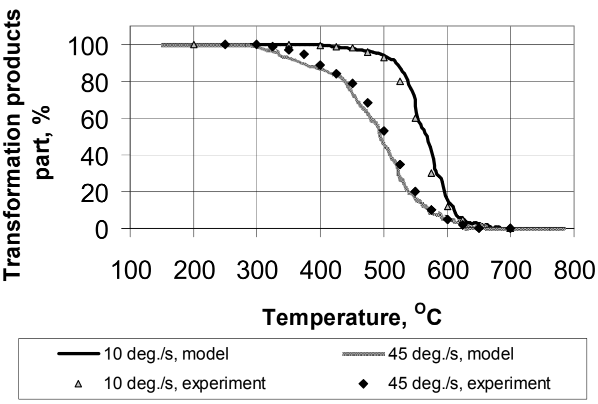


Figure 1. Comparison of the experimental data with the results obtained by the computer model.

Temperatures of actual beginning of the transformation predicted quite accurately. Thus, according to experimental data, they are 676°C (for 10 deg./s) and 653°C (for 45 deg./s), by the results of the computer model, they are, respectively, 675°C and 652°C. The displacement of the curve to the left with a cooling rate increase is seen. It also corresponds to the experiment that at a cooling rate of 10 deg./s approximately 95% of the austenite is already transformed at 500°C, after which the transformation slows down. When the cooling rate is 45 deg./s the transformation is actually completed at about 300°C. On the theoretical and experimental curves for a cooling rate 45 deg./s there is a "kink" in the region about 410...430°C corresponding to the beginning of the shear (martensitic) transformation.

Thus although the developed computer model allows quickly obtaining of sufficient for practical purposes, and quite reliable data about the kinetics of austenite transformation in a given steel.

4. Studied Material and Its Properties

The studied material was an ordinary low-carbon steel with composition given in table 2.

Table 2. 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°C, A_2 = 902.1°C. Using the thermodynamic calculations module of the developed computer model a part of a quasi-binary phase diagram Fe-C was calculated in para-equilibrium approach. The calculations were performed for the temperature range from 200 to 1000°C and carbon content range from 0 to 1.5%. Concentrations of the other elements corresponds to the table 2 data. The calculated diagram is shown on figure 2. Calculated diagram lines extrapolated to non-equilibrium (super-cooled) area are shown as dashed. The current steel carbon content is shown by a vertical gray line.

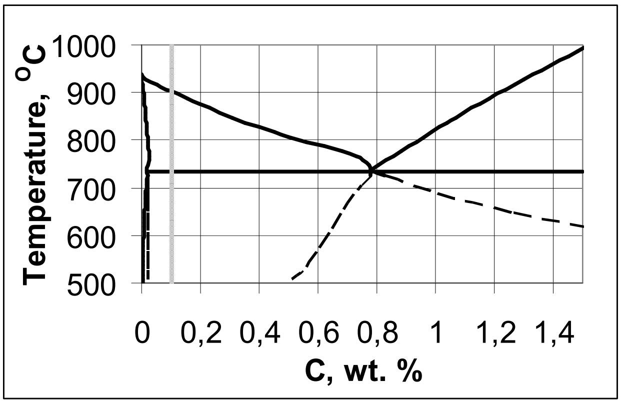


Figure 2. Calculated part of quasi-binary section of Fe-C phase diagram for the studied steel.

As it could be seen from figure 2 the Fe-C phase diagram fore this steel is very close to one of not alloyed Fe-C binary system.

5. 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 3 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.

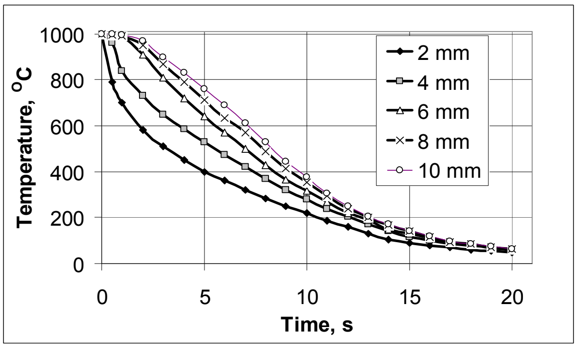


Figure 3. Simulated cooling curves in different distances from the surface of the sample.

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. The simulated austenite transformation kinetic curves are shown on the figure 4 and the results of structure formation simulation are shown on the figure 5.

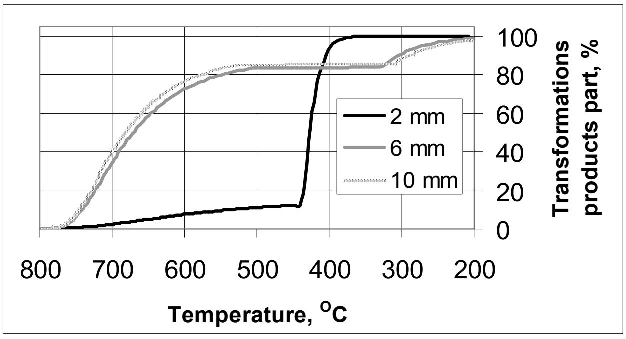


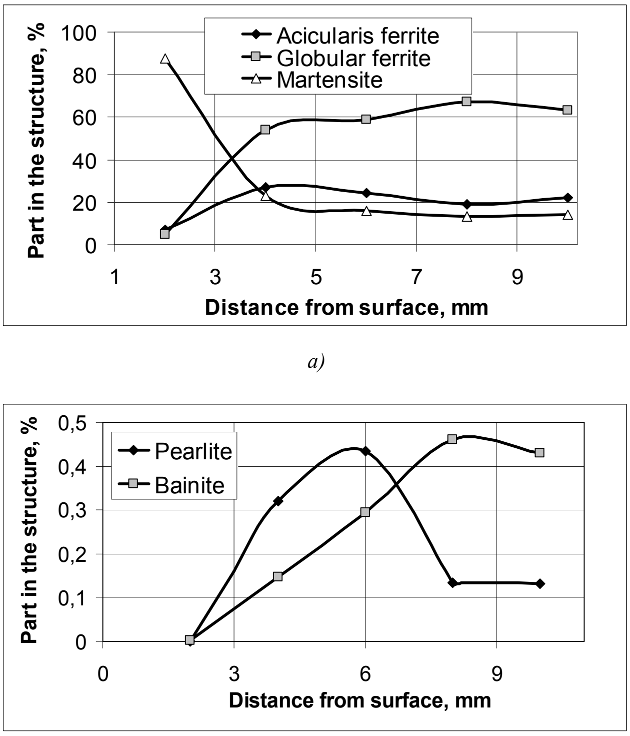
Figure 4. Simulated kinetic curves of austenite transformations at the different distances from the sample surface.

The kinetic curves shown on the figure 4 demonstrate the austenite transformation process at three different distances from the surface: 2 mm, 6 mm and 10 mm (center axis).

Near the surface a cooling rate at the first seconds of the process is quite rapid. So that, as it could be seen from the curve shape for 2 mm distance, competently small part (about 12%) of austenite transformed to ferrite at the temperature range where this type of transformation is possible. At the 440°C martensitic transformation starts and it completes at about 370°C. During the ferritic transformation (which is a diffusion type one) a carbon exchange process between austenite and ferrite occurs. In this process the current carbon content in austenite increases. But the process proceeds (especially when fast cooling) by not equilibrium schema also the content of carbon become not equal inside an austenite grain: higher near the grain boundary (where the ferrite formation is going) and lower in the middle (because diffusion process is not instantaneous). According to the simulation by the moment of martensitic transformation start (at the distance 2 mm from the surface) the average carbon concentration in austenite is about 0.104%. That is only slightly more then at the process beginning. Thus the obtained martensite will be low carbon one.

The kinetic curves for distances 6 and 10 mm have minor difference. Ferritic transformation in these areas is more complete. Before the 500°C temperature arrival ~83…85% of austenite already turns to ferrite. Then the transformation process becomes slower. The carbon exchange between ferrite and austenite in this case is more significant. The average carbon concentration in austenite at 650°C in this case (area near the central axis of the sample) is about 0.23%. At 520°C its content becomes there 0.53%. According to the thermodynamically calculation it is enough (at this temperature) for the pearlite formation start. But actually the amount of pearlite forms is very small (see figure 5 below). Also there forms an insignificant part ob bainite. Because of carbon content in austenite increasing the temperature of martensitic transformation start becomes lower. So in the distance 6 mm from the surface it starts at 327°C and in the central at 308°C. Thus in spite of significantly smaller part of martensite than near the sample surface in the center it contains more carbon, so could be some harder.

Figure 5 shows the simulated results of structure type distribution in the sample traverse section.



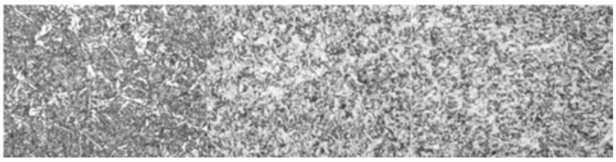
a)

b)

Figure 5. *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 les than 0,5%. At the distance ater 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 simulated results of the structure formation prediction were proofed by a real experiment of such sample quenching. The sample was made from a casted and then annealed steel with a similar composition. That means that there was no deformation influence on the phase transformation in the experiment. The microstructure of the sample was studied at the areas near 2 mm, 6 mm and 10 mm from the surface. The obtained photographs of the structures (optical metallography) are shown on the figure 6.



a) b) c)

Figure 6. *Microstructure of the sample after quenching (magnification ×500): a) 2 mm from the surface; b) 6 mm from the surface; c) near the central axis*

From the shown photographs of the structures it could be seen that the metal in the distance 2 mm from the sample surface consist mostly of low carbon martensite which is in the matrix of ferrite. But ferrite content is rather small. In 6 mm from the surface structure becomes more ferritic but some content (~15%) of martensite is seen which is mostly outside ferrite grains. The structure in the center is almost the same one in the distance 6 mm from the surface.

Measured values of hardness in different areas of the sample traverse section also corresponds the structure changes. The obtained values of hardness (by Rockwell scale) are:

2 mm – 27±2 HRC;
6 mm – 90±3 HRB;
Near the central axis – 89±3 HRB

Thus 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.

6. 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. By a verification experiment using low carbon alloyed steel samples the developed model usability was successfully proofed. Although the developed computer model is not a complete alternative to the experimental studies, but it allows obtaining result with sufficient for most of practical purposes precision and reliability.

3. 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 qunching 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.

4. The simulation allowed studying the austenite transformation process in different distances from the sample surface. Thus the temperature ranges of ferrite and martensite formation processes in different parts of the sample traverse section were defined. Also there was studied the process of carbon exchange between austenite and forming ferrite and the average carbon content in austenite by the martensite transformation start moment was predicted.

5. 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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